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Section A :
Physique théorique.

Asymptotic $\hbar$-expansions of stationary quantum states

by

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ABSTRACT. — We discuss the mathematical framework for uniform asymptotic expansions in the parameter $\hbar$ of non-relativistic quantum mechanics. Quantum observables of interest are taken in an algebra of pseudo-differential operators defined with the help of the Wigner transformation. We define a class of asymptotic quantum states as certain linear functionals on those operators. These functionals are microlocal, and we study their supports in phase space in analogy with wave front set theory; they are also shown to be covariant under the « metaplectic representation » of the affine symplectic transformations in phase space. In this asymptotic framework we can formulate the eigenstate problem for the most general observable. This problem is formally solved by quadratures for one-dimensional systems: a Bohr-Sommerfeld formula correct to all orders in $\hbar$ is the obtained for the discrete spectrum.

RÉSUMÉ. — Nous formulons un cadre mathématique pour développer la mécanique quantique non-relativiste en séries asymptotiques uniformes dans le paramètre $\hbar$. Il faut se restreindre à des observables quantiques appartenant à une certaine algèbre d'opérateurs pseudo-différentiels, définie à l'aide de la transformation de Wigner. Nous définissons alors une classe d'états quantiques asymptotiques comme fonctionnelles linéaires sur ces observables. Ces fonctionnelles sont microlocales, et nous étudions leurs supports dans l'espace de phase en analogie avec la théorie des fronts d'onde; nous montrons aussi qu'elles sont covariantes par la « représen-

(*) Détaché du C. N. R. S.

tation métaplectique » du groupe symplectique affine sur l'espace de phase. Dans ce formalisme asymptotique, nous pouvons formuler le problème des fonctions propres pour une observable quelconque. Ce problème est formellement résolu par quadratures pour les systèmes à une dimension : on obtient alors pour le spectre discret une formule de Bohr-Sommerfeld correcte à tous les ordres en $\hbar$

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1. INTRODUCTION

The purpose of this article is to provide the mathematical background to the treatment of some quantum mechanical problems by regular asymptotic expansions in the parameter $\hbar$ (Planck's constant) around the corresponding solution in classical mechanics. We sketch an application (developed in more detail in [*62*]) to the Schrödinger eigenfunction problem (for a non-relativistic, spinless system in flat space).

The WKB treatment of the Schrödinger equation [*1*]-[*4*], among others, establishes a close analogy between the small $\hbar$ behaviour of quantum mechanics, and the high frequency behaviour of light waves as described by geometrical optics [*5*] [*6*]. In today's mathematics, geometrical optics has become a part of the theory of pseudo-differential operators [*7*] [*8*] [*9*]: it governs the propagation of singularities of the solutions. We assume the reader to be reasonably acquainted with the C^∞ theory of pseudo-differential operators in its standard form, as found for instance in [*8*] (we shall not use here the alternative but parallel approach based on hyperfunctions [*10*]).

We shall insist on the many geometrical features of the theory in phase space (i. e. the cotangent bundle of the coordinate manifold): the symplectic structure of phase space, microlocality of the asymptotics, the classical behaviour of wave front sets, the role of lagrangian manifolds [*11*]-[*13*].

Well before the advent of pseudo-differential operators, physicists had developed various types of so-called « semi-classical methods » (1) to solve —sometimes heuristically—various quantum problems in powers of $\hbar$: the WKB method [*1*] [*4*], the Wigner transformation [*14*]-[*17*] (or quantum mechanics on classical phase space), the Thomas-Fermi methods [*1*] [*2*] [*18*] [*19*], Feynman's path integral [*20*], the Balian-Bloch spectral density expansion [*21*], etc. (for a review see [*22*]). All these methods explain, or compute, certain features of the quantum theory in terms of the underlying classical structure.

The relevance of these physical methods (and of the results) to pseudo-

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(1) In this work, we shall reserve the word *semi-classical* to denote the dominant asymptotic corrections to the classical terms (the word *asymptotic* referring to the complete formal expansions in $\hbar$).

differential operator theory and *vice versa*, has been established rather lately and incompletely, and it still remains to be fully exploited. Maslov's contributions to the WKB theory [*4*] have been interpreted and generalized in the light of pseudo-differential operator theory [*7*] [*8*] [*23*] and of geometric quantization (R. Blattner, K. Gawedzki, B. Kostant, E. Onofri, D. Simms, A. Weinstein in [*11*]; [*24*]-[*26*]). The Wigner transformation for quantum observables has been identified as a kind of symbol calculus [*15*] [*27*]. Results about the spectrum of the Laplace-Beltrami operator [*28*]-[*30*] are related to the work of Balian-Bloch. Quantization along closed paths [*31*] has been related by Guillemin [*32*] to the Kostant-Sternberg theory of symplectic spinors [*33*]. Also, the occurrence of the parameter $\hbar$ in quantum asymptotics has received several, essentially equivalent, interpretations [*4*] [*12*] [*27*].

The present work is intended as another step towards blending many asymptotic methods of quantum physics, in spite of their formal differences, into one single pseudo-differential operator calculus (we follow ideas expressed at the semi-classical level in [*27*]). Among the obstacles against such a program, we have found that: on one hand, part of the sophistication of the mathematical theory essentially arises from its generality (working on manifolds) and some of it might just be superfluous to understand the Schrödinger equation on an affine space. On the other hand, standard pseudo-differential operators also have several undesirable features regarding their use in quantum theory—and this fact should be corrected first. As for the extension of our methods to manifolds, we leave it as an open problem; it probably requires the use of symplectic spinors as in [*32*].

Our plan is the following: in section 2 we review the essential facts about pseudo-differential operators on an affine space and we adapt the theory to quantum mechanics by a *reduction* procedure followed by a symmetrization between position and momentum coordinates. In section 3, the new theory is shown to have the structure of an algebra of Wigner symbols under twisted multiplication. Section 4 is group theoretical and deals with the metaplectic representations, using some ideas of prequantization theory. Section 5 gives a new application of a very old notion of quantum theory, that of density operator, or linear functional associated to a wave function (to a half-form): we use it to define a space of *admissible linear functionals*, which we use in the following sections. In section 6, the eigenstate problem is discussed in the asymptotic theory, with a more thorough application to one-dimensional problems (including the eigenvalue condition) sketched in section 7. The reader mainly interested in physical applications can skip section 2 and all the proofs.

Also, ref. [*58*] forms an outline of this article.

The reference list does not claim to be comprehensive and it essentially mentions the works which we have found the most convenient for our purposes.

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2. REDUCED PSEUDO-DIFFERENTIAL OPERATORS

We shall modify the usual definition of pseudo-differential operators (in short: PDO) to adapt them to quantum mechanical purposes, in the same way as geometrical optics becomes the WKB method in order to describe the transition from the Schrödinger equation to the Hamilton-Jacobi equation of classical mechanics [*1*]-[*4*].

2.1. Some facts of standard PDO theory [*8*]

As indicated, we restrict our interest to problems defined on an affine space $\tilde{Q} \approx \mathbb{R}^{l+1}$. For our own later purposes, $\tilde{Q}$ will have the distinguished form: $\tilde{Q} = \mathbb{R} \oplus Q(Q \approx \mathbb{R}^l, l \geq 1)$ with adapted cartesian coordinates $\tilde{q} = (s, q)$. We let $\tilde{\xi} = (\lambda, \xi)$ be the dual coordinates on the dual space $\tilde{Q}^*$.

An integral operator $\tilde{A}$ with kernel $\tilde{A}(\tilde{q}, \tilde{q}') \in \mathscr{D}'(\tilde{Q} \times \tilde{Q})$:

$$(\tilde{A}\tilde{f})(\tilde{q}) = \langle \tilde{A}(\tilde{q}, .), \tilde{f} \rangle \qquad (\tilde{f} \in C_0^\infty(\tilde{Q})) \tag{2.1}$$

is called a *pseudo-differential operator* (a PDO) iff the following expression:

$$\tilde{a}(\tilde{q}, \tilde{\xi}) = \int_{\tilde{Q}} \tilde{A}(\tilde{q}, \tilde{q} + \tilde{r}) e^{i\tilde{\xi}\tilde{r}} d\tilde{r} \tag{2.2}$$

makes sense and defines a function $\tilde{a} \in C^\infty(T^*\tilde{Q}, \mathbb{C})$ called the (full) *symbol* of $\tilde{A}$ (here: $T^*\tilde{Q} \approx \tilde{Q} \oplus \tilde{Q}^*$), that admits an expansion:

$$\tilde{a}(\tilde{q}, \tilde{\xi}) \sim \sum_0^\infty \tilde{a}_{m-j}(\tilde{q}, \tilde{\xi}) \tag{2.3}$$

where each $\tilde{a}_r(\tilde{q}, \tilde{\xi})$ is C^∞ outside of $\tilde{\xi} = 0$, and positively homogeneous of degree r in ξ for fixed q:

$$\tilde{a}_r(\tilde{q}, \tau\tilde{\xi}) = \tau^r \tilde{a}_r(\tilde{q}, \tilde{\xi}) \qquad (\forall \tau > 0) \tag{2.4}$$

and (2.3) is an asymptotic series in the sense that:

$$\partial_{\tilde{\xi}}^{\alpha}\left(\tilde{a}(\tilde{q}, \tilde{\xi}) - \sum_{j=0}^{k-1} \tilde{a}_{m-j}(\tilde{q}, \tilde{\xi})\right) \leqslant \mathcal{O}(\| \tilde{\xi} \|^{m-k-|\alpha|}) \tag{2.5}$$

for all $\alpha \in \mathbb{N}^{l+1}$ and for $\| \tilde{\xi} \| \to \infty$ (locally uniformly in $\tilde{Q}$; $\partial_{\tilde{\xi}}^{\alpha}$ means: $\dfrac{\partial^{|\alpha|}}{\partial_{\lambda}^{\alpha_0}\partial_{\xi_1}^{\alpha_1} \dots \partial_{\xi_l}^{\alpha_l}}$; $| \alpha | = \sum_0^l \alpha_j\Big)$.

The *order* of $\tilde{A}$ is the real number m in Eq. (2.3); the term of highest degree $\tilde{a}_m(\tilde{q}, \tilde{\xi})$ is called the *principal symbol* of $\tilde{A}$. The *characteristic set* of $\tilde{A}$ is the closed subset $\gamma(\tilde{A}) = \tilde{a}_m^{-1}(0)$ of $T^*\tilde{Q}\backslash\{0\}$, which is conical in every fiber. The characteristic equation (5):

$$\tilde{a}_m(\tilde{q}, d\Sigma(\tilde{q})) = 0$$

is a first order *homogeneous* differential equation (when $\tilde{A}$ is the Maxwell operator of electromagnetic wave propagation, that is just the Hamilton-Jacobi equation of geometrical optics [5] [6]).

Any PDO $\tilde{A}$ defines a linear map $\mathscr{E}'(Q) \to \mathscr{D}'(Q)$ [8] with important geometrical relations between the *local* singularities of a distribution $\tilde{\psi}$ and those of $\tilde{A}\tilde{\psi}$. The singularities of a distribution $\tilde{\psi} \in \mathscr{D}'(\tilde{Q})$ are reflected by its *wave front set* $WF(\tilde{\psi})$, which is the closed subset of $T^*\tilde{Q}\backslash\{0\}$ (conical along the fibers) such that:

$$(\tilde{q}', \tilde{\xi}') \notin WF(\tilde{\psi}) \Leftrightarrow \exists \varphi \in \mathscr{D}(\tilde{Q}) : \quad \varphi(\tilde{q}') \neq 0$$

and:

$$\int_{\tilde{Q}} \varphi(\tilde{q})\tilde{\psi}(\tilde{q})e^{-i\tau\tilde{\xi}\tilde{q}}d\tilde{q} = o(\tau^{-N}) \qquad \forall N > 0 \tag{2.6}$$

as $\tau \to +\infty$, uniformly in $\tilde{\xi}$ in some neighborhood of $\tilde{\xi}'$ (for instance, $\tilde{\psi}$ is C^∞ at $\tilde{q}'$ iff $WF(\tilde{\psi})$ is empty above $\tilde{q}'$).

We quote a few important results [7] [8]:

— $$WF(\tilde{\psi}) = \bigcap_{\tilde{A} | WF(\tilde{A}\tilde{\psi}) = \varnothing} \gamma(\tilde{A}) \tag{2.7}$$

($\tilde{A}$ runs over all PDO's such that $\tilde{A}\tilde{\psi}$ is a C^∞ function).

— $$\tilde{A}\tilde{\psi} \in C^\infty \Rightarrow WF(\tilde{\psi}) \subset \gamma(\tilde{A}), \tag{2.8}$$

and $WF(\tilde{\psi})$ is invariant under the hamiltonian flow of $\tilde{a}_m(\tilde{q}, \tilde{\xi})$ on $T^*(\tilde{Q})\backslash\{0\}$ (provided this flow is regular on $\gamma(\tilde{A})$).

Such a framework clearly produces an asymptotic description of PDO's and of their solutions in terms of the dilation-along-fibers parameter τ, and we shall call it the *homogeneous* theory. Accordingly, the geometrical objects of the theory (characteristic sets, wave front sets) are conical along the fibers, and it is customary to view them as sections of the sphere bundle $S^*\tilde{Q} = (T^*\tilde{Q}\backslash\{0\})/\mathbb{R}^*_+$ [7] [*10*]).

As it stands, the theory is unfit to describe the semi-classical behaviour of even the most typical Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\Delta_q + V(q)\right)\psi$$

in terms of the classical Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V(q) = 0$$

predicted by physics. Here there is no obvious homogeneity in the momentum variables, and the extra parameter $\hbar$ does not seem to fit into the picture. Heuristically speaking, we shall lift both obstacles at once by ascribing to $\hbar$ a degree of homogeneity (-1), as follows.

2.2. **The reduction procedure** [*12*] [*27*]

Let $\tilde{A}$ be a PDO on $\tilde{Q}$, satisfying (2.1)-(2.5), and moreover *translation-invariant* in the variable s: $\tilde{A}(\tilde{q}, \tilde{q}') = \tilde{A}(s - s', q, q')$; equivalently: $\tilde{a}(\tilde{q}, \tilde{\xi})$ is independent of s. Let $\mathcal{F} : \mathcal{S}'(\tilde{Q}) \to \mathcal{S}'(\mathbb{R} \times Q)$ be the Fourier transformation:

$$(\mathcal{F}\tilde{\psi})(\lambda, q) = \psi(\lambda, q) = \int_{\mathbb{R}} \tilde{\psi}(s, q)e^{-i\lambda s}ds.$$

We define the *reduced* PDO as: $A = \mathcal{F}\tilde{A}\mathcal{F}^{-1}$, or explicitly:

$$\psi(\lambda, q) \mapsto (A\psi)(\lambda, q) = \int_Q A(\lambda; q, q')\psi(\lambda, q')dq' \tag{2.9}$$

The variable λ, dual of s, has been diagonalized and can be considered as a parameter of the theory; A now has a reduced kernel on $(Q \times Q)$ related to the original symbol by:

$$\tilde{a}(\tilde{q}, \tilde{\xi}) = \tilde{a}(q, \xi; \lambda) = \int_Q A(\lambda; q, q + r)e^{i\xi r}dr \tag{2.10}$$

hence A is a λ-dependent operator looking like a PDO on the space Q, but without the homogeneity properties (2.3)-(2.4). For example, the wave operator $\tilde{A} = \partial^2/\partial s^2 - \Delta_q$ leads to the well-known reduced operator: $A = -\Delta_q - \lambda^2$ (physically: s is time, λ is frequency) [5].

For quantum mechanics a different interpretation of reduction is needed. We put $\lambda = \frac{1}{\hbar}$ (> 0 by convention) and we represent each cotangent ray in the $\lambda > 0$ half-space by its trace p on the affine hyperplane

$P : \left\{ \lambda = \frac{1}{\hbar} \right\}$ (for fixed $\hbar$) : the points $p \in P$ will represent the physical momenta. In coordinates, we have : $p = \frac{\xi}{\lambda}$, so the original variables $\tilde{\xi} = (\lambda, \xi)$ are *projective* coordinates for the physical momenta. The homogeneous theory can now be translated in terms of the physical variables (q, p) to produce a « reduced theory ». The Schrödinger time-dependent operator, for instance (assuming here that one variable of Q represents time, t) : $H = i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \Delta_q - V(q)$ is indeed the reduced operator of

$$\tilde{H} = \hbar^2 \left(- \frac{\partial^2}{\partial s \partial t} + \Delta_q + V(q) \frac{\partial^2}{\partial s^2} \right) \qquad \text{(homogeneous)}$$

and the principal symbol is $E - \frac{p^2}{2m} - V(q)$, the correct classical energy function (E is conjugate to t).

In terms of the reduced symbol $a(q, p ; \hbar) \equiv a(q, \xi)$, the relations (2.2)-(2.5) get translated as:

$$a(q, p ; \hbar) = \int_Q A\left(\frac{1}{\hbar} ; q, q + r \right) e^{\frac{ipr}{\hbar}} dr \tag{2.11}$$

and:

$$\hbar^m a(q, p ; \hbar) \sim \sum_{j=0}^{\infty} a_j(q, p) \hbar^j \tag{2.12}$$

where $a_j(q, p) \equiv \tilde{a}_{m-j}(q, \lambda = 1, \xi = p)$ is no longer homogeneous, but only satisfies the estimate (for any norm on P):

$$(\forall \alpha \in \mathbb{N}^l) : \qquad | \partial_p^\alpha a_j(q, p) | \leqslant \mathcal{O}(\| p \|^{m-j-|\alpha|}) \tag{2.13}$$

and (2.12) is asymptotic in the following sense:

$$(\forall \alpha \in \mathbb{N}^l) : \qquad \partial_p^\alpha \left[\hbar^m a(q, p ; \hbar) - \sum_{j=0}^{n-1} a_j(q, p) \hbar^j \right] \leqslant \mathcal{O}(\hbar^n \| p \|^{m-n-|\alpha|}) \tag{2.14}$$

for $\hbar \to 0^+$ and/or $\| p \| \to +\infty$.

The form of the homogeneous Schrödinger operator $\tilde{H}$, and the Eq. (2.12), suggest that the physically relevant operators have the form : $A = \hbar^m \times$ (a reduced PDO of arbitrary order m), so that their symbols have regular expansions in $\hbar$, by Eq. (2.12).

We can define the *reduced characteristic set* of a reduced PDO :

$$R\gamma(A) = \{ (q, p) \in Q \oplus P \mid \exists (s, \lambda > 0) : (s, q, \lambda, \lambda p) \in \gamma(\tilde{A}) \}$$
$$\equiv a_0^{-1}(\{0\}).$$

For the time-independent Schrödinger operator on $Q = \mathbb{R}^l$:

$$H = \left(-\frac{\hbar^2 \Delta_q}{2m} + V(q) - E \right) :$$

$R\gamma(H)$ is the classical energy surface of equation $\frac{p^2}{2m} + V(q) = E$, in the « classical phase space » $X = Q \oplus P$. The principal symbol also has the correct interpretation as the classical hamiltonian.

We shall say that a distribution $\psi(\lambda, q) \in \mathcal{S}'^{\mathbb{C}}(\mathbb{R} \times Q)$ belongs to $\hat{\mathcal{S}}'^{\mathbb{C}}_M(Q)$ if for some $\lambda_0 > 0$, $N > 0$ and for all $\varphi \in \mathcal{S}(Q)$, the map:

$$\lambda \in [\lambda_0, \infty) \longrightarrow \langle \psi(\lambda), \varphi \rangle_Q$$

is C^∞, and the set $\{ \lambda^{-N}\psi(\lambda, .) \mid \lambda > \lambda_0 \}$ is bounded in $\mathcal{S}'^{\mathbb{C}}(Q)$.

For a reduced PDO A, and for $\psi \in \hat{\mathcal{S}}'^{\mathbb{C}}_M(Q)$ of compact Q-support, $A\psi$ is defined as a λ-dependent distribution. This fact can be used to make local statements about singularities of a distribution $\psi \in \hat{\mathcal{S}}'^{\mathbb{C}}_M(Q)$: we define its *reduced wave front set* $RWF(\psi)$ as the closed subset of $X = Q \oplus P$ such that:

$$(q', p') \notin RWF(\psi) \Leftrightarrow \exists \theta \in \mathcal{D}(Q) : \qquad \theta(q') \neq 0$$

and :

$$\int_Q \theta(q)\psi(\lambda, q)e^{-i\lambda pq}dq = o(\lambda^{-N}) \qquad \forall N > 0 \tag{2.15}$$

in some neighborhood of p', uniformly in p, as $\lambda \to +\infty$.

We note : $\psi \sim 0$ for : $RWF(\psi) = \emptyset$: such distributions ψ are $o(\lambda^{-\infty})$ as $\lambda \to +\infty$ (they are the analogs of the C^∞ distributions of the homogeneous theory). Let again: $\tilde{\psi} = \mathcal{F}^{-1}\psi$ $(\in \mathcal{S}'(\tilde{Q}))$. Then we have:

THEOREM 2.2.1. — (*i*) Let

$$E = \{ (q, p) \in X \mid \exists (s, \lambda > 0) : (s, q, \lambda, \lambda p) \in WF(\tilde{\psi}) \}.$$

Then $E \subset RWF(\psi)$, and if Supp $\tilde{\psi}$ is compact : $E = RWF(\psi)$.

(*ii*) $RWF(\psi) = \bigcap_{A \mid A\psi \sim 0} R\gamma(A)$ (A : reduced PDO).

(*iii*) $A\psi \sim 0 \Rightarrow RWF(\psi) \subset R\gamma(A)$, and $RWF(\psi)$ is invariant under the hamiltonian flow of $a_0(q, p)$ on X (provided this flow is regular on $R\gamma(A)$).

Proof. — (*i*) Eq. (2.15) reads:

$$\int_Q dq\, \theta(q)e^{-i\lambda pq} \int_{\mathbb{R}} ds\, \tilde{\psi}(s, q)e^{-i\lambda s} = \int_{\tilde{Q}} d\tilde{q}\, \theta(q)\tilde{\psi}(\tilde{q})e^{-i\tilde{\xi}\tilde{q}} = o(\lambda^{-N})$$

hence if $(q', p') \notin RWF(\psi)$, by taking $\varphi(\tilde{q}) = \theta(q)$ in Eq. (2.6) we see that for all $s \in \mathbb{R}$: $(s, q', \lambda, \lambda p') \notin WF(\tilde{\psi})$, so that $E \subset RWF(\psi)$. Conservely if Supp $\tilde{\psi}$ is compact and if for all s : $(s, q', \lambda, \lambda p') \notin WF(\tilde{\psi})$ then the function

$\varphi(\tilde{q})$ in Eq. (2.6) can be chosen independent of s (by a partition of unity argument) to yield the relation (2.15).

(*ii*) and (*ii*) are proved in the same way as the results (2.7) and (2.8) of the homogeneous theory.

Point (*i*) shows that the reduced wave front is essentially the $\lambda > 0$ part of the homogeneous wave front, cut by the hyperplane $\lambda = \frac{1}{\hbar}$ and integrated over s; (*ii*) and (*iii*) show the relevance of this set in the reduced theory.

2.3. Symmetrization of the reduced theory

At this point the reduced theory is essentially equivalent to the original homogeneous theory through conjugation by the mapping $\mathscr{F}$, and it now has a form adapted to asymptotic ($\hbar \to 0$) problems of quantum mechanics. But it fails to reflect an essential symmetry of these problems: canonical invariance.

Classical hamiltonian mechanics on the phase space $X = Q \oplus P$ is covariant with respect to the group of *symplectic* diffeomorphisms of X $\left(\text{those preserving the symplectic form } \omega = \sum_{1}^{l} dq^i \wedge dp_i\right)$.

Although there is no representation of this group as a unitary symmetry group of the quantum theory [*34*], there does exist such a (projective) representation for the subgroup of *affine* (resp. *linear*) symplectic mappings of X, denoted $i\mathrm{S}p(\mathrm{X})$ (resp. $\mathrm{S}p(\mathrm{X})$) : the well known *metaplectic* representation of van Hove-Segal-Shale-Weil [*11*] [*33*]-[*35*]). Several authors have stressed the necessity for an asymptotic theory of quantum mechanics to reflect metaplectic symmetry [*4*] [*15*] [*23*], and our reduced PDO theory definitely fails in this respect; the definition (2.14) of a reduced PDO is not even invariant under interchange of q and p.

This defect has an easy remedy, in two steps. First, instead of the non-invariant symbol map (2.11), we shall define the symbols by a Wigner transformation, which enjoys explicit metaplectic covariance (see section 4). Next, we shall require the symbol of a (reduced) operator to satisfy growth conditions like (2.13)-(2.14), but equally strong in the q and p variables ([2]). While the first step could be viewed as just a matter of convenience concerning the choice of a symbol map, the second step restricts in a nontrivial way the class of « admissible » operators (as we shall call them, to avoid confusion): these are more regular than reduced PDO's. For example, reduced PDO's like their homogeneous counterparts, cannot be composed

([2]) We could have symmetrized the homogeneous theory as well, but the operation would not have made much sense — especially if $\tilde{Q}$ were a manifold.

(multiplied) without support assumptions irrelevant for quantum mechanics [7] [8], while our admissible operators will form an algebra without any assumptions (this algebra is very close to the ones studied in [15]).

3. ADMISSIBLE OPERATORS AND THE WIGNER SYMBOLIC CALCULUS

In this section we define and discuss an algebra of quantum operators along the lines suggested by section 2.

3.1. Notations

Let $Q \approx \mathbb{R}^l$ be an affine space ($l < \infty$). We shall use on Q (and on other linear spaces) conventional multi-index notations:

$$\alpha = (\alpha_1, \ldots, \alpha_l)_{\alpha_i \in \mathbb{N}} ; \qquad |\alpha| = \sum_1^l \alpha_i ; \qquad \alpha ! = \prod_1^l \alpha_i !$$

$$q^\alpha = \prod_1^l q_i^{\alpha_i} ; \qquad \partial_q^\alpha f = \frac{\partial^{|\alpha|} f}{\partial q^\alpha} = \frac{\partial^{\alpha_1 + \ldots + \alpha_l}}{\partial_{q_1}^{\alpha_1} \ldots \partial_{q_l}^{\alpha_l}} f(q_1, \ldots, q_l)$$

We begin with notions borrowed from classical mechanics [24] [35]-[37]. Let $P = Q^*$ (³) (dual of Q). The *phase space* is the symplectic manifold $(X, \omega) = \left(Q \oplus P, \sum_1^l dq_j \wedge dp_j\right)$; its points are noted $x = (q, p)$. As the Lie algebra $\mathfrak{A}_{cl}$ of *classical observables*, we choose the function space $\mathcal{O}_M(X)$ defined in [38] [39] (³), with the Poisson bracket law:

$$\{ f, g \} = \sum_1^l \left(\frac{\partial f}{\partial q_j} \frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial g}{\partial q_j} \right).$$

For $h \in \mathfrak{A}_{cl}$ we define its hamiltonian vector field $\mathcal{X}_h = (\nabla_p h, -\nabla_q h)$ and its flow U_t^h (the classical evolution operator) [36]-[38].

Let $\langle \ , \ \rangle_{cl}$ be the inner product on $L^2_{\mathbb{C}}(X, \omega^l = d^{2l}x)$:

$$\langle f, g \rangle_{cl} = \int_X f^*(x) g(x) d^{2l}x \tag{3.1}$$

This « classical pairing » naturally extends (with the same notation) to other spaces in duality, like $\mathcal{S}^{\mathbb{C}}(X)$ and $\mathcal{S}'^{\mathbb{C}}(X)$.

(³) With real-valued functions. If we want complex-valued functions we shall write $\mathcal{O}_M^{\mathbb{C}}(X)$ (and likewise for other function or distribution spaces).

A *classical state* is a *positive* measure μ on X (physically, it should be normalizable to $\int_X \mu = 1$, in order to be interpreted as the probability density of presence in phase space, but we shall not worry about this ([4]) here) [*38*].

Quantum mechanics suggests the study of various classes of linear operators acting on a complex Hilbert space $\mathscr{H}$ whose elements are called *state vectors* and noted $| \psi \rangle$ (the antidual of $| \varphi \rangle$ is noted $\langle \varphi |$ and the inner product is noted $\langle \varphi | \psi \rangle$. The quantum observables are the self-adjoint operators on $\mathscr{H}$; a quantum state is a positive operator ρ (a « density matrix » : again we shall omit its normalization ([4]), which should be: $\operatorname{Tr} \rho = 1$). Any state vector $| \psi \rangle$ defines a *pure state* $\rho = | \psi \rangle \langle \psi |$ (the orthogonal projector onto the ray spanned by $| \psi \rangle$) [*38*].

The space of Hilbert-Schmidt operators $\mathrm{HS}(\mathscr{H})$ admits the inner product or « quantum pairing »:

$$\langle \mathrm{B}, \mathrm{A} \rangle_{qu} = \operatorname{Tr} \mathrm{B}^\dagger \mathrm{A} \tag{3.2}$$

which extends (with the same notation) to other operator spaces in duality, e. g. : A bounded and B of trace-class, etc. ([*40*], vol. 1).

We impose on our Hilbert space $\mathscr{H}$ an additional structure: that of being an irreducible representation space of the *Heisenberg algebra* $\{ \mathrm{Q}_j, \mathrm{P}_j, \mathbb{1} \}_{j=1,\dots,l}$ with the commutation rules: $[\mathrm{Q}_j, \mathrm{P}_k]_- = i\hbar\, \delta_{jk}\mathbb{1}$. Up to unitary equivalence (see section 4), the solution to this problem is the *position representation*: $\mathscr{H} \approx \mathrm{L}^2_{\mathbb{C}}(\mathrm{Q}, d^lq)$, the vectors of $\mathscr{H}$ being *wave functions* $q \longmapsto \psi(q)$, the algebra $\{ \mathrm{Q}_j, \mathrm{P}_j, \mathbb{1} \}$ being represented by the self-adjoint operators:

$$(\hat{q}_j\psi)(q) = q_j\psi(q)\,; \qquad (\hat{p}_j\psi)(q) = -\,i\hbar\frac{\partial\psi}{\partial q_j}(q)\,; \qquad (\hat{1}\psi)(q) = \psi(q) \tag{3.3}$$

This additional structure depends on the parameter $\hbar (0 < \hbar < \infty)$, therefore we shall allow vectors of $\mathscr{H}$, operators on $\mathscr{H}$ ... to depend explicitly on $\hbar$, too.

3.2. **The Weyl quantization rule** [*41*]

This rule associates to any function $f \in \mathfrak{A}^{\mathbb{C}}_{\mathrm{cl}}(\mathrm{X})$ an $\hbar$-dependent operator on $\mathscr{H}$ denoted $\hat{f}$, defined by its kernel in the position representation:

$$\hat{f}(q, q'\,; \hbar) = \langle q \,|\, \hat{f}(\hbar) \,|\, q' \rangle = \frac{1}{(2\pi\hbar)^l} \int_{\mathrm{P}} f\left(\frac{q+q'}{2}, p\right) e^{\frac{ip(q-q')}{\hbar}} d^lp \tag{3.4}$$

([4]) Instead, we shall say that two measures (resp. operators) differing by a scalar factor define the same classical (resp. quantum) state. Generalized (non-normalizable) states are thus allowed.

The canonical coordinate functions (q_j, p_j) precisely get quantized as the operators $(\hat{q}_j, \hat{p}_j)$ occurring in Eq. (3.3), and also:

$$\hat{1} = \mathbb{1}\,;\ \widehat{T(p) + V(q)} = T(\hat{p}) + V(\hat{q})$$

for arbitrary functions T and V.

The Weyl rule has the following symmetry properties:

$$\begin{cases} \hat{f^*} = \hat{f}^\dagger \quad \text{(formally)} & (3.5\,a) \\ \widehat{\exp i(\alpha q + \beta p)} = \exp i(\alpha\hat{p} + \beta\hat{q}) \quad (\forall \alpha, \beta \in \mathbb{R}^l) & (3.5\,b) \end{cases}$$

Eq. (3.5 *b*) characterizes the Weyl rule, in a representation-free way, as a symmetric ordering of quantum operators. The Weyl rule also has group-theoretical properties to be seen in section 4.

3.3. The Wigner symbol map

Wigner has introduced a transformation on operators of $\mathscr{H}$ which is just the inverse of the map $f \rightarrow \hat{f}$ of Eq. (3.4). To an operator $A(\hbar)$ it associates a complex function A_W on X, now also $\hbar$-dependent in general. In terms of the kernel $A(q, q')$ in the position representation, formally [*14*]:

$$A_W(q, p\,;\hbar) = \int_Q A\left(q - \frac{r}{2}, q + \frac{r}{2}\,;\hbar\right)e^{\frac{ipr}{\hbar}} d^l r \tag{3.6}$$

Since A_W is some sort of classical equivalent of the operator A, we shall view Eq. (3.6) as a symbol map and call A_W the *Wigner symbol* of A. We expect this (full) symbol to be more symmetrical in q and p than the analogous symbol defined by (2.11). For instance, this symbol is *real iff* A *is symmetric.*

For fixed $\hbar$, the Parseval identity applied to Eq. (3.6) implies that this symbol map is *unitary* from $HS(\mathscr{H}) \approx L^2_{\mathbb{C}}(Q \times Q, d^l q \times d^l q)$ to $L^2_{\mathbb{C}}\left(X, \frac{d^{2l}x}{(2\pi\hbar)^l}\right)$:

$$\left.\begin{aligned} \langle B(\hbar), A(\hbar)\rangle_{qu} (= \operatorname{Tr} B^\dagger A) &= \frac{1}{(2\pi\hbar)^l}\int_X B^*_W(x\,;\hbar)A_W(x\,;\hbar)d^{2l}x \\ &\equiv \frac{1}{(2\pi\hbar)^l}\langle B_W(\hbar), A_W(\hbar)\rangle_{cl} \end{aligned}\right\} \tag{3.7}$$

Also, if A is of trace-class and $A_W \in L^1_{\mathbb{C}}(X, d^{2l}x)$:

$$\operatorname{Tr} A(\hbar) = \int_Q A(q, q)d^l q = \frac{1}{(2\pi\hbar)^l}\int_X A_W(x\,;\hbar)d^{2l}x \tag{3.8}$$

3.4. **Admissible operators** [27]

We define an operator $A(\hbar)$ on $\mathcal{H}$ to be *admissible* iff its symbol $A_W(x;\hbar)$ is a C^∞ function of $x \in X$ and $\hbar \in [0, \hbar_0)$ (for some unspecified $\hbar_0 \in (0, \infty]$) with an expansion as $\hbar \to 0^+$:

$$A_W(x;\hbar) \sim \sum_{n=0}^{\infty} A_n(x)\hbar^n \tag{3.9}$$

where all « coefficients » $A_n \in \mathcal{O}_M^{\mathbb{C}}(X)$ satisfy, for some $m \in \mathbb{R}$ and for all $\alpha \in \mathbb{N}^{2l}$:

$$|\partial_x^\alpha A_n(x)| \leqslant C_{n,\alpha} \| x \|^{m-|\alpha|-2n} \tag{3.10}$$

as $\| x \| \to \infty$ (for an arbitrary norm $\| \,.\, \|$ on X), and with an asymptotic condition imposed on (3.9):

$(\forall n \in \mathbb{N},\ \forall \alpha \in \mathbb{N}^{2l})$:

$$\left| \partial_x^\alpha \left(A_W(x;\hbar) - \sum_0^{n-1} A_j(x)\hbar^j \right) \right| \leqslant C_{n,\alpha}\hbar^n \| x \|^{m-|\alpha|-2n} \tag{3.11}$$

$$\left(\text{with the convention: } \sum_0^{-1} [\text{anything}] = 0 \right)$$

when $\hbar \to 0^+$ and/or $\| x \| \to +\infty$. Compared to Eq. (2.14), Eq. (3.11) is symmetrical in q and p, and « scale-invariant » under the homothety $(\hbar, x) \mapsto (\tau\hbar, \sqrt{\tau}x)$; physically $\hbar$ has the dimension of a product $q.\,p$.

The operators satisfying (3.11) for a given $m \in \mathbb{R}$ form the space $\hat{\mathfrak{A}}_m^{\mathbb{C}}(X)$. We have $\hat{\mathfrak{A}}_{m_1}^{\mathbb{C}} \subseteq \hat{\mathfrak{A}}_{m_2}^{\mathbb{C}}$ for $m_1 \leqslant m_2$, and we set:

$$\hat{\mathfrak{A}}^{\mathbb{C}}(X) = \bigcup_{-\infty < m < \infty} \hat{\mathfrak{A}}_m^{\mathbb{C}}(X):$$

the space of all admissible operators;

$$\hat{\mathcal{S}}^{\mathbb{C}}(X) = \hat{\mathfrak{A}}_{-\infty}^{\mathbb{C}}(X) = \bigcap_{-\infty < m < \infty} \hat{\mathfrak{A}}_m^{\mathbb{C}}(X):$$

the space of all admissible operators A such that A_W and all coefficients A_n belong to $\mathcal{S}^{\mathbb{C}}(X)$.

DÉFINITIONS 3.4.1. — The dominant term $A_0(x)$ is called the *principal symbol*, or the *classical limit*, of the operator A.

— The operators $A \in \hat{\mathfrak{A}}_m^{\mathbb{C}}$ with real-valued symbols form the real space $\hat{\mathfrak{A}}_m$; if moreover $A_0(x) > 0$ for all x, we write $A \in \hat{\mathfrak{A}}_m^+$.

— An operator $N \in \hat{\mathfrak{A}}^{\mathbb{C}}$ is *negligible* iff $N_W \sim 0$, hence according to (3.10):

$N \in \hat{\mathcal{S}}^{\mathbb{C}}$, and all seminorms of N_W in $\mathcal{S}^{\mathbb{C}}$ are $\sigma(\hbar^\infty)$. These operators form the space $\hat{\mathcal{N}}^{\mathbb{C}}(X)$.

Our admissible operators form a smaller space than Leray's pseudo-differential operators [*23*] due to the growth restrictions as $\|x\| \to \infty$ in Eq. (3.11) (the Wigner symbol in [*23*], noted a_0, is any C^∞ function), and they differ from the operators of [*15*] by obeying explicit behaviour laws in $\hbar$, which we view as important (see section 2). However, for the proof of the forthcoming theorems, we shall find it convenient to assume sometimes $\hbar$ fixed and forget about the $\hbar$-dependence. Then Eq. (3.11) reduces to:

$$(\forall \alpha \in \mathbb{N}^{2l}): \quad |\partial_x^\alpha A_W(x)| \leqslant C_{n,\alpha} \|x\|^{m-|\alpha|} \quad (\|x\| \to \infty) \qquad (3.11')$$

which appears in ref. [*15*].

Grushin's quasi-homogeneous operators [*42*] [*43*] are also defined by estimates analogous to (3.11).

THEOREM 3.4.2. — $\hat{\mathfrak{A}}^{\mathbb{C}}$ is an algebra for operator multiplication, with $\hat{\mathfrak{A}}^{\mathbb{C}}_{m_1}\hat{\mathfrak{A}}^{\mathbb{C}}_{m_2} \subseteq \hat{\mathfrak{A}}^{\mathbb{C}}_{m_1+m_2}$. The symbol of a product is:

$$(AB)_W(x\,;\hbar) = \frac{1}{(\pi\hbar)^{2l}} \int_{X^2} A_W(x + x_1\,;\hbar) B_W(x + x_2\,;\hbar) e^{\frac{2i}{\hbar}\omega(x_1,x_2)} d^{2l}x_1 d^{2l}x_2 \qquad (3.12)$$

and it has the expansion (Groenowold's rule [*14*] [*16*], or Wick's theorem):

$$(AB)_W(x\,;\hbar) \sim \sum_{n=0}^{\infty} \frac{(i\hbar)^n}{2^n.n!} [(\partial_{q_1}\partial_{p_2} - \partial_{q_2}\partial_{p_1})^n A_W(x_1) B_W(x_2)]_{x_1=x_2=x}$$

denoted: (3.13)

$$(AB)_W \sim A_W(x)\left[\exp \frac{i\hbar \overleftrightarrow{\Lambda}}{2}\right] B_W(x)$$

$\left(\text{where } \overleftrightarrow{\Lambda} = \overleftarrow{\partial}_q \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_q\,;\ \text{note that } \exp\left(\frac{i\hbar\overleftrightarrow{\Lambda}}{2}\right) \text{ is « scale-invariant »}\right)$

Remarks. — The operation (3.12) is known as the *twisted product* of symbols [*15*] [*17*]. When $\hbar = 0$ it reduces to the ordinary commutative product of the principal symbols: $(AB)_0(x) = A_0(x)B_0(x)$. If A_W (or B_W) is a polynomial in x, the series (3.13) terminates and gives the exact value of $(AB)_W$.

COROLLARY 3.4.3. — *a*) The anticommutator of two operators has the symbol expansion:

$$([A, B]_+)_W(x\,;\hbar) \sim A_W(x\,;\hbar)\left[2 \cos \frac{\hbar \overleftrightarrow{\Lambda}}{2}\right] B_W(x\,;\hbar) \qquad (3.13')$$

b) The commutator of two operators has the expansion:

$$([\mathrm{A}, \mathrm{B}]_-)_{\mathrm{W}}(x\,;\hbar) \sim \mathrm{A}_{\mathrm{W}}(x\,;\hbar)\left[2i \sin \frac{\hbar \overleftrightarrow{\Lambda}}{2}\right]\mathrm{B}_{\mathrm{W}}(x\,;\hbar) \qquad (3.13'')$$

$\hat{\mathfrak{A}}^{\mathbb{C}}$ is a Lie algebra for the commutator; also $\hat{\mathfrak{A}}$ is a Lie algebra for the operation $(\mathrm{A}, \mathrm{B}) \mapsto \dfrac{[\mathrm{A}, \mathrm{B}]_-}{i\hbar}$ (with principal symbol $\{\mathrm{A}_0, \mathrm{B}_0\}$), and $\dfrac{[\hat{\mathfrak{A}}_{m_1}, \hat{\mathfrak{A}}_{m_2}]_-}{i\hbar} \subset \hat{\mathfrak{A}}_{m_1+m_2-2}$.

c) If A_{W} (*or* B_{W}) is a polynomial in x *of degree* $\leqslant 2$:

$$([\mathrm{A}, \mathrm{B}]_-)_{\mathrm{W}} = i\hbar\{\mathrm{A}_{\mathrm{W}}, \mathrm{B}_{\mathrm{W}}\} \qquad (3.14)$$

PROOF OF THEOREM 3.4.2. — In a first step, we omit the $\hbar$-dependence of symbols, hence we only assume the estimates (3.11′) for $\mathrm{A} \in \hat{\mathfrak{A}}^{\mathbb{C}}_{m_1}$ and $\mathrm{B} \in \hat{\mathfrak{A}}^{\mathbb{C}}_{m_2}$. The formula (3.12) for $(\mathrm{AB})_{\mathrm{W}}$ is easy to derive formally using (3.4) and (3.6), but we must show that it makes sense and that $(\mathrm{AB})_{\mathrm{W}}$ satisfies (3.11′) for $m = m_1 + m_2$. The idea is that the integrand in (3.12) is tempered in the x variables, and it is rapidly decreasing as a distribution in the variables $y = (x_1, x_2)$ thanks to the oscillations of the phase (Eq. (3.11) will make sense as an « oscillatory integral »).

More precisely we want the following equality *and* bound:

$$\frac{\partial_x^\alpha(\mathrm{AB})_{\mathrm{W}}}{(1+\|x\|^2)^{\frac{m-|\alpha|}{2}}} = \frac{1}{(\pi\hbar)^{2l}}\int_{\mathrm{X}^2} \frac{\partial_x^\alpha[\mathrm{A}_{\mathrm{W}}(x+x_1)\mathrm{B}_{\mathrm{W}}(x+x_2)]}{(1+\|x\|^2)^{\frac{m-|\alpha|}{2}}}\, e^{\frac{2i}{\hbar}\omega(x_1,x_2)}\, dx_1 dx_2 = \mathcal{O}(1) \qquad (3.15)$$

with $m = m_1 + m_2$. The Leibniz formula produces in (3.15) sums of terms $\partial_x^{\alpha_1}\mathrm{A}_{\mathrm{W}}(x+x_1)\,.\,\partial_x^{\alpha_2}\mathrm{B}_{\mathrm{W}}(x+x_2)$ with $\alpha = \alpha_1 + \alpha_2$.

By hypothesis:

$$\frac{\partial_x^{\alpha_1}\mathrm{A}_{\mathrm{W}}(x+x_1)}{(1+\|x+x_1\|^2)^{\frac{m_1-|\alpha_1|}{2}}} \quad \text{and} \quad \frac{\partial_x^{\alpha_2}\mathrm{B}_{\mathrm{W}}(x+x_2)}{(1+\|x+x_2\|^2)^{\frac{m_2-|\alpha_2|}{2}}}$$

and all their derivatives in x, x_1 and x_2 are uniformly bounded. This is also true for the function $\dfrac{(1+\|x+x_1\|^2)^{\frac{m_1-|\alpha_1|}{2}}}{(1+\|x\|^2)^{\frac{m_1-|\alpha_1|}{2}}(1+\|y\|^2)^{\left|\frac{m_1-|\alpha_1|}{2}\right|}}$ and for its analog with x_2, m_2, α_2. Hence the integrand in (3.15) can be written as:

$$\Phi(x, y)(1+\|y\|^2)^k e^{\frac{2i}{\hbar}\omega(x_1,x_2)}$$

where Φ and all its derivatives are uniformly bounded in X^3 if $k \in \mathbb{N}$ is chosen large enough. But for every $n \in \mathbb{N}$:

$$\left(1 + \sum_1^{4l} y_i^2\right)^n e^{\frac{2i}{\hbar}\omega(x_1,x_2)} = P_n(\partial_{x_1}, \partial_{x_2}) e^{\frac{2i}{\hbar}\omega(x_1,x_2)}$$

for some polynomial P_n, because ω is nondegenerate; therefore (as for the case of e^{ix^2} proved in [39]) : $\left(1 + \sum_1^{4l} y_i^2\right)^k e^{\frac{2i}{\hbar}\omega(x_1,x_2)} \in \mathcal{O}_c'^{\mathbb{C}}(\mathbb{R}^{4l})$ and we can integrate the y variables in (3.15). Also, derivation under $\int$ is legitimate in this case, so the RHS of (3.15) is equal indeed to $\dfrac{(\partial_x^\alpha(AB)_W}{(1 + \|x\|^2)^{\frac{m-|\alpha|}{2}}}$ and is bounded uniformly in x.

Now we look again at the $\hbar$-dependence of our expressions: $A_W(x + x_1)B_W(x + x_2)$ depends smoothly on $\hbar$ with an expansion to any order, and control over the remainder by Eq. (3.11). Also, in the space $\mathcal{O}_c'^{\mathbb{C}}(\mathrm{R}^{4l})$ we have the asymptotic expansion in powers of $\hbar$:

$$\frac{e^{\frac{2i}{\hbar}\omega(x_1,x_2)}}{(\pi\hbar)^{2l}} \sim \sum_{n=0}^{\infty} \frac{1}{n!}\left[\frac{i\hbar}{2}(\nabla_{q_1}\nabla_{p_2} - \nabla_{q_2}\nabla_{p_1})\right]^n \delta(x_1)\delta(x_2)$$

Proof. — The Fourier transform:

$$\int_{X^2} \frac{e^{\frac{2i}{\hbar}\omega(x_1,x_2)}}{(\pi\hbar)^{2l}} e^{i(\eta_1 p_1 + \eta_2 p_2 - \zeta_1 q_1 - \zeta_2 q_2)} dx_1 dx_2 = e^{\frac{i\hbar}{2}(\zeta_1\eta_2 - \zeta_2\eta_1)}$$

has the asymptotic Taylor series $\sum_0^{\infty} \frac{(i\hbar)^n}{2^n.n!}(\zeta_1\eta_2 - \zeta_2\eta_1)^n$ in the Fourier transformed space $\mathcal{O}_M^{\mathbb{C}}(\mathbb{R}^{4l})$.

Hence substitution term by term in (3.12) makes sense and yields Eq. (3.13). Equivalently we could have evaluated the expansion by the stationary phase method, or by successive integrations by parts. The latter method makes it obvious that for a polynomial A_W (or B_W), the finite RHS of Eq. (3.13) gives the symbol of the product exactly.

The proof of the corollary is straightforward.

We now turn to miscellaneous properties of admissible operators.

THEOREM 3.4.4. — If $A \in \hat{\mathfrak{A}}^{\mathbb{C}}(X)$, if $A_0(x) \neq 0$ for all x, and if for $\|x\| \to +\infty$:

$$(\forall \alpha \in \mathbb{N}^{2l},\ \forall n \in \mathbb{N}): \qquad |\partial_x^\alpha A_n(x)| \leqslant C_{n,\alpha}|A_0(x)| \,.\, \|x\|^{-|\alpha|-2n} \quad (3.16)$$

then A^{-1} exists in $\hat{\mathfrak{A}}^{\mathbb{C}}$ with principal symbol $(A^{-1})_0 = \frac{1}{A_0}$, for $\hbar$ small enough.

Proof. — We shall adapt the parametrix method of homogeneous PDO theory [8]. First we construct the inverse symbol as a formal power series in $\hbar$: $B_W \sim \sum_0^\infty B_n(x)\hbar^n$, solution of:

$$1 \sim (AB)_W \sim [A_W e^{\frac{i\hbar\overleftrightarrow{\Lambda}}{2}}]B_W = \left(\sum_{n=0}^\infty \mathscr{A}_n(x, \partial_x)\hbar^n\right)\left(\sum_{k=0}^\infty B_k(x)\hbar^k\right)$$

where the $\mathscr{A}_n$ are linear partial differential operators of order $\leqslant n$ depending linearly on the coefficients $A_{n'}(n' \leqslant n)$; in particular: $\mathscr{A}_0(x, \partial_x) \equiv A_0(x)$. That equation has the recursive solution (see also § 6.3):

$$B_0(x) = \frac{1}{A_0(x)}; \; \dots \; ; B_n(x) = \frac{-1}{A_0(x)}\left(\sum_{k=0}^{n-1} \mathscr{A}_{n-k}(x, \partial_x)B_k(x)\right) \quad (3.17)$$

Eq. (3.16) implies: $\| \nabla_x(\log | A_0(x) |) \| \leqslant \frac{m'}{\| x \|}$ for $m' = \max_{|\alpha|=1} \{ C_{0,\alpha} \}$, hence $\left| \frac{1}{A_0(x)} \right| < C \| x \|^{m'}$ as $\| x \| \to \infty$. Repeated use of Eq. (3.16) and some dimensional analysis on the $\mathscr{A}_n$ (related to scale invariance) yields: $| \partial_x^\alpha B_n(x) | \leqslant C_{n,\alpha} \| x \|^{m'-2n-|\alpha|}$. Again adapting a standard argument of PDO theory, we can assert the existence of an approximate inverse $B \in \hat{\mathfrak{A}}_{m'}^{\mathbb{C}}$ with $B_W \sim \sum_0^\infty B_n \hbar^n$ and $A(\hbar)B(\hbar) - \mathbb{1} = N(\hbar) \in \mathscr{N}^{\mathbb{C}}$ (a negligible operator) so that: $\| N \|_{H.S.} = \sigma(\hbar^\infty)$ by Eq. (3.7). Then the existence of $A^{-1} = B(1+N)^{-1}$ is guaranteed by a Neumann series or a Fredholm type argument, for $\hbar < \hbar'_0$ (if $\hbar'_0$ is chosen small enough) $\left(\text{and } (A^{-1})_W \text{ has the same expansion } \sum_0^\infty B_n\hbar^n\right)$.

The condition (3.16) essentially keeps the symbol of A from decreasing too rapidly as $\| x \| \to \infty$.

We now introduce an important class of comparison operators: the powers of the quantized harmonic oscillator.

LEMMA 3.4.5. — Let $H = \hat{h}$ with $h(x) = \frac{1}{2}(q^2 + p^2)$. Then for all $n \in \mathbb{Z}$: $(1 + H)^n \in \hat{\mathfrak{A}}_{2n}^+(X)$ and has principal symbol $(1 + h)^n$.

This is obvious for $n = 0,1$. Theorem 3.4.2 then proves it for $n \geqslant 2$, and theorem 3.4.4 for $n < 0$ (the lemma is certainly true for any $n \in \mathbb{R}$, but we have not proved it).

THEOREM 3.4.6. — If $A \in \hat{\mathfrak{A}}^+$ (definition 3.4.1) and if A satisfies (3.16), then it is a semi-bounded operator (positive for $\hbar$ small enough).

Proof. — as we know, (3.16) implies: $A_0(x) \geq C \| x \|^{-m'} > 0$ for some $m' \in \mathbb{R}$. Let $A' = (1 + H)^n A (1 + H)^n$, with H as in lemma 3.4.5, and $n \in \mathbb{N}$ is chosen $\geq \frac{m'}{4}$. Then $A'_0(x) \geq c > 0$. Now there exists a symmetric operator $B \in \hat{\mathfrak{A}}$ which is an approximate square root of $\left(A' - \frac{c}{2}\mathbb{1}\right)$ in the sense that $B^2 = \left(A' - \frac{c}{2}\mathbb{1}\right) + N$, $N \in \hat{\mathcal{N}}$; the principal symbol of B is $\sqrt{A'_0(x) - c/2}$. The proof is patterned exactly on the proof of theorem 3.4.4, except that B and N come out with real symbols, hence they are symmetric. But N is bounded so it is self-adjoint, then: $A' = B^2 + \left(\frac{c}{2}\mathbb{1} - N\right)$ is a semi-bounded operator, and so is $A = (1 + H)^{-n} A' (1 + H)^{-n}$. Since $\| N \| = \mathcal{O}(\hbar^\infty)$, A' and A are positive for $\hbar$ small enough.

THEOREM 3.4.7 (5). — As an operator $\mathcal{H} \to \mathcal{H}$, $A(\hbar) \in \hat{\mathfrak{A}}^{\mathbb{C}}_m$ satisfies:

a) if $m = 0$: $A(\hbar)$ is bounded.
b) if $m < 0$: $A(\hbar)$ is compact.
c) if $m < -l$: $A(\hbar)$ is of Hilbert-Schmidt (H-S) class.
d) if $m < -2l$: $A(\hbar)$ is of trace-class.
e) for all m (and all $\mathbb{N} \ni n \geqslant m/2$): $A(1 + H)^{-n}$ is bounded, hence A is defined on the dense domain of H^n in $\mathcal{H}$ (H as in lemma 3.4.5).

Proof. — in the following order: *c*), *b*), *d*), *a*), *e*).

c) if $m < -l$, $A_W \in L^2(X)$, and we apply Eq. (3.7).

b) if $m < 0$, some power $A^k \in \hat{\mathfrak{A}}^{\mathbb{C}}_{mk} (k \in \mathbb{N})$ is H-S by *c*), so A is compact.

d) if $m < -2l$, A can be written as a product of two H-S operators, e. g. $A = B(B^{-1}A)$ with $B = \widehat{(1 + h)^{m/4}}$ (h as in lemma 3.4.5): B and $B^{-1}A$ are in $\hat{\mathfrak{A}}^{\mathbb{C}}_{m/2}$, and we apply *c*).

a) if A_W is real and $| A_0(x) | \leq M$, then for some $\varepsilon > 0$, $A + (M + \varepsilon).\mathbb{1}$ and $(M + \varepsilon).\mathbb{1} - A$ are positive operators by theorem 3.4.6 (they satisfy condition (3.16) automatically), hence A is bounded. This extends to complex-valued symbols, using: $A = \widehat{\mathrm{Re}\, A_W} + i\, \widehat{\mathrm{Im}\, A_W}$.

e) if $m \leq 2n$: by lemma 3.4.5: $A(1 + H)^{-n} \in \hat{\mathfrak{A}}^{\mathbb{C}}_0$, so it is bounded, by *a*) (as for the lemma, the restriction $n \in \mathbb{N}$ is certainly avoidable).

(5) For more detailed proofs and further properties of admissible operators, see [*61*]-[*62*].

Concerning the symmetric operators $A \in \hat{\mathfrak{A}}$, the question of their self-adjointness is a very difficult problem in general (40, vol. II). A semi-bounded operator (as in theorem 3.4.6) does have self-adjoint extensions by Friedrichs' theorem. On the other hand, an operator as simple as $\hat{q}\hat{p}\hat{q} \in \hat{\mathfrak{A}}_3(\mathbb{R}^2)$ has unequal deficiency indices, hence no self-adjoint extensions [*44*].

3.5. Asymptotic operators

The space of negligible operators $\hat{\mathcal{N}}^{\mathbb{C}}$ forms an ideal of $\hat{\mathfrak{A}}^{\mathbb{C}}$ by theorem 3.4.2. The quotient algebra $\tilde{\mathfrak{A}}^{\mathbb{C}} = \hat{\mathfrak{A}}^{\mathbb{C}}/\hat{\mathcal{N}}^{\mathbb{C}}$ can be identified as the algebra of *formal* power series $\tilde{A} = \sum_0^\infty A_n(x)\hbar^n$ satisfying Eq. (3.10), with the multiplication law (3.13) (which is *microlocal*, i. e. local in phase space). $\tilde{\mathfrak{A}}^{\mathbb{C}}$ is the relevant framework for the asymptotic study of operator of $\hat{\mathfrak{A}}^{\mathbb{C}}$: we call the elements $\tilde{A}$ of $\tilde{\mathfrak{A}}^{\mathbb{C}}$ *asymptotic operators.*

4. THE METAPLECTIC REPRESENTATIONS

The covariance of quantization under linear canonical transformations of X is realized via the « metaplectic representation » Mp(l), of the group Sp(l) on $\mathcal{H}$; there is an extensive literature on this subject, for instance [*11*] [*23*] [*34*]-[*35*] [*45*]-[*47*], and also on the related notions of half-forms and symplectic spinors [*32*] [*33*]. Here we shall only give a few basic facts of the theory, but our treatment will: 1) stress the special relevance of Weyl's quantization procedure (§3.2) as *the one* that is *explicitly* covariant under the representation Mp(l), and also as a way to build the representation itself; 2) incorporate the Weyl representation of the translation group of X at the same time.

An affine symplectic frame R on X is defined by an origin $x_0 \in X$ and by independent vectors $e_1, \ldots, e_{2l}$ at x_0 such that $\omega(e_j, e_{l+k}) = \delta_{jk}$ for $j, k = 1, \ldots, l$. Those frames form a manifold F. Let Q_R and P_R be the affine subspaces of X spanned by $\{ e_j \}_{j=1,\ldots,l}$ and $\{ e_k \}_{k=l+1,\ldots,2l}$ respectively, and q_{Rj}, p_{Rk} be the corresponding canonical coordinate functions.

Let $Sp(l) \subset GL(2l, \mathbb{R})$ be the real symplectic group [*37*] on $\mathbb{R}^{2l}$ (we shall call « rotations » the matrices $U \in Sp(l)$), and iSp(l) be the usual semi-direct product group $Sp(l) \times_{Sp(l)} \mathbb{R}^{2l}$: the affine (or inhomogeneous) symplectic group on $\mathbb{R}^{2l}$; the elements $(\mathbb{1}, a)$ with $a \in \mathbb{R}^{2l}$ are the translations on $\mathbb{R}^{2l}$. There is a right action of the group iSp(l) on F:

$$R = \{ x_0 ; e_1, \ldots, e_{2l} \} \longrightarrow R(U, a) = \left\{ x_0 + \sum_1^{2l} a_j e_j ; \sum_1^{2l} U_{j1} e_j, \ldots, \sum_1^{2l} U_{j,2l} e_j \right\}$$

where $U \in Sp(l)$, $a \in \mathbb{R}^{2l}$, $(U, a) \in i\mathrm{Sp}(l)$.

4.1. Canonical quantization

Let $\mathcal{Q}_2$, $\mathcal{Q}_1$, $\mathcal{Q}_0$ respectively denote the spaces of (real) quadratic, linear and constant functions on X. They are stable under linear symplectic transformations of X; $\mathcal{Q}_2$, $\underline{\mathcal{Q}}_1 = \mathcal{Q}_1 \oplus \mathcal{Q}_0$ and $\underline{\underline{\mathcal{Q}}} = \mathcal{Q}_2 \oplus \mathcal{Q}_1 \oplus \mathcal{Q}_0$ are Lie algebras for the Poisson brackets; $\underline{\mathcal{Q}}_1$ is called the *Heisenberg algebra.*

Canonical quantization consists in taking an irreducible faithful representation of $\underline{\mathcal{Q}}_1$ by self-adjoint operators on a (separable) Hilbert space $\mathcal{H}$: $\underline{\mathcal{Q}}_1 \rightharpoonup \hat{\underline{\mathcal{Q}}}_1$, with:

$$(\forall \varphi_1, \varphi_2 \in \underline{\mathcal{Q}}_1): \qquad [\hat{\varphi}_1, \hat{\varphi}_2]_- \equiv i\hbar \, \widehat{\{\varphi_1, \varphi_2\}} \tag{4.1}$$

($\hbar > 0$ a given parameter) (6); cf. § 3.1. We know that this structure is at the basis of quantum mechanics [36] [38] [41]. To avoid cumbersome domain problems for the (unbounded) operators $\hat{\varphi}$, we shall replace Eq. (4.1) by its exponentiated version (Weyl [41]). For this, we define the *Heisenberg group* (or Weyl group) as the fiber bundle $W = X \times \mathbb{T} \xrightarrow{\varpi} X$: $w = (x, z) \xrightarrow{\varpi} x \in X$ ($\mathbb{T}$ is the unit circle in $\mathbb{C}$), carrying the multiplication law [17] [38]:

$$(x_1, z_1)(x_2, z_2) = (x_1 + x_2, z_1, z_2 e^{-\frac{i}{2\hbar}\omega(x_1,x_2)}) \tag{4.2}$$

Under the exponential map: $\varphi(x) = \omega(x_0, x) + c_0 \longrightarrow \exp(\varphi) = (x_0, e^{\frac{c_0}{i\hbar}})$, the Lie algebra of W is isomorphic to $\underline{\mathcal{Q}}_1$.

In terms of the Lie group W, canonical quantization is the choice of an irreducible, faithful, unitary Hilbert space representation of W. By the Stone-von Neumann theorem [17] [48] this problem has a solution, *unique* up to unitary equivalence. To express it, we first fix a symplectic frame on X, i. e. we identify X with the « canonical » symplectic space $\left(\mathbb{R}^{2l}, \sum_1^l dq_i \wedge dp_i\right)$: $\underline{\mathcal{Q}}_1$ is then generated by the functions q_j, p_j, 1; we then take $\mathcal{H} = L^2_{\mathbb{C}}(\mathbb{R}^l, d^l r)$ and we define the map $\underline{\mathcal{Q}}_1 \rightharpoonup \hat{\underline{\mathcal{Q}}}_1$ by:

$$\hat{q}_j = \text{multiplication by } r_j; \qquad \hat{p}_j = -i\hbar\frac{\partial}{\partial r_j}; \qquad \hat{1} = \mathbb{1}. \tag{4.3}$$

A unitary representation of W is then the bijection $W \xrightarrow{\sigma^{-1}} \tilde{W}$ = Lie group generated by $\hat{\underline{\mathcal{Q}}}_1$ in $U(\mathcal{H})$ (the group of unitary operators on $\mathcal{H}$):

$$\left.\begin{aligned} w = \exp(\varphi) &\xrightarrow{\sigma^{-1}} \exp\left(\frac{\hat{\varphi}}{i\hbar}\right) \\ \text{or:} \quad \sigma^{-1}(x_0, z_0) &= z_0 \exp\left(\frac{\omega(x_0, \hat{x})}{i\hbar}\right) \end{aligned}\right\} \tag{4.4}$$

(6) Strictly speaking, φ is « represented » by $\hat{\varphi}/i\hbar$, but we shall keep this abuse of notation throughout.

with:

$$\omega(x_0, \hat{x}) = \sum_1^l (q_{0j}\hat{p}_j - p_{0j}\hat{q}_j).$$

But for any $V \in i\mathrm{Sp}(l)$, the map:

$$w = \exp(\varphi) \in W \rightarrow \exp \frac{(\widehat{\varphi \circ V^{-1}})}{i\hbar} \in \tilde{W}$$

defines another irreducible faithful representation of W, hence by the Stone-von Neumann theorem there exists $\mathscr{V} \in U(\mathscr{H})$ such that:

$$(\forall \varphi' \in \mathscr{Q}_1): \qquad \exp \frac{(\widehat{\varphi' \circ V^{-1}})}{i\hbar} = \mathscr{V} \exp\left(\frac{\hat{\varphi}'}{i\hbar}\right)\mathscr{V}^\dagger \tag{4.5}$$

Irreducibility implies that $\mathscr{V}$ is uniquely defined up to a phase factor; as a consequence of this and of Eq. (4.5), the operators $\mathscr{V}$ form a group G with $\mathbb{T}.\mathbb{1}_{\mathscr{H}} \subset G \subset U(\mathscr{H})$, and the map $V \twoheadrightarrow \mathscr{V}$ is a faithful projective representation of $i\mathrm{Sp}(l)$ by G.

4.2. **The manifold of quantum representations**

Before building the group G explicitly, we show its role in the covariance of canonical quantization with respect to $i\mathrm{Sp}(l)$. We shall describe this fact together with the physical interpretation which establishes its importance.

By Eqs. (4.3), each r_j is a spectral value of $\hat{q}_j$, and it is physically the analog (under the correspondence principle between quantum and classical mechanics) of the classical variable q_j: the physicist will thus identify r_j with q_j, and $L^2_{\mathbb{C}}(\mathbb{R}^l, d^l r)$ with $L^2_{\mathbb{C}}(Q, d^l q)$. But Eqs. (4.3)-(4.4) for the representation $\tilde{W}$ were relative to a particular frame on X; the same formulas in various frames $R \in F$ lead to different maps $\hat{}^R$ and representations $\tilde{W}^R$, each expressed on a Hilbert space $L^2_{\mathbb{C}}(Q_R, d^l q_R)$. Since the description of the physical world should privilege no particular frame, we should consider all the $\tilde{W}^R$ as realizations of one abstract representation of W on an intrinsic Hilbert space $\mathscr{H}$. For each $R \in F$, any two realizations of $\mathscr{H}$ as $L^2(Q_R, d^l q_R)$ can differ at most by a constant phase (since the irreducible representation $\tilde{W}^R$ is given). We call each such realization of $\mathscr{H}$ a « representation of quantum mechanics », or *quantum representation*, corresponding to the frame R.

Let $\mathscr{F}$ be the set of all quantum representations $\mathscr{R}$. What structure should we put on $\mathscr{F}$? Clearly it should be a fiber bundle over F, of structure group $\mathbb{T}$. Also, if $\varphi \in \mathscr{Q}_1$, and φ_R denotes its expression in the frame $R \in F$, and if we perform a change of frame $R' = RV$ ($V \in i\mathrm{Sp}(l)$; $\varphi_R = \varphi_{R'} \circ V^{-1}$), then Eq. (4.5) implies:

$$(\forall \varphi \in \mathcal{Q}_1): \qquad \exp\left(\frac{\hat{\varphi}_R^R}{i\hbar}\right) = \mathscr{V} \exp\left(\frac{\hat{\varphi}_{R'}^{R'}}{i\hbar}\right) \mathscr{V}^\dagger \tag{4.6}$$

hence $\mathscr{V}: L^2_{\mathbb{C}}(Q_{R'}, d^l q_{R'}) \to L^2_{\mathbb{C}}(Q_R, d^l q_R)$ is an intertwining operator between $\tilde{W}^{R'}$ and $\tilde{W}^R$. If $\mathscr{R}, \mathscr{R}' \in \mathscr{F}$ are two quantum representations corresponding to R and R', if $\psi \in \mathscr{H}$, and $\psi^{\mathscr{R}} \in L^2(Q_R, d^l q_R)$ denotes its expression in the representation $\mathscr{R}$, we want to specify entirely $\mathscr{V}$ by the condition:

$$(\forall \psi \in \mathscr{H}): \qquad \psi^{\mathscr{R}} = \mathscr{V} \psi^{\mathscr{R}'} \tag{4.7}$$

so that $\mathscr{F}$ must be a space for the transitive, right action of the group G. The correct answer for the structure of $\mathscr{F}$ is then to describe it as the *product fiber bundle* $F \times_{i\mathrm{Sp}(l)} G$: the set of all pairs $(R, \mathscr{V}) \in F \times G$ quotiented by the equivalence relation: $(R, \mathscr{V}) \approx (RV_0, \mathscr{V}_0^{-1}\mathscr{V})$ for any $\mathscr{V}_0 \in G$, $\mathscr{V}_0$ representing a unique $V_0 \in i\mathrm{Sp}(l)$; the projection $\mathscr{F} \to F$ is: $(R, \mathscr{V}) \to RV$.

Eqs. (4.6) and (4.7) express the fact that all the $\tilde{W}^R$ are realizations of a same intrinsically defined representation of W on $\mathscr{H}$. This covariance property implies that all quantum representations in $\mathscr{F}$ are equivalent. Physically, in a representation $\mathscr{R}$ over a frame R, the commuting observables $\{ \hat{q}_{Rj} \}$ are diagonalized, and one more often diagonalizes the position coordinates: the $\mathscr{R}$ such that $Q_R = Q$ are called *position representations*.

All discussions henceforth will take place in some particular representation: usually it will be fixed and not mentioned explicitly (then we shall assume it is a « standard » *position* representation, and identify: $(X, \omega) = \left(\mathbb{R}^{2l}, \sum_1^l dq_i \wedge dp_i\right)$, $Q_R = Q$, $P_R = P$, $\mathscr{H} = L^2_{\mathbb{C}}(Q, d^l q)$, etc.), but sometimes we shall let the representation vary explicitly, only when specified.

4.3. The metaplectic group Mp(l)

First we shall only describe a subgroup of G representing the homogeneous group Sp(l). Maslov [*4*] already considered the representation of the discrete subgroup of Sp(l) generated by rotations by $\pi/2$ in the 2-planes $(q_j, p_j) \subset X$: the corresponding operators in G are partial Fourier transformations [*23*] [*27*]; they allow to pass from position to momentum representations, for instance, and to regularize the WKB theory. But it is more elegant to represent at once the full Lie group Sp(l), because for this we only need the infinitesimal representation of the Lie algebra sp(l) (since Sp(l) is connected), which is very simple to find.

The Lie algebra sp(l) consists of the $2l \times 2l$ matrices: $\begin{pmatrix} b & a \\ -c & -b \end{pmatrix}$

where a, b, c are real $l \times l$ matrices with a and c symmetric [37]. This algebra is isomorphic to the Poisson bracket algebra $\mathcal{Q}_2$ under the map:

$$\varphi = \frac{1}{2}\sum_{j,k=1}^{l}(a_{jk}p_jp_k + 2b_{jk}q_jp_k + c_{jk}q_jq_k) \overset{u}{\longleftrightarrow} u(\varphi) = \begin{pmatrix} b & a \\ -c & -b \end{pmatrix}$$

(which is such that $e^{tu(\varphi)} \equiv U_t^\varphi \in Sp(l)$), U_t^φ defined in § 3.1.

By corollary 3.4.3.c):

$$\forall \varphi_1, \varphi_2 \in \mathcal{Q}_2, \qquad [\hat{\varphi}_1, \hat{\varphi}_2]_- = i\hbar\,\widehat{\{\varphi_1, \varphi_2\}},$$

so that $\mathcal{Q}_2$ is isomorphic by the map $\varphi \longleftrightarrow \dfrac{\hat{\varphi}}{i\hbar}$ to the Weyl-quantized operator Lie algebra $\hat{\mathcal{Q}}_2$, where:

$$\hat{\varphi} = \frac{1}{2}\sum_{j,k}\left[a_{jk}\left(-\frac{i\hbar\partial}{\partial q_j}\right)\left(-\frac{i\hbar\partial}{\partial q_k}\right) + 2b_{jk}q_j\left(-\frac{i\hbar\partial}{\partial q_k}\right) + c_{jk}q_jq_k\right] - \frac{i\hbar}{2}\sum_{j=1}^{l} b_{jj}$$

This gives a representation of sp(l) by $\hat{\mathcal{Q}}_2$, found by van Hove [34], who also proved the self-adjointness on $\mathcal{H}$ of the operators $\hat{\varphi} \in \hat{\mathcal{Q}}_2$.

Let Mp(l) (the *metaplectic group* (7)) be the subgroup of U($\mathcal{H}$) generated by the operators $\exp\left(\dfrac{\hat{\varphi}}{i\hbar}\right)$ for $\hat{\varphi} \in \hat{\mathcal{Q}}_2$. The map: $\exp\left(\dfrac{\hat{\varphi}}{i\hbar}\right) \overset{\pi}{\rightarrow} e^{u(\varphi)} \in Sp(l)$ is clearly a local group isomorphism between neighborhoods of the identities in Mp(l) and Sp(l). Applying again corollary 3.4.3c) with now $A = \hat{\varphi} \in \hat{\mathcal{Q}}_2$ and $B = \hat{f}$, $f \in \mathcal{O}_M^{\mathbb{C}}(X)$:

$$(\forall \varphi \in \mathcal{Q}_2,\ \forall f \in \mathcal{O}_M^{\mathbb{C}}(X)): \qquad [\hat{\varphi}, \hat{f}] = i\hbar\,\widehat{\{\varphi, f\}}\,. \tag{4.8}$$

Let $f(t) = f \circ U_{-t}^\varphi$: $f(t) \in \mathcal{O}_M^{\mathbb{C}}(X)$ for all t, hence by (4.8):

$$\text{Ad}\,\frac{\hat{\varphi}}{i\hbar}\,.\,(\hat{f}(t)) = \left[\frac{\hat{\varphi}}{i\hbar}, \hat{f}(t)\right]_- = \widehat{\{\varphi, f(t)\}} = \widehat{\frac{df}{dt}}(t)\,.$$

Then: $\widehat{f(t)} = \exp\left(t.\text{Ad}\,\dfrac{\hat{\varphi}}{i\hbar}\right)(\hat{f})$, or:

$$(\forall \varphi \in \mathcal{Q}_2,\ \forall f \in \mathcal{O}_M^{\mathbb{C}}(X)): \qquad \left(\exp\frac{\hat{\varphi}}{i\hbar}\right)\hat{f}\left(\exp\frac{\hat{\varphi}}{i\hbar}\right)^\dagger = \widehat{f \circ U_{-1}^\varphi} = \widehat{f \circ e^{-u(\varphi)}}$$

Any $\mathcal{U} \in Mp(l)$ can be written as a product: $\mathcal{U} = \exp\dfrac{\hat{\varphi}_1}{i\hbar} \ldots \exp\dfrac{\hat{\varphi}_n}{i\hbar}$: then if $\pi(\mathcal{U}) = e^{u(\varphi_1)} \ldots e^{u(\varphi_n)}$ we also have:

$$(\forall f \in \mathcal{O}_M^{\mathbb{C}}(X)): \qquad \mathcal{U}\hat{f}\mathcal{U}^\dagger = \widehat{f \circ \pi(\mathcal{U})^{-1}} \tag{4.9}$$

Eq. (4.9) shows that $\pi(\mathcal{U})$ is unique, therefore the map π extends to a group

(7) There is no universal agreement upon this denomination.

homomorphism $\mathrm{Mp}(l) \xrightarrow{\pi} \mathrm{Sp}(l)$, locally $1-1$, and surjective since $\mathrm{Sp}(l)$ is connected: $\mathrm{Mp}(l)$ is a *covering* of $\mathrm{Sp}(l)$. Then it must be a quotient space of the universal covering $\widetilde{\mathrm{Sp}(l)}$ by a subgroup Γ of the homotopy group of $\mathrm{Sp}(l)$; this group is $\pi_1(\mathrm{Sp}(l)) = \mathbb{Z}$ [*23*] [*45*]: it is generated by a single homotopy class, so any covering of $\mathrm{Sp}(l)$ is characterized by its multiplicity $\gamma = \operatorname{card}\{\mathbb{Z}/\Gamma\}$ $(1 \leq \gamma \leq \infty)$.

The detailed analysis of $\mathrm{Mp}(l)$ shows that $\pi^{-1}(\mathbb{1}_X) = \{+\mathbb{1}_{\mathscr{H}}, -\mathbb{1}_{\mathscr{H}}\}$ consists of exactly two points, hence $\gamma = 2$: $\mathrm{Mp}(l)$ *double-covers* $\mathrm{Sp}(l)$.

Eqs. (3.5 *b*) and (4.9) together imply:

$$(\forall \varphi' \in \mathcal{Q}_1,\ \forall \mathscr{U} \in \mathrm{Mp}(l)): \qquad \mathscr{U} \exp\left(\frac{\hat{\varphi}'}{i\hbar}\right)\mathscr{U}^\dagger = \exp\left(\frac{\widehat{\varphi' \circ \pi(\mathscr{U})^{-1}}}{i\hbar}\right)$$

so that the projective representation of $\mathrm{Sp}(l)$ by $\mathrm{Mp}(l)$ does solve Eq. (4.5); and it does not reduce to a true representation because of the double-covering property (in analogy with the SO(3) spinor theory).

4.4. Mp(l) and the Maslov index

We still have to find the explicit form of the covering map $\mathrm{Mp}(l) \xrightarrow{\pi} \mathrm{Sp}(l)$ « in the large ». The general study of $\mathrm{Mp}(l)$ is done explicitly in refs [*23*] [*45*] [*49*]. Here we shall only explicit π along a 1-parameter group $\mathscr{U}(t) = \exp \frac{\hat{\varphi}}{i\hbar}$, $\hat{\varphi} \in \hat{\mathcal{Q}}_2$. We can choose a frame in which φ has the normal form $\sum_1^l \lambda_j \varphi_j(q_j, p_j)$: $\lambda_j \in \mathbb{R}$, and each φ_j is a quadratic form on $\mathbb{R}^2$ of one of these types: $\frac{q^2}{2}$, qp, $\frac{q^2+p^2}{2}$. Then $\mathscr{U}(t)$ is a tensor product of operators in $\mathrm{Mp}(l)$ of one of the following types:

$$a) \qquad \varphi = \frac{q^2}{2}: \quad \left(\exp\left(\frac{t\hat{\varphi}}{i\hbar}\right) . \ \psi\right)(q) = e^{\frac{-iq^2t}{2\hbar}}\psi(q) \tag{4.10}$$

and:

$$\exp\left(\frac{t\hat{\varphi}}{i\hbar}\right) \xrightarrow{\pi} e^{tu(\varphi)} = \begin{pmatrix} 1 & 0 \\ -t & 1 \end{pmatrix}$$

$$b) \qquad \varphi = qp: \quad \left(\exp\left(\frac{t\hat{\varphi}}{i\hbar}\right)\psi\right)(q) = e^{-t/2}\psi(e^{-t}q) \tag{4.11}$$

and:

$$\exp\left(\frac{t\hat{\varphi}}{i\hbar}\right) \xrightarrow{\pi} e^{tu(\varphi)} = \begin{pmatrix} e^t & 0 \\ 0 & e^{-t} \end{pmatrix}$$

(these are trivial cases since the orbit is simply connected and no multiple covering can occur).

c) $\mathscr{q} = \frac{1}{2}(q^2 + p^2)$ (the hamiltonian of the harmonic oscillator): $\left(\exp\left(\frac{t\hat{\mathscr{q}}}{i\hbar}\right)\psi\right)(q) =$ (for $t \neq 0 \bmod \pi$):

$$\int_{\mathbb{R}} \left(\frac{e^{-\frac{i\pi}{4}} i^{-\left[\frac{t}{\pi}\right]}}{(2\pi\hbar\,|\sin t\,|)^{1/2}} e^{\frac{i}{2\hbar\sin t}(\cos t(q^2+q'^2)-2qq')} \right) \psi(q')dq' \qquad (4.12)$$

with $[c] =$ integer part of c;

(for $t = 2n\pi$): $\qquad (-1)^n\psi(q) \qquad (4.12')$

(for $t = (2n+1)\pi$): $\qquad (-1)^{n+1} i\psi(-q) \qquad (4.12'')$

and

$$\exp\left(\frac{t\hat{\mathscr{q}}}{i\hbar}\right) \xrightarrow{\pi} e^{tu(\mathscr{q})} = \begin{pmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{pmatrix}$$

(note that for $t = \pi/2$, eq. (4.12) defines a plain Fourier transformation).

This cyclic group of period 4π now double-covers its projection onto Sp(l), which has period 2π: $\exp\frac{(t+2\pi)\hat{\mathscr{q}}}{i\hbar} = -\exp\frac{t\hat{\mathscr{q}}}{i\hbar}$. The factor (-1) results from the phase jumps of $i^{-[t/\pi]}$ at $t = k\pi$, which have a semiclassical interpretation: for fixed q', the kernel in Eq. (4.12) is a WKB function corresponding to the classical motions induced by $\mathscr{q}$, with initial data $q(t=0) = q'$ defining a lagrangian space $\lambda_{t=0}$ in X. This space is transported by the hamiltonian flow as λ_t, and the WKB phase is $i^{-\nu(t)} e^{\frac{i}{\hbar}\int_{\lambda_t} pdq}$, where $\nu(t)$ is the Keller-Maslov index [*3*] [*4*] [*23*], jumping (by $+1$ in this case, as t increases) every time λ_t does not intersect the fixed lagrangian space P transversally: here $\nu(t) = [t/\pi]$.

In any dimension l, Mp(l) is generated by elementary transformations of the types (4.10-4.12), so its structure, and also the projection π, are determined — in principle, because the actual discussion requires careful stationary phase arguments [*23*]. We only mention here two results stressing the semi-classical character of the elements $\mathscr{U} \in$ Mp(l):

— a generic $\mathscr{U} \in$ Mp(l) has a kernel on $L^2_{\mathbb{C}}(Q, d^lq)$:

$$\frac{e^{\frac{il\pi}{4}} i^{\varepsilon} e^{\frac{i}{\hbar}K(q,q')}}{(2\pi\hbar)^{l/2} \left|\det \frac{\partial^2 K}{\partial q_j dq'_k}\right|^{1/2}}$$

where K, a real quadratic form on Q $\times$ Q $\approx \mathbb{R}^{2l}$, is the generating function of the map U $= \pi(\mathscr{U}) \in$ Sp(l), i. e.:

$$x = Ux' \Leftrightarrow \frac{\partial K}{\partial q_j}(q, q') = p_j \quad \text{and} \quad \frac{\partial K}{\partial q'_j}(q, q') = -p'_j \qquad (\forall j)$$

and the matrix $\left(\frac{\partial^2 K}{\partial q_j \partial q'_k}\right)$ is invertible, $(-1)^\varepsilon$ being the sign of its determinant; but there are many exceptional cases with singular kernels, corresponding to generating functions with $\det\left(\frac{\partial^2 K}{\partial q_j \partial q'_k}\right) = 0$ such as the examples (4.10, 4.11, 4.12′, 4.12″) for $l = 1$, and those cases must be studied separately.

— let $\Gamma = \{ \lambda(t) \}_0^T$ be a closed continuous curve in the manifold Λ of all lagrangian subspaces of X. For a fixed $\lambda_0 \in \Lambda$, the subset of Λ: $\Lambda_{\lambda_0} = \{ \lambda \in \Lambda \mid \lambda$ non-transversal to $\lambda_0 \}$ essentially forms an oriented $(l-1)$-cycle of Λ. The intersection index $\nu(\Gamma)$ of Γ with that cycle ([8]) is an integer independent of λ_0 called the *Maslov index* of Γ; as a map from 1-cycles to integers: $\nu \in H^1(\Lambda, \mathbb{Z})$. Unfortunately, $\nu(\Gamma)$ can be hard to compute using this definition; the following relation can sometimes reduce it to a simpler homotopy problem : *if* $\lambda(t) = U(t)\lambda$ where $\gamma = \{ U(t) \}_0^T$ is a continuous closed curve in $Sp(l)$, and $\lambda \in \Lambda$ is fixed, then $\nu(\Gamma) = 2n(\gamma)$, where $n(\gamma)$ is the homotopy class of the loop γ in $\pi_1(Sp(l)) = \mathbb{Z}$ [*23*] [*45*] [*49*]. Let then $\{ \mathscr{U}(t) \}_0^T$ be a continuous lift-up (unique up to the overall sign) of the curve γ to $Mp(l)$. The double covering structure implies:

$$\mathscr{U}(T) = (-1)^{n(\gamma)}\mathscr{U}(0) = (-1)^{\frac{\nu(\Gamma)}{2}}\mathscr{U}(0) \tag{4.13}$$

4.5. The affine metaplectic group iMp(l)

We now want to extend the metaplectic group so as to represent on $\mathscr{H}$ the affine symplectic group iSp(l); we call $i$sp(l) its Lie algebra, and we try to follow the pattern of § 4.3.

To represent $i$sp(l) as a Poisson bracket algebra, we must add to $\mathscr{Q}_2$ the linear functions; but $\mathscr{Q}_2 \oplus \mathscr{Q}_1$ generates the Lie algebra $\underline{\underline{\mathscr{Q}}} = \mathscr{Q}_2 \oplus \mathscr{Q}_1 \oplus \mathscr{Q}_0$. The condition: $e^{tv(\varphi)} \equiv U_t^\varphi \in iSp(l)$ defines a Lie algebra homomorphism : $\varphi \in \underline{\underline{\mathscr{Q}}} \xrightarrow{v} v(\varphi) \in isp(l)$ giving the exact sequence:

$$0 \to \mathscr{Q}_0 \hookrightarrow \underline{\underline{\mathscr{Q}}} \xrightarrow{v} isp(l) \to 0$$

hence $isp(l) \approx \underline{\underline{\mathscr{Q}}}/\mathscr{Q}_0$.

By corollary (3.4.3.*c*), exactly as before, the Weyl quantization $\underline{\underline{\mathscr{Q}}} \to \hat{\underline{\underline{\mathscr{Q}}}}$ is a Lie algebra isomorphism. We call iMp(l) (*the affine metaplectic group*) the Lie group generated by $\hat{\underline{\underline{\mathscr{Q}}}}$ in U($\mathscr{H}$). Exactly as for Eq. (4.9), one proves that the map $\hat{\varphi} \in \hat{\underline{\underline{\mathscr{Q}}}} \leftrightarrow v(\varphi) \in isp(l)$ induces a group homomorphism $iMp(l) \xrightarrow{\pi} iSp(l)$ (onto) satisfying:

$$(\forall \mathscr{V} \in iMp(l),\ \forall f \in \mathscr{O}_M^{\mathbb{C}}(X)): \qquad \mathscr{V}\hat{f}\mathscr{V}^\dagger = \widehat{f \circ \underline{\pi}(\mathscr{V})^{-1}} \tag{4.14}$$

([8]) Physically, intersection points of Γ with Λ_{P_R} are semi-classical *caustic* points in the representations $\mathscr{R}$ over the frame R.

but $\underline{\pi}$ is no longer locally $1 - 1$ and it defines not a covering, but a *fibration* of $i\mathrm{Sp}(l)$ by $i\mathrm{Mp}(l)$.

We can give another description of $i\mathrm{Mp}(l)$, suggested by Souriau [*49*], as a double covering, using a « prequantization » formalism [*24*] [*25*]. The idea is that $\underline{\underline{\mathcal{Q}}}$ itself generates a group of geometrical transformations (of a semi-classical nature): $\underline{\underline{\mathcal{Q}}}(= \mathcal{Q}_2 + \underline{\underline{\mathcal{Q}}}_1)$ is the Lie algebra of the semi-direct product group $\mathrm{Sp}(l) \times \mathrm{W}$, which we denote $\mathrm{WSp}(l)$, and which acts on W by diffeomorphisms (« quantomorphisms » in [*24*] [*49*]):

$$w_0 = (x_0, z_0) \mapsto g(w_0) = w(\mathrm{U}x_0, z_0) = \left(\mathrm{U}x_0 + a,\ \eta z_0 e^{\frac{1}{2i\hbar}\omega(a,\mathrm{U}x_0)}\right)$$

where $g = (\mathrm{U}, w) \in \mathrm{WS}p(l)$, $w = (a, \eta) \in \mathrm{W}$. The product law in $\mathrm{WSp}(l)$ is:

$$\begin{aligned} g_1 g_2 &= (\mathrm{U}_1, a_1, \eta_1)(\mathrm{U}_2, a_2, \eta_2) \\ &= \left(\mathrm{U}_1\mathrm{U}_2,\ \mathrm{U}_1 a_2 + a_1,\ \eta_1\eta_2 e^{\frac{1}{2i\hbar}\omega(a_1,\mathrm{U}_1 a_2)}\right) \end{aligned} \tag{4.15}$$

$\mathrm{WSp}(l)$ is also a fiber bundle over $i\mathrm{Sp}(l)$, of fiber $\mathbb{T}$, for the projection $(\mathrm{U}, w) \to (\mathrm{U}, \varpi(w)) = (\mathrm{U}, a)$.

The Lie algebra isomorphism $\underline{\underline{\mathcal{Q}}} \approx \hat{\underline{\underline{\mathcal{Q}}}}$ then implies that $i\mathrm{Mp}(l)$ is the semi-direct product $\mathrm{Mp}(l) \times \tilde{\mathrm{W}}$ ($\hat{\mathcal{Q}}_2$ generates $\mathrm{Mp}(l)$ and $\hat{\underline{\underline{\mathcal{Q}}}}_1$ generates $\tilde{\mathrm{W}}$), which double-covers $\mathrm{WSp}(l)$, since $\tilde{\mathrm{W}} \xrightarrow{\sigma} \mathrm{W}$ is an isomorphism. We now have a complete picture of fibrations and coverings, all compatible with the group and semi-direct product structures:

$$\begin{array}{c|lcccc|l}
 & i\mathrm{Mp}(l) & = & \mathrm{Mp}(l) & \times & \tilde{\mathrm{W}} & \text{(where for simplicity } \varpi \text{ also denotes} \\
 & \downarrow{\scriptstyle \pi\times\sigma} & & \downarrow{\scriptstyle \pi} & & \downarrow{\scriptstyle \sigma} & \\
\underline{\pi} & \mathrm{WSp}(l) & = & \mathrm{Sp}(l) & \times & \mathrm{W} & id_{\mathrm{Sp}(l)} \times \varpi, \text{ and X stands for } \mathbb{R}^{2l}, \text{ etc.} \\
 & \downarrow{\scriptstyle \varpi} & & \downarrow{\scriptstyle id} & & \downarrow{\scriptstyle \varpi} & \\
 & i\mathrm{Sp}(l) & = & \mathrm{Sp}(l) & \times & \mathrm{X} & \text{since we work in a fixed frame).}
\end{array}$$

4.6. **Covariance revisited**

Eqs. (3.5 *b*) and (4.14) imply that $i\mathrm{Mp}(l)$ is a projective representation of $i\mathrm{Sp}(l)$ that solves Eq. (4.5); since the covariance group G for canonical quantization (§ 4.1) is uniquely determined up to phases, we can, and shall henceforth, identify G with $i\mathrm{Mp}(l)$. Since a change of reference frame induces an inner automorphism of $i\mathrm{Mp}(l)$, we can also view $i\mathrm{Mp}(l)$ as an image of an intrinsic representation $i\mathrm{Mp}(\mathcal{H})$ (as for $\tilde{\mathrm{W}}$ in § 4.2).

We now indicate an important extension of the domain of the representation $i\mathrm{Mp}(l)$: the restriction of any $\mathcal{V} \in i\mathrm{Mp}(l) \subset \mathrm{U}(\mathrm{L}^2_{\mathbb{C}}(\mathrm{Q}, d^l q))$ to the subspace $\mathcal{S}^{\mathbb{C}}(\mathrm{Q})$ (of rapidly decreasing test functions) is a continuous isomorphism of $\mathcal{S}^{\mathbb{C}}(\mathrm{Q})$; hence by duality $\mathcal{V}$ extends to a *continuous isomorphism of* $\mathcal{S}'^{\mathbb{C}}(\mathrm{Q})$.

This result is classic for $\mathrm{Mp}(l)$ [*11*] [*23*] but we sketch a proof valid for

$i\mathrm{Mp}(l)$ too. We can take as a family of seminorms on $\mathcal{S}^{\mathbb{C}}(\mathrm{Q})$ all maps: $\{\varphi \in \mathcal{S}^{\mathbb{C}} \mapsto \|\hat{\mathfrak{p}}\varphi\|_{\mathrm{L}^2}\}$, where $\mathfrak{p}(x)$ is an arbitrary polynomial on X. For any $\mathscr{V} \in i\mathrm{Mp}(l) : \mathcal{S}^{\mathbb{C}} \xrightarrow{\mathscr{V}} \mathcal{S}^{\mathbb{C}}$ continuously if:

$$(\forall \mathfrak{p}\ \exists \mathfrak{p}'\ \forall \varphi \in \mathcal{S}^{\mathbb{C}}(\mathrm{Q})): \quad \|\hat{\mathfrak{p}}\mathscr{V}\varphi\|_{\mathrm{L}^2} \leqslant \|\hat{\mathfrak{p}}'\varphi\|_{\mathrm{L}^2}.$$

But

$$\|\hat{\mathfrak{p}}\mathscr{V}\varphi\|_{\mathrm{L}^2} = \|\mathscr{V}^{\dagger}\hat{\mathfrak{p}}\mathscr{V}\varphi\|_{\mathrm{L}^2} = \|\widehat{\mathfrak{p} \circ \underline{\pi}(\mathscr{V})}\varphi\|_{\mathrm{L}^2}$$

by the unitarity of $\mathscr{V}$ and by Eq. (4.14): so $\mathscr{V}$ is continuous. It clearly admits $\mathscr{V}^{\dagger}$ as inverse, so it is an isomorphism. The extension to $\mathcal{S}'^{\mathbb{C}}(\mathrm{Q})$ by duality is done exactly as for the Fourier transformation:

$$\psi' = \mathscr{V}\psi \quad \text{for} \quad \psi \in \mathcal{S}'^{\mathbb{C}}(\mathrm{Q}) \Leftrightarrow \forall \varphi \in \mathcal{S}^{\mathbb{C}}(\mathrm{Q}): \quad \langle \psi' \mid \varphi \rangle = \langle \varphi \mid \mathscr{V}^{\dagger}\varphi \rangle.$$

For various representations $\mathscr{R}$, the spaces $\mathcal{S}^{\mathbb{C}}(\mathrm{Q_R}) \subset \mathrm{L}^2_{\mathbb{C}}(\mathrm{Q_R}, d^l q_{\mathrm{R}}) \subset \mathcal{S}'^{\mathbb{C}}(\mathrm{Q_R})$ are intertwined by the operators of $i\mathrm{Mp}(l)$, so they are the images by $\mathscr{R}$ of an intrinsic Gelfand triplet [50]: $\mathcal{S}^{\mathbb{C}}(\mathscr{H}) \subset \mathscr{H} \subset \mathcal{S}'^{\mathbb{C}}(\mathscr{H})$. The extension $\mathcal{S}'^{\mathbb{C}}(\mathscr{H})$ is a space of *symplectic spinors* on X [33]; it will play a role in WKB theory (§§ 5.4 and 7.2).

We finally indicate the connection of $i\mathrm{Mp}(l)$ with the space of admissible operators, which is a direct consequence of Eq. (4.14).

THEOREM 4.6.1. — If $\mathrm{A} \in \hat{\mathfrak{A}}^{\mathbb{C}}_m$ and $\mathscr{V} \in i\mathrm{Mp}(l)$, then: $\mathscr{V}\mathrm{A}\mathscr{V}^{\dagger} \in \hat{\mathfrak{A}}^{\mathbb{C}}_m$, and:

$$\text{so that:} \qquad (\forall n \in \mathbb{N}): \quad \left.\begin{array}{l} (\mathscr{V}\mathrm{A}\mathscr{V}^{\dagger})_{\mathrm{W}} = \mathrm{A}_{\mathrm{W}} \circ \underline{\pi}(\mathscr{V})^{-1} \\ (\mathscr{V}\mathrm{A}\mathscr{V}^{\dagger})_n(x) = \mathrm{A}_n(\underline{\pi}(\mathscr{V})^{-1}.x) \end{array}\right\} \tag{4.16}$$

The spaces $\hat{\mathfrak{A}}^{\mathbb{C}}_m(\mathrm{X})$ of admissible operators (for any m) are thus explicitly $i\mathrm{Mp}(l)$-covariant, to all orders in $\hbar$. The same holds for asymptotic operators.

4.7. **Parallel transport on** $\mathrm{WSp}(l)$

The natural inclusion $i\mathrm{Sp}(l) \subset \mathrm{WSp}(l)$ defined by: $\mathrm{V} \mapsto (\mathrm{V}, 1)$ fails to be a group homomorphism due to the curvature term $e^{\omega(a_1, \mathrm{U}_1 a_2)/2i\hbar}$

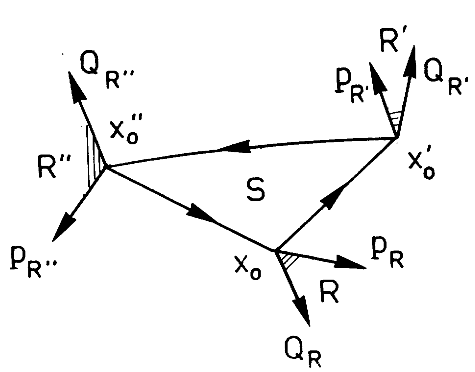

FIG. 1.

in Eq. (4.15), which can be visualized as follows: for an arbitrary frame R, consider the circuit in $F : R \to R' = RV_1 \to R'' = RV_1V_2 \to R = RV_1V_2V_3$, where $V_j \in i\mathrm{Sp}(l)$, $V_1V_2V_3 = \mathrm{id}$. Then:

$$(V_1, 1)(V_2, 1)(V_3, 1) = (\mathrm{id}, e^{\frac{1}{i\hbar}\int_S \omega}) \in \mathbb{T}(\subset \mathrm{WSp}(l))$$

where S is the oriented triangle in X described by the motion of the origin of $R : x_0 \to x_0' \to x_0'' \to x_0$ (fig. 1). The extension of this to differentiable motions $R(t)$ involves a natural *affine connection* on $\mathrm{WSp}(l)$.

DEFINITIONS 4.7.1. — We call $\underline{\mathcal{Q}} = \mathcal{Q}_2 \oplus \mathcal{Q}_1 \subset \underline{\underline{\mathcal{Q}}}$ the *horizontal subspace* of $\underline{\underline{\mathcal{Q}}}$. The *horizontal lift-up* of $v \in i\mathrm{sp}(l)$ $(\approx \underline{\underline{\mathcal{Q}}}/\mathcal{Q}_0)$ to $\underline{\mathcal{Q}}$ is the image $\varphi^h(v)$ of v in $\underline{\mathcal{Q}}$ under the vector space isomorphism $\underline{\underline{\mathcal{Q}}}/\mathcal{Q}_0 \approx \underline{\mathcal{Q}}$. A horizontal lift-up of a connected C^1 curve $\{ V(t) = (U(t), a(t)) \} \subset i\mathrm{Sp}(l)$ is a connected curve $\{ L_V(t) = (U(t), a(t), \eta_V(t)) \} \subset \mathrm{WSp}(l)$ whose velocity vector in $\underline{\underline{\mathcal{Q}}}$: $T_*(L_V(t))^{-1}(\dot{L}_V(t))$ is the horizontal lift-up of the velocity vector of $V(t)$: $T_*(V(t))^{-1}(\dot{V}(t))$. This defines a *left-invariant* affine connection on the bundle of Lie groups $\mathrm{WSp}(l) \overset{\varpi}{\to} i\mathrm{Sp}(l)$ [51]; the curve $\{ \eta_V(t) \} \subset \mathbb{T}$ is called a *parallel transport curve along* V between fibers.

THEOREM 4.7.2. — *a*) The curve $\eta_V(t)$ solves the equation:

$$\frac{\dot{\eta}_V(t)}{\eta_V(t)} = \frac{1}{2i\hbar}\,\omega(a(t), \dot{a}(t)) \tag{4.17}$$

b) for given $\eta_V(t_0) \in \mathbb{T}$, Eq. (4.17) has the unique solution:

$$\eta_V(t) = \eta_V(t_0)e^{\frac{1}{i\hbar}\int_{S_{t_0t}} \omega} \tag{4.18}$$

where S_{t_0t} is the oriented 2-surface swept by the vector $a(\tau)$ from $\tau = t_0$ to $\tau = t$ (fig. 2).

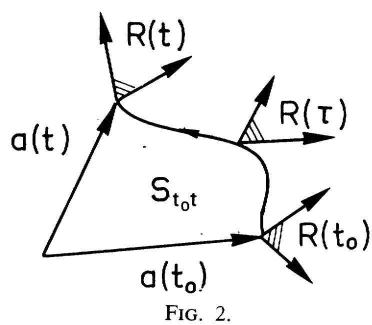

FIG. 2.

c) (Stokes theorem): if $\{ a(t) \}_0^T = \Gamma \subset X$ is a closed loop:

$$\eta_V(T) = \eta_V(0)e^{\frac{1}{i\hbar}\int_S \omega} \tag{4.19}$$

where $S \subset X$ is now any oriented 2-surface of boundary Γ (fig. 3).

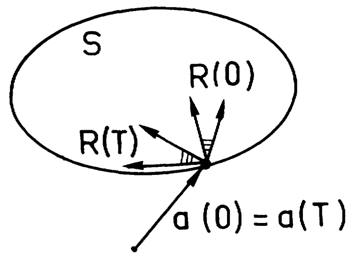

FIG. 3.

Proof. — *a*)

$T_*(L_V(t))^{-1}(\dot{L}_V(t))$

$$= \lim_{\Delta_t \to 0} \frac{1}{\Delta t} [(U(t), a(t), \eta_V(t))^{-1}(U(t + \Delta t), a(t + \Delta t), \eta_V(t + \Delta t) - \mathbb{1}]$$

has the component along $\mathcal{Q}_0$, by Eq. (4.15):

$$\lim_{\Delta_t \to 0} \frac{1}{\Delta t} [\eta_V(t)^{-1}\eta_V(t + \Delta t)e^{\frac{\omega(-U^{-1}(t)a(t), U^{-1}(t)a(t+\Delta t)}{2i\hbar}} - 1] = \frac{\dot{\eta}_V(t)}{\eta_V(t)} + \frac{i}{2\hbar}\omega(a(t), \dot{a}(t))$$

and this must vanish to make the vector horizontal. The proof of *b*) and *c*) is immediate; *b*) implies the existence and uniqueness of the parallel transport associated to the connection (this connection can also be defined as the transfer to WSp(l) of the Sp(l)-invariant connection on W having curvature ω, which is defined in prequantization theory [*24*] [*25*] [*49*]).

4.8. **Parallel transport on** *i*Mp(l)

A connected lift-up of the curve $L_V(t)$, previously defined in WSp(l), to the double covering iMp(l) will be called a horizontal lift-up $\mathcal{L}_V(t)$ of the curve $\{V(t)\}$ to iMp(l): it is clear that $\mathcal{L}_V(t)$ exists and is uniquely specified by fixing one point $\mathcal{L}_V(t_0) \in \underline{\pi}^{-1}(V(t_0))$. But his notion of parallel transport on iMp(l) is now also directly linked with *Weyl quantization*: the horizontal lift-up to the Lie algebra $\hat{\underline{\mathcal{Q}}}$ (of iMp(l)) of a vector $v \in i$sp(l) is $\hat{\varphi}$, where $\varphi = \varphi^h(v)$ (the unique vector in $\underline{\mathcal{Q}}$ such that $v(\varphi) = v$ as in § 4.4).

THEOREM 4.8.1. — *a*) The lift-up $\mathcal{L}_V(t)$ satisfies the operator equation:

$$i\hbar\, \dot{\mathcal{L}}_V(t) = \mathcal{L}_V(t)\hat{\varphi}(t) \tag{4.20}$$

where $\varphi(t) = \varphi^h[T_*(V(t))^{-1}(\dot{V}(t))] \in \underline{\mathcal{Q}}$.

b) We have the identity (for $t > 0$, T exp denoting the Dyson time-ordered exponential):

$$\mathcal{L}_V(t)^\dagger = \mathrm{T}\exp\left(\frac{-1}{i\hbar}\int_{t_0}^{t} \hat{\varphi}(\tau)d\tau\right) . \mathcal{L}_V(t_0)^\dagger = [(\pi \times \sigma)^{-1}L_V(t)]^\dagger \tag{4.21}$$

where the last term is completely determined by Eq. (4.18) and by the point $\mathscr{L}_V(t_0)$ as initial data.

c) (Stokes theorem): if $\{ V(t) \}_0^T = \{ (U(t), a(t)) \}_0^T \subset i\mathrm{Sp}(l)$ is a closed loop:

$$\mathscr{L}_V(T) = (-1)^{n(\gamma)} e^{\frac{1}{i\hbar}\int_S \omega} \mathscr{L}_V(0) \tag{4.22}$$

where $n(\gamma)$ is the homotopy class of the loop $\gamma = \{ U(t) \}_0^T \subset \mathrm{Sp}(l)$, and $S \subset X$ is any 2-surface of boundary $\Gamma = \{ a(t) \}_0^T$.

Proof. — *a)* the velocity vector in $\hat{\mathscr{Q}}$ of $\mathscr{L}_V(t)$ is:

$$T_*(\mathscr{L}_V(t))^{-1}\dot{\mathscr{L}}_V(t) = \mathscr{L}_V(t)^{-1}\dot{\mathscr{L}}_V(t)$$

and it must be $\hat{q}(t)$, hence Eq. (4.20); *b)* Eq. (4.20) is equivalent to: $-i\hbar\dot{\mathscr{L}}_V(t)^\dagger = \hat{q}(t)\mathscr{L}_V(t)^\dagger$ which has the standard Dyson solution involving time-ordered exponentials; Eq. (4.21) is thus an explicit formula for the time-ordered exponential of a time-dependent quadratic operator, because $L_V(t)$ is known through Eq. (4.18) and its lift-up to $i\mathrm{Mp}(l)$ is determined by the initial data; *c)* is a direct consequence of *b)*, using Eqs. (4.13) and (4.19).

4.9. Parallel transport on $\mathscr{F}$

Up to this point, we could have equivalently defined and used the right-invariant connection on $\mathrm{WSp}(l)$ having $\mathscr{Q}$ as horizontal subspace at $\mathrm{id}_{\mathrm{WSp}(l)}$ (it is conjugate to the left-invariant one under the map $V \to V^{-1}$). But, due to the definition of $\mathscr{F}$ as a right $i\mathrm{Mp}(l)$-space, only the previously given left-invariant connection defines a parallel transport on quantum representations, as follows.

We recall that $\mathscr{F}$ is a bundle over F (§ 4.2). A connected curve $\{ \mathscr{R}(t) \} \subset \mathscr{F}$ which is a lift-up of the connected C^1 curve $\{ R(t) \} \subset F$ (i. e. for all t, $\mathscr{R}(t)$ projects onto $R(t)$), is a *horizontal lift-up* of $\{ R(t) \}$ if moreover, for some $\mathscr{R}_0 \in \mathscr{F}$ (and for all t): $\mathscr{R}(t) = \mathscr{R}_0\mathscr{V}(t)$, with $\mathscr{V}(t)$: a *horizontal* curve in $i\mathrm{Mp}(l)$ (this then holds for all $\mathscr{R}_0 \in \mathscr{F}$ because the connection on $i\mathrm{Mp}(l)$ is left-invariant). The map $[\mathscr{R}_0] : \mathscr{V} \in i\mathrm{Mp}(l) \xrightarrow{[\mathscr{R}_0]} \mathscr{R}_0\mathscr{V} \in \mathscr{F}$ induces the isomorphism: $\hat{\mathscr{Q}} \xrightarrow{T_{id}[\mathscr{R}_0]} T_{\mathscr{R}_0}\mathscr{F}$; and there is a similar isomorphism: $i\mathrm{sp}(l) \xrightarrow{T_{id}[R_0]} T_{R_0}F$. Then the horizontality condition for $\{ \mathscr{R}(t) \}$ becomes: $\dot{\mathscr{R}} = T_{id}[\mathscr{R}(t)]\hat{q}(t)$, with $q(t) \in \mathscr{Q}$ for all t. Summing up:

THEOREM 4.9.1. — A horizontal lift-up $\{ \mathscr{R}(t) \}$ of $\{ R(t) \}$ satisfies:

$$\dot{\mathscr{R}}(t) = T_{id}[\mathscr{R}(t)]\hat{q}(t) \tag{4.23}$$

where $q(t) = q^h(v(t))$ is defined by the condition:

$$\dot{R}(t) = T_{id}[R(t)]v(t) \tag{4.23'}$$

Eq. (4.23) has a unique solution for any specified initial value $\mathscr{R}(t_0)$ over $R(t_0)$.

The proof is adapted from that of theorem 4.8.1.

For fixed $x \in X$ the motion $\{ R(t) \}$ induces an apparent motion on the coordinates $x_{R(t)} = \begin{pmatrix} q_{R(t)} \\ p_{R(t)} \end{pmatrix} \in \mathbb{R}^{2l}$; similarly for fixed $\psi \in \mathscr{H}$ (or $\psi \in \mathscr{S}'^{\mathbb{C}}(\mathscr{H})$) we have an apparent motion of the representative $\psi^{\mathscr{R}(t)} \in L^2_{\mathbb{C}}(\mathbb{R}^l, d^l r)$ (or $\psi^{\mathscr{R}(t)} \in \mathscr{S}'^{\mathbb{C}}(\mathbb{R}^l)$). In terms of these apparent motions theorem 4.9.1 becomes:

THEOREM 4.9.2. — The apparent motion of any $\psi \in \mathscr{S}'^{\mathbb{C}}(\mathscr{H})$ satisfies the « Schrödinger equation of motion »:

$$i\hbar \frac{\partial}{\partial t} \psi^{\mathscr{R}(t)} = - \hat{\varphi}(t) \psi^{\mathscr{R}(t)} \tag{4.24}$$

where $\varphi(t) \in \mathscr{Q}$ is determined as inducing the « classical apparent motion » by:

$$(\forall x \in X): \qquad \frac{d}{dt}(x_{R(t)}) = \{ x_{R(t)}, - \varphi(t) \} \tag{4.24'}$$

This results from the classic formulas for coordinate changes:

$$x^R = V x_{R'} \qquad \text{if} \qquad R' = RV \qquad \text{in} \qquad F \tag{4.25}$$

$$\psi^{\mathscr{R}} = \mathscr{V} \psi^{\mathscr{R}'} \qquad \text{if} \qquad \mathscr{R}' = \mathscr{R}\mathscr{V} \qquad \text{in} \qquad \mathscr{F} \tag{4.7}$$

Clearly the apparent motions go in reverse of the frame motions, hence the minus signs in theorem 4.9.2 if we keep the notations of theorem 4.9.1. Eq. (4.24') is just the differential expression of the identity: $e^{-tv(\varphi)} = U_t^{-\varphi} (\forall t)$. Also in this theorem, φ is understood as a function on $\mathbb{R}^{2l}$ and $\hat{\varphi}$ as the Weyl-quantized operator on $L^2(\mathbb{R}^l, d^l r)$ according to Eqs. (4.3).

We shall need this framework in § 7.3 to get spectrum quantization conditions for the Schrödinger equation.

4.10. A concluding remark

This section was written from the viewpoint of group theory and geometrical quantization. But the subject of quantum evolution operators of quadratic hamiltonians has received wide attention in the physical literature from many various viewpoints. To mention only some: Bogoliubov transformations [*52*], Moshinsky-Quesne transformations [*47*], Feynman path integrals [*20*], second quantization [*53*]...

5. SYMBOLIC CALCULUS ON QUANTUM STATES

We are going to extend the Wigner symbolic calculus from $\hat{\mathfrak{A}}^{\mathbb{C}}$ to a larger class hopefully containing interesting quantum states. The extension is inspired from the pattern of Gelfand triplets ($\mathscr{S} \subset L^2 \subset \mathscr{S}'$) [*50*], but with the inner product taking $\hbar$-dependent values.

5.1. Admissible functionals, asymptotic functionals

An operator B on $\mathcal{H}$ can be viewed as a linear functional on other operators through the quantum pairing (3.2); for an operator-as-functional we shall use the following Wigner symbol:

$$B^W = \frac{1}{(2\pi\hbar)^l} B_W \tag{5.1}$$

For the pairing (3.2), the space HS($\mathcal{H}$) is self-dual and the Parseval identity (3.7) reads:

$$\langle B, A \rangle_{qu} = \langle B^W, A_W \rangle_{cl} \tag{5.2}$$

Eq. (5.2) naturally extends to the cases where $A_W \in \mathcal{S}^{\mathbb{C}}(X)$ and $B^W \in \mathcal{S}'^{\mathbb{C}}(X)$. This suggests defining a space of linear functionals on the subspace $\hat{\mathcal{S}}^{\mathbb{C}} \subset \hat{\mathfrak{A}}^{\mathbb{C}}$ of admissible operators with rapidly decreasing symbols. A necessary and sufficient condition for the inner product $\langle B, A \rangle_{qu}$ to be defined as a C^∞ function of $\hbar$ for all $A \in \hat{\mathcal{S}}^{\mathbb{C}}$ is the following:

DÉFINITION 5.1.1. — An operator $B(\hbar)$ on $\mathcal{H}$ is an *admissible functional* (denoted $B \in \hat{\mathcal{S}}'^{\mathbb{C}}(X)$) iff its symbol $B^W(\hbar)$ is a C^∞ function of $\hbar$ ($\in [0, \hbar_0)$) taking values in $\mathcal{S}'^{\mathbb{C}}(X)$, and has an asymptotic expansion at $\hbar = 0$ in $\mathcal{S}'^{\mathbb{C}}(X)$:

$$B^W(\hbar) \sim \sum_0^\infty B_n \hbar^n \qquad (B_n \in \mathcal{S}'^{\mathbb{C}}(X)) \tag{5.3}$$

Remark. — There is a natural imbedding $\hat{\mathfrak{A}}^{\mathbb{C}}(X) \subset \hat{\mathcal{S}}'^{\mathbb{C}}(X)$.

THEOREM 5.1.2. — Eq. (5.3) is equivalent to the weak asymptotic condition: for any $A \in \hat{\mathcal{S}}^{\mathbb{C}}$ with $A_W(\hbar) \sim \sum_0^\infty A_n \hbar^n$:

$$\langle B(\hbar), A(\hbar) \rangle_{qu} \sim \sum_{n=0}^\infty \left(\sum_{n'=0}^n \langle B_{n-n'}, A_{n'} \rangle_{cl} \right) \hbar^n \tag{5.4}$$

Proof. — eq. (5.3) means: $B_0 = \text{s-lim}_{\hbar_j \to 0} B^W(\hbar_j)$, $B_1 = \text{s-lim}_{\hbar_j \to 0} \frac{B^W(\hbar_j) - B_0}{\hbar_j}, \ldots$ for all sequences $\{ \hbar_j \} \to 0$; eq. (5.4) means the same thing with strong limits replaced by weak limits. The theorem then follows from the equivalence of weak and strong convergence of sequences in $\mathcal{S}'$ [*40*, vol. 1].

DÉFINITION 5.1.3. — If $B \in \hat{\mathcal{S}}'^{\mathbb{C}}(X)$ and $B(\hbar)$ is a positive operator for all $\hbar$, we call it an *admissible state* [*27*].

Admissible states form a convex cone $\hat{\mathcal{S}}'^{+}(X)$ in $\hat{\mathcal{S}}'^{\mathbb{C}}(X)$. If $B \in \hat{\mathcal{S}}'^{+}$, then B_0 must be a positive measure and all B_n are real-valued (these conditions are not sufficient).

DÉFINITION 5.1.4. — We call $B \in \hat{\mathcal{S}}'^{\mathbb{C}}(X)$ *negligible* on the open set $\Omega \subset X$ (denoted: $B_{|\Omega} \sim 0$), iff for all $\varphi \in \mathcal{S}^{\mathbb{C}}(\Omega)$ $(= \{ \varphi \in \mathcal{S}^{\mathbb{C}}(X) \mid \mathrm{Supp}\, \varphi \subset \Omega \})$, we have: $\langle B^W(\hbar), \varphi \rangle_{cl} = o(\hbar^\infty)$. The *essential support* of B is the smallest closed set $ES(B) \subset X$ such that $B_{|X \setminus ES(B)} \sim 0$. Equivalently, if $B^W(\hbar) \sim \sum_0^\infty B_n \hbar^n$:

$$ES(B) = \overline{\bigcup_0^\infty \mathrm{Supp}\, B_n} \tag{5.4}$$

DÉFINITION 5.1.5. — The quotient space of $\hat{\mathcal{S}}'^{\mathbb{C}}(X)$ by the equivalence relation $(B_1 - B_2)_{|\Omega} \sim 0$ is called the space of *asymptotic functionals* on Ω: $\tilde{\mathcal{S}}'^{\mathbb{C}}(\Omega)$.

Every $B \in \hat{\mathcal{S}}'^{\mathbb{C}}(X)$ has an equivalence class $\tilde{B} \in \tilde{\mathcal{S}}'^{\mathbb{C}}(X)$ which can be represented as the formal expansion: $\tilde{B} = \sum_0^\infty B_n \hbar^n$. The essential support of B only depends on $\tilde{B}$, so we can denote it $ES(\tilde{B})$. The class of B in $\tilde{\mathcal{S}}'^{\mathbb{C}}(\Omega)$ can be interpreted as the restriction $\tilde{B}_{|\Omega}$.

5.2. Examples

Our ultimate goal is to describe as asymptotic functionals quantum pure states, i. e. density operators $\rho = |\psi\rangle\langle\psi|$ (of kernel in the position representation: $\rho(q, q') = \psi(q)\psi^*(q')$), for suitably chosen state vectors ψ. The symbol is then:

$$\rho^W(q, p\,; \hbar) = \frac{1}{(2\pi\hbar)^l} \int_Q \psi\left(q - \frac{r}{2}\right)\psi^*\left(q + \frac{r}{2}\right) e^{\frac{ipr}{\hbar}} d^l r \tag{5.5}$$

Some examples

a) plane waves: if $\psi(q) = e^{\frac{i}{\hbar} p_0 \cdot q}$: $\rho^W(q, p\,; \hbar) = \delta(p - p_0)$ (an l-dimensional δ-function: stands for $\delta(p_1 - p_{01}) \otimes \delta(p_2 - p_{02}) \otimes \ldots \otimes \delta(p_l - p_{1l})$) and $ES(\tilde{\rho}) = \{ p = p_0 \}$.

b) the harmonic oscillator ground state, $l = 1$: if ψ is the ground state vector of the operator $\hat{h} = \frac{1}{2}\left(-\hbar^2 \frac{d^2}{dq^2} + q^2\right)$, then: $\rho^W(q, p\,; \hbar) = \frac{1}{\pi\hbar} e^{-\frac{q^2+p^2}{\hbar}}$

The obvious expansion in $\mathcal{S}'^{\mathbb{C}}(X^*)$:

$$\int_X \rho^W e^{-i(\xi q + \eta p)} d^{2l}x = e^{-\frac{\hbar}{4}(\xi^2+\eta^2)} \sim \sum_0^\infty \frac{1}{n!}\left(\frac{-1}{4}\right)^n (\xi^2 + \eta^2)^n \hbar^n$$

leads to [27]:

$$\rho^{W}(q, p ; \hbar) = \frac{1}{\pi\hbar} e^{-\frac{q^2+p^2}{\hbar}} \sim \sum_{0}^{\infty}\left(\frac{(\Delta_q + \Delta_p)^n}{4^n . n!}\delta(x)\right)\hbar^n \qquad (5.6)$$

Hence $ES(\tilde{p}) = \{ x = 0 \}$. This is an illustration of microlocality: the exact ρ^W is spread over the whole phase space but mostly over an area given by: $\sqrt{\langle p^2 \rangle \langle q^2 \rangle} = \frac{\hbar}{2}$ (in agreement with the uncertainty principle), but the asymptotic state (the RHS of eq. (5.6)) is strictly localized *to all orders* at the point $x = 0$, which is the support of the classical ground state.

c) the Airy function, $l = 1$: for $\psi(q) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}\left(\frac{p^3}{6} - pq\right)} dp$, eq. (5.5) yields in $\mathscr{S}'^{\mathbb{C}}(X)$:

$$\rho^{W}(q, p ; \hbar) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}\left[\frac{(p-\tau/2)^3-(p+\tau/2)^3}{6}+q\tau\right]} d\tau = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{-\frac{i\tau^3}{24\hbar}} e^{\frac{i\tau}{\hbar}(q-p^2/2)} d\tau$$

To show that ρ^W has an expansion in $\hbar$, we apply the general formula of symbolic calculus valid for any dimension l:

$$\int_{\mathbb{R}^l} f(\tau, \hbar)\varphi(\tau)e^{-\frac{i\tau\sigma}{\hbar}} d^l\tau \sim f(- i\hbar\partial_\sigma, \hbar)\left[\int_{\mathbb{R}^l} \varphi(\tau)e^{-\frac{i\tau\sigma}{\hbar}} d^l\tau\right] \qquad (5.7)$$

which holds if $\varphi \in \mathscr{S}'^{\mathbb{C}}(\mathbb{R}^l)$, $f \in \mathscr{O}_M^{\mathbb{C}}(\mathbb{R}^l)$ and if $\int_{\mathbb{R}^l} \varphi(\tau)e^{-\frac{i\tau\sigma}{\hbar}} d\tau$ has an $\hbar$-expansion in $\mathscr{S}'^{\mathbb{C}}$ and $f(\hbar\tau, \hbar)$ has an $\hbar$-expansion in $\mathscr{O}_M^{\mathbb{C}}(\mathbb{R}^l)$. Putting $l = 1$, $\varphi(\tau) = 1$, $f(\tau, \hbar) = e^{-\frac{i\tau^3}{24\hbar}}$ yields:

$$\rho^{W}(q, p ; \hbar) \sim \left(\exp \frac{\hbar^2}{24}\partial_q^3\right) . \delta\left(q - \frac{p^2}{2}\right)$$
$$= \delta\left(q - \frac{p^2}{2}\right) + \frac{\hbar^2}{24}\delta'''\left(q - \frac{p^2}{2}\right) + \ldots \qquad (5.8)$$

and $ES(\tilde{\rho})$ is the parabola $\left\{ q = \frac{p^2}{2} \right\}$. This result will appear as a particular case of theorem 5.4.2.

For an arbitrary $\psi(\hbar) \in \hat{\mathscr{S}}'^{\mathbb{C}}_M(Q)$, the class $\tilde{\rho}$ of the symbol (5.5) expresses *local* properties of $\psi(\hbar)$:

THEOREM 5.2.1. — If $\psi(q ; \hbar) = o(\hbar^\infty)$ (in the weak sense) on an open set $V \subset Q$, then $ES(\rho^W) \cap (V \times P) = \emptyset$.

Proof. — We test $\rho^W(\hbar)$ upon $\varphi \in \mathcal{S}^{\mathbb{C}}(X)$ with Supp $\varphi \subset V \times P$:

$$\langle \rho^W(\hbar), \varphi \rangle_{cl} = \frac{1}{(2\pi\hbar)^l} \int_{Q\times X} \psi\left(q - \frac{r}{2}\right)\psi^*\left(q + \frac{r}{2}\right)\varphi(q, p)e^{\frac{ipr}{\hbar}} d^lr d^lq d^lp$$

Applying the stationary phase principle with respect to the variable p we find that nonnegligible contributions can arise only at $r = 0$, but there the integrand is negligible by hypothesis. Q. E. D.

Weinstein [*54*] has defined a different type of (principal) symbol for a distribution g in the homogeneous theory; this symbol also lives on X and expresses the local properties of g; it has the advantage of being linear in g, but its covariance rules are rather complicated.

5.3. Symbolic calculus on admissible functionals

The calculus on admissible states is the obvious extension — when possible — of the calculus on admissible operators.

a) *Metaplectic covariance.* — If $B \in \hat{\mathcal{S}}'^{\mathbb{C}}$ and $\mathcal{V} \in i\mathrm{Mp}(l)$ then $\mathcal{V}B\mathcal{V}^\dagger \in \hat{\mathcal{S}}'^{\mathbb{C}}$ and:

$$(\mathcal{V}B\mathcal{V}^\dagger)^W = B^W \circ \underline{\pi}(\mathcal{V})^{-1} \tag{5.9}$$

This follows from the extension procedure of $i\mathrm{Mp}(l)$ to tempered distributions (§ 4.5): we can define $\mathcal{V}B\mathcal{V}^\dagger$ by the identity:

$$\langle \mathcal{V}B\mathcal{V}^\dagger, A \rangle_{qu} = \langle B, \mathcal{V}^\dagger A \mathcal{V} \rangle_{qu} \qquad \forall A \in \hat{\mathcal{S}}^{\mathbb{C}}(X)$$

or:

$$\langle (\mathcal{V}B\mathcal{V}^\dagger)^W, A_W \rangle_{cl} = \langle B^W, A_W \circ \underline{\pi}(\mathcal{V}) \rangle_{cl} = \langle B^W \circ \underline{\pi}(\mathcal{V})^{-1}, A_W \rangle_{cl} .$$

b) *Multiplication.* — The product of a functional $B \in \hat{\mathcal{S}}'^{\mathbb{C}}$ by an operator $A \in \hat{\mathfrak{A}}^{\mathbb{C}}$ can be defined, by extension of the operator product, as the functional $AB \in \hat{\mathcal{S}}'^{\mathbb{C}}$ satisfying the identity:

$$(\forall C \in \hat{\mathcal{S}}^{\mathbb{C}}): \qquad \langle AB, C \rangle_{qu} = \langle B, A^\dagger C \rangle_{qu} \tag{5.10}$$

from which one obtains the explicit expansion formula (see also [*55*]):

$$\widetilde{AB} = \tilde{A}\left(\exp \frac{i\hbar \overleftrightarrow{\Lambda}}{2}\right)\tilde{B} \in \tilde{\mathcal{S}}'^{\mathbb{C}} \tag{5.11}$$

which yields a multiplication law: $\tilde{\mathfrak{A}}^{\mathbb{C}} \times \tilde{\mathcal{S}}'^{\mathbb{C}} \to \tilde{\mathcal{S}}'^{\mathbb{C}}$.

On the other hand there seems to be no satisfactory extension of the multiplication law when both factors are asymptotic functionals [*62*].

5.4. WKB states

A basic motivation for introducing admissible states is that they can provide a uniformly regular representation of WKB wave functions, so that WKB computations can be replaced by regular operations of the symbolic calculus just introduced. Besides, our framework will be more general than the WKB method, because most admissible states cannot be expressed as WKB states. To discuss these questions, we shall rely mainly on Leray's [*23*] definition of WKB functions as inspired from Maslov [*4*], with some technical conditions added.

Let $\Lambda \subset X$ be a C^∞ submanifold, without boundary or self-intersections, and *lagrangian*, i. e. maximally isotropic for the 2-form ω ($\Leftrightarrow \omega_{|\Lambda} = 0$ and $\dim \Lambda = l$) [*4*] [*45*] [*46*]. For any frame $R \in F$ (cf. section 4), if π_R is the projection $\Lambda \twoheadrightarrow Q_R$ parallel to P_R, we call $\Sigma_R = \{ x \in \Lambda \mid T_x(\pi_R) \text{ not injective} \}$ the *singular set* of π_R, $\pi_R(\Sigma_R)$ the *caustic set* of Λ in Q_R (fig. 4), and $S^R_\Lambda(x) = \int_{x_0}^{x} p_R(x')dq_R(x')$ the *generating function* of Λ in the frame R (the integral is taken along an arbitrary path on Λ of endpoints x_0 and x : S^R is multivalued on Λ and defined up to an overall additive constant given by the choice of x_0). For any quantum representation $\mathcal{R} \in \mathcal{F}$ corresponding to the frame R, $a^{\mathcal{R}}(x\,;\hbar) = \sum_0^\infty a_n^{\mathcal{R}}(x)\hbar^n$ will denote a formal power series with coefficients $a_n^{\mathcal{R}} \in \mathcal{O}_M^{\mathbb{C}}(\Lambda \backslash \Sigma_R)$ (these can become infinite on Σ_R).

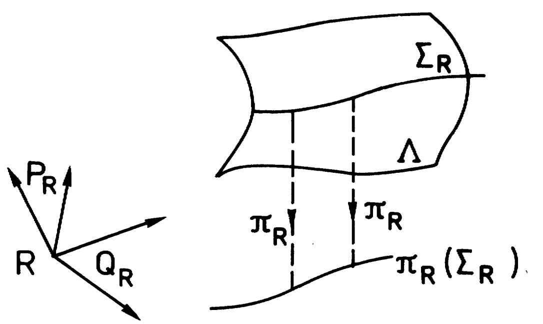

FIG. 4.

DÉFINITION 5.4.1. — We shall call a wave function $\psi(\hbar) \in \mathcal{S}'^{\mathbb{C}}(\mathcal{H})$ a WKB *state vector* if: *a*) $\psi(\hbar) \in \widehat{\mathcal{S}'^{\mathbb{C}}_M}(\mathcal{H})$: the subspace of distributions belonging in any representation to the (iMp(l)-$i$nvariant) space $\widehat{\mathcal{S}'^{\mathbb{C}}_M}$ defined in § 2.2; *b*) there is a lagrangian manifold $\Lambda \subset X$ carrying for any $\mathcal{R} \in \mathcal{F}$ a formal series $a^{\mathcal{R}}(x\,;\hbar)$ such that $\psi^{\mathcal{R}}(\hbar)$ admits the weak expansion in $Q_R \backslash \pi_R(\Sigma_R)$:

$$(\forall q_R \notin \pi_R(\Sigma_R)): \qquad \psi^{\mathcal{R}}(q_R\,;\hbar) \sim \sum_{x_j[q_R] \in \pi_R^{-1}(q_R)} a^{\mathcal{R}}(x_j[q_R]\,;\hbar) e^{\frac{i}{\hbar} S^R_\Lambda(x_j[q_R])} \tag{5.12}$$

Commentary. — *a*) Is a technical condition stating that $\psi(\hbar)$ depends

smoothly on $\hbar$ and remains bounded in $\mathcal{S}'^{\mathbb{C}}(\mathcal{H})$ by some $\mathcal{O}(\hbar^{-k})$ as $\hbar \to 0$.
b) Means the following: on any connected open set $\Xi \subset Q_R \backslash \pi_R(\Sigma_R)$ we can decompose:

$$\psi^{\mathcal{R}}(q_R ; \hbar) = \sum_j a^{\mathcal{R}}_{(j)}(q_R ; \hbar) e^{\frac{i}{\hbar} S^R_{\Lambda_j}(q_R)}$$

the Λ_j denoting the distinct branches (assumed in finite number) of Λ above Ξ, and $S^R_{\Lambda_j}(q_R) = S^R_{\Lambda}(x_j[q_R])$; each « amplitude » $a^{\mathcal{R}}_{(j)}(q_R ; \hbar) \in \mathcal{S}'^{\mathbb{C}}(Q_R)$ is then uniquely defined above Ξ, and it admits a weak expansion: for all $\varphi \in \mathcal{S}^{\mathbb{C}}(Q_R)$ with Supp $\varphi \subset \Xi$:

$$\langle \hat{a}^{\mathcal{R}}_{(j)}(q_R ; \hbar), \varphi \rangle_{Q_R} \sim \sum_0^{\infty} \langle a^{\mathcal{R}}_n(x_j[q_R]), \varphi(q_R) \rangle_{Q_R} \hbar^n .$$

Condition *b*) is consistent under a change of representation $\mathcal{R}' = \mathcal{R}\mathcal{V}$ provided:

$$\sum_{j'} a^{\mathcal{R}'}_{(j')}(q_{R'} ; \hbar) e^{\frac{i}{\hbar} S^{R}_{\Lambda_{j'}}(q_{R'})} =$$

(the stationary phase expansion of) $\mathcal{V}^{-1}\left(\sum_j a^{\mathcal{R}}_{(j)}(q_R ; \hbar) e^{\frac{i}{\hbar} S^R_{\Lambda_j}(q_R)} \right)$.

This yields an explicit *microlocal* transformation rule for the amplitudes: $a^{\mathcal{R}}(x ; \hbar) \mapsto a^{\mathcal{R}'}(x ; \hbar)$ [23].

Hence the set $\bigcup_0^{\infty}$ Supp $a^{\mathcal{R}}_n \subset \Lambda$ is independent of $\mathcal{R}$ and noted Supp *a*.

THEOREM 5.4.2. — For any open set $\Omega \subset X$ such that $\bar{\Omega} \cap \Lambda \overset{\pi_R}{\to} Q_R$ is an injective regular map for some frame R, the projector onto the WKB state $\psi(\hbar)$ of def. 5.4.1 has an asymptotic class $\tilde{\rho}_{\Omega}$ in $\tilde{\mathcal{S}}'^{\mathbb{C}}(\Omega)$ with $ES(\tilde{\rho}_{\Omega}) = \Omega \cap$ Supp *a*.

Proof. — The local expansions (5.12) define $\psi(\hbar)$ modulo $\sigma(\hbar^{\infty})$ in $\widehat{\mathcal{S}'^{\mathbb{C}}_M}$, hence they define $\rho = |\psi\rangle\langle\psi|$ modulo a negligible distribution of $\mathcal{S}'^{\mathbb{C}}(X)$. There remains to show that ρ^W has an $\hbar$-expansion in Ω under the assumptions for Ω. We recall that $\tilde{\rho}_{\Omega}$ is defined as the functional: $\varphi \in \mathcal{S}^{\mathbb{C}}(\Omega) \mapsto \langle \rho^W(\hbar), \varphi \rangle_{cl}$ [mod $\hbar^{\infty}$].

In any representation $\mathcal{R}$ this is, using Eq. (5.5):

$$\langle \tilde{\rho}(\hbar), \varphi \rangle_{cl} = \frac{1}{(2\pi\hbar)^l} \int_{\mathbb{R}^{3l}} \psi^{\mathcal{R}}\left(q_R - \frac{r}{2}\right) \psi^{\mathcal{R}}\left(q_R + \frac{r}{2}\right)^* \varphi^{\mathcal{R}}(q_R, p_R) e^{\frac{i}{\hbar} p_R \cdot r} d^l r \, d^l q_R \, d^l p_R \text{ [mod } \hbar^{\infty}]$$

Non-zero contributions to $\langle \tilde{\rho}, \varphi \rangle_{\text{cl}}$ can only come from the critical manifold of the phase in the integrand. Stationarity with respect to p_{R} implies $r = 0$, hence $\tilde{\rho}(q_{\text{R}}, p_{\text{R}})$ is determined by (the germ of) $\psi^{\mathscr{R}}$ [mod $\hbar^{\infty}$] at q_{R}. We can thus replace $\psi^{\mathscr{R}}$ by its local expansion (5.12) (cf. theorem 5.2.1) wherever it holds. Its contribution to $\langle \tilde{\rho}(\hbar), \varphi \rangle_{\text{cl}}$ is:

$$\frac{1}{(2\pi\hbar)^l} \sum_{j,k} \int_{\mathbb{R}^{3l}} a^{\mathscr{R}}\left(x_j\left[q_{\text{R}} - \frac{r}{2}\right]\right) a^{\mathscr{R}}\left(x_k\left[q_{\text{R}} + \frac{r}{2}\right]\right)^* \varphi^{\mathscr{R}}(q_{\text{R}}, p_{\text{R}}) \\ e^{\frac{i}{\hbar}\left[S^{\text{R}}_{\Lambda}\left(x_j\left[q_{\text{R}} - \frac{r}{2}\right]\right) - S^{\text{R}}_{\Lambda}\left(x_k\left[q_{\text{R}} + \frac{r}{2}\right]\right) + p_{\text{R}}.r\right]} d^l r\, d^l q_{\text{R}}\, d^l p_{\text{R}}$$

Stationarity of the phase with respect to q_{R} and r_{R} now yields, at $r = 0$: $x_j = x_k = (q_{\text{R}}, p_{\text{R}})$. Since Λ has no self-intersections, this happens only for $j = k$: the distinct branches of the expansion (5.12) do not interfere asymptotically, so each branch gives to $\tilde{\rho}$ an independent, additive, and microlocal contribution: the branch $a^{\mathscr{R}}(x_j)e^{\frac{i}{\hbar}S^{\text{R}}_{\Lambda}(x_j)}$ contributes to $\tilde{\rho}$ at x_j. Under the hypothesis of theorem 5.3.2, $\tilde{\rho}_{\Omega}$ is then determined by a single branch $a^{\mathscr{R}}(x_j\,;\,\hbar)e^{\frac{i}{\hbar}S^{\text{R}}_{\Lambda}(x_j)}$: the one such that $x_j[q_{\text{R}}] \in \Omega \cap \Lambda$. Dropping all indices j, R, $\mathscr{R}$, and calling $\partial_q S_{\Lambda}(q) = p_{\Lambda}(q)$ so that $x[q] = \begin{pmatrix} q \\ p_{\Lambda}(q) \end{pmatrix}$, we obtain for this branch:

$$\tilde{\rho}_{\Omega}(q, p\,;\,\hbar) = \frac{1}{(2\pi\hbar)^l} \int_{\text{Q}_{\text{R}}} a\left(q - \frac{r}{2}\,;\,\hbar\right) a\left(q + \frac{r}{2}\,;\,\hbar\right)^* e^{\frac{i}{\hbar}\left[S_{\Lambda}\left(q - \frac{r}{2}\right) - S_{\Lambda}\left(q + \frac{r}{2}\right) + pr\right]} d^l r \\ \int_{\text{Q}_{\text{R}}} a\left(q - \frac{r}{2}\,;\,\hbar\right) a\left(q + \frac{r}{2}\,;\,\hbar\right)^* e^{\frac{i}{\hbar}\mathscr{S}_{\Lambda}(q, r)} e^{\frac{i}{\hbar}(p - p_{\Lambda}(q))r} \frac{d^l r}{(2\pi\hbar)^l}$$

where

$$\mathscr{S}_{\Lambda}(q, r) = S_{\Lambda}\left(q - \frac{r}{2}\right) - S_{\Lambda}\left(q + \frac{r}{2}\right) + p_{\Lambda}(q) \, . \, r = \mathcal{O}(r^3)$$

because $p_{\Lambda}(q) = \partial_q S_{\Lambda}(q)$; hence:

$$\tilde{\rho}_{\Omega}(q, p\,;\,\hbar) = \left[a\left(q + \frac{i\hbar}{2}\partial_p\,;\,\hbar\right) a^*\left(q - \frac{i\hbar}{2}\partial_p\,;\,\hbar\right) \right. \\ \left. \exp \frac{i}{\hbar}\mathscr{S}_{\Lambda}(q, -i\hbar\partial_p) \right] . \, \delta(p - p_{\Lambda}(q)) \quad (5.13)$$

where we have used Eq. (5.7), thanks to the fact that the exponential has a regular $\hbar$-expansion $\left(\frac{i}{\hbar}\mathscr{S}_{\Lambda}(q, -i\hbar\partial_p) = \mathcal{O}(\hbar^2)\right)$; and again:

$$\delta(p - p_{\Lambda}(q)) = \delta(p_1 - p_{\Lambda 1}(q)) \otimes \ldots \otimes \delta(p_l - p_{\Lambda l}(q)) = \int_{\text{Q}} e^{\frac{i}{\hbar}(p - p_{\Lambda}(q))r} \frac{d^l r}{(2\pi\hbar)^l}.$$

Hence [27]:

$$\tilde{\rho}_\Omega(q, p ; \hbar) = \left(\sum_0^\infty \hbar^n \gamma_n(q, \partial_p)\right)\delta(p - p_\Lambda(q))_{|\Omega}$$

$$= |a_0(q)|^2 \delta(p - p_\Lambda(q))_{|\Omega} + \mathcal{O}(\hbar) \quad (5.14)$$

where the γ_n are polynomials in ∂_p. The semi-classical term in (5.14) is the square of the Maslov half-density, and it is obvious from Eqs. (5.13) and (5.14) that $\tilde{\rho}_\Omega \in \tilde{\mathcal{S}}'^{\mathbb{C}}(\Omega)$ and $\mathrm{ES}(\rho_\Omega) = \Omega \cap \mathrm{Supp}\, a$ (a closed subset of Ω). Q. E. D.

The local expansions $\tilde{\rho}_\Omega^{\mathrm{R}}(q_{\mathrm{R}}, p_{\mathrm{R}} ; \hbar)$ given by formulas of the type (5.13) are consistent with one another: if $\tilde{\rho}_\Omega^{\mathrm{R}}$ and $\tilde{\rho}_{\Omega'}^{\mathrm{R}'}$ are two local expansions, then:

$$\tilde{\rho}_{\Omega'|\Omega\cap\Omega'}^{\mathrm{R}'} = \widetilde{|\psi^{\mathcal{R}'}\rangle\langle\psi^{\mathcal{R}'}|}_{|\Omega\cap\Omega'} = (\mathcal{V}^\dagger \tilde{\rho}_\Omega^{\mathrm{R}} \mathcal{V})_{|\Omega\cap\Omega'}$$

where $\mathcal{R}' = \mathcal{R}\mathcal{V}$ with $\mathcal{V} \in i\mathrm{Mp}(l)$; using Eq. (5.9):

$$\tilde{\rho}_{\Omega'|\Omega\cap\Omega'}^{\mathrm{R}'}(x_{\mathrm{R}'} ; \hbar) = \tilde{\rho}_\Omega^{\mathrm{R}}(\underline{\pi}(\mathcal{V})x_{\mathrm{R}'} ; \hbar)_{|\Omega\cap\Omega} = \tilde{\rho}_{\Omega|\Omega\cap\Omega'}^{\mathrm{R}}(x_{\mathrm{R}} ; \hbar)$$

Hence all $\tilde{\rho}_\Omega$ could arise in principle from one *global* asymptotic functional $\tilde{\rho} \in \tilde{\mathcal{S}}'^{\mathbb{C}}(x)$ with $\mathrm{ES}(\tilde{\rho}) = \mathrm{Supp}\, a$. But we must be careful here: we know that definition 5.4.1 makes sense globally only if Λ satisfies the Bohr-Sommerfeld-Maslov conditions [4] [56] which (when not vacuous) depend on $\hbar$. Such a restriction should also be felt if we try to define a global $\tilde{\rho} \in \tilde{\mathcal{S}}'^{\mathbb{C}}(x)$: quantization conditions for the spectrum should appear when we try to patch together a global $\tilde{\rho}$ from its local expansions. Unfortunately, those conditions can be explicitly obtained only for a limited class of systems (completely integrable or quasi-separable), as *Bohr-Sommerfeld rules* (see section 7); we shall postpone this difficulty for the moment.

We also remark that the essential support of a WKB state is the closure of a non-empty open subset of a lagrangian manifold Λ (typically it is all of Λ). So an asymptotic state of $\tilde{\mathcal{S}}'^{\mathbb{C}}(\mathrm{X})$, which may have any closed subset of X as essential support (proof: as for the analogous theorem in [32]), is much more general.

5.5. General properties of essential supports

THEOREM 5.5.1. — Let $\psi(q ; \hbar) \in \hat{\mathcal{S}}'^{\mathbb{C}}_{\mathrm{M}}(\mathrm{Q})$ such that $\rho = |\psi\rangle\langle\psi| \in \hat{\mathcal{S}}'(\mathrm{X})$. Then $\mathrm{ES}(\rho)$ coincides with the reduced wave front of ψ (defined in § 2.2).

Proof. — We first assume $\mathrm{ES}(\rho) = \emptyset$. Then $\rho(\hbar) = \sigma(\hbar^\infty)$ in $\mathcal{S}'^{\mathbb{C}}(\mathrm{Q} \times \mathrm{Q})$, so $\psi = \sigma(\hbar^\infty)$ in $\mathcal{S}'^{\mathbb{C}}(\mathrm{Q})$, $\theta\psi = \sigma(\hbar^\infty)$ in $\mathcal{O}'^{\mathbb{C}}_c(\mathrm{Q})$ for $\theta \in \mathcal{D}(\mathrm{Q})$, so that $\displaystyle\int_{\mathrm{Q}} \theta\psi e^{-\frac{ipq}{\hbar}} dq = \sigma(\hbar^\infty)$ in $\mathcal{O}^{\mathbb{C}}_{\mathrm{M}}(\mathrm{P})$, then Eq. (2.15) holds for all $(q', p') \in \mathrm{X}$, and $\mathrm{RWF}(\psi) = \emptyset$.

For the general case, we remark that Eq. (5.11) implies: $ES(\rho) = \bigcap_A R\gamma(A)$ where A runs over the admissible operators such that $ES(A\rho A^\dagger) = \emptyset$, or (by the fact just proved): $RWF(A\psi) = \emptyset$. The relation between admissible operators and reduced PDO's, and theorem 2.2.1 (*ii*) achieve the proof.

This result means that, by their definition 5.1.5, asymptotic functionals are somewhat analogous to the *microfunctions* of the homogeneous theories [*7*]-[*10*]. Our essential support plays the same role as the *singular spectrum* of a hyperfunction [*10*] or the *microsupport* of a quasi-mode [*29*].

THEOREM 5.5.2. — If $\psi_1(\hbar), \psi_2(\hbar) \in \hat{\mathcal{S}}'^{\mathbb{C}}_M(Q)$, if $\rho_1 = |\psi_1\rangle\langle\psi_1|$, $\rho_2 = |\psi_2\rangle\langle\psi_2|$, and $|\psi_1\rangle\langle\psi_2|$ all belong to $\hat{\tilde{\mathcal{S}}}'^{\mathbb{C}}(X)$, and if $\rho = |\lambda_1\psi_1 + \lambda_2\psi_2\rangle\langle\lambda_1\psi_1 + \lambda_2\psi_2|$ for $\lambda_1, \lambda_2 \in \mathbb{C}$:

i) $ES(\tilde{\rho}) \subseteq ES(\rho_1) \cup ES(\rho_2)$

ii) $ES(|\psi_1\rangle\langle\psi_2|) = ES(|\psi_2\rangle\langle\psi_1|) \subseteq ES(\rho_1) \cap ES(\rho_2)$

Proof. — *i*) follows from *ii*). But we have $ES(A|\psi_1\rangle\langle\psi_2|) = \emptyset$ for any $A \in \hat{\mathfrak{A}}^{\mathbb{C}}$ such that $R\gamma(A) \supset RWF(\psi_1) = ES(\rho_1)$, hence $ES(|\psi_1\rangle\langle\psi_2|) \subset ES(\rho_1)$ and similarly for ρ_2.

A consequence of *ii*) is that $\tilde{\rho}_{|\Omega} = (|\lambda_1|^2\tilde{\rho}_1 + |\lambda_2|^2\tilde{\rho}_2)_{|\Omega}$ (the asymptotic superposition state is indistinguishable from an asymptotic mixture state) whenever $\Omega \cap (ES(\rho_1) \cap ES(\rho_2)) = \emptyset$. This suggests (cf. analogous definition in [*29*]):

DÉFINITION 5.5.3. — Two asymptotic functionals $\tilde{\rho}_1$ and $\tilde{\rho}_2$ are *pseudo-orthogonal* (denoted $\tilde{\rho}_1 \tilde{\perp} \tilde{\rho}_2$) iff $ES(\tilde{\rho}_1) \cap ES(\tilde{\rho}_2) = \emptyset$.

6. ASYMPTOTIC EIGENSTATES

6.1. Definitions

A *time-independent Schrödinger equation* has the form:

$$(A(\hbar) - E)\psi_E(\hbar) = 0 \tag{6.1}$$

where $A \in \hat{\mathfrak{A}}(X)$ is self-adjoint (9), E is a real constant (the eigen-value) and $\psi_E(\hbar) \in \mathcal{H}$ (true eigenvector) or $\psi_E(\hbar) \in \widehat{\mathcal{S}'^{\mathbb{C}}_M}(\mathcal{H})$ (generalized eigenvector). The problem is to solve Eq. (6.1) explicitly under suitable eigenvalue conditions (also to be found), assuming a smooth behaviour in $\hbar$ throughout.

In terms of the state $\rho_E(\hbar) = |\psi_E(\hbar)\rangle\langle\psi_E(\hbar)| = \rho_E^\dagger(\hbar)$, eq. (6.1) reads:

$$(A(\hbar) - E)\rho_E(\hbar) = \rho_E(\hbar)(A(\hbar) - E) = 0 \tag{6.2}$$

(9) In physics, A is the hamiltonian operator $\dfrac{\hat{p}^2}{2m} + \widehat{V(q)}$, but here we do not restrict the explicit form of A.

We can restrict the problem to the search for the *admissible* states $\rho_E \in \hat{\mathcal{S}}'^{+}(X)$ solving eq. (6.2). In power series of $\hbar$, we then get equations for the *asymptotic class* $\tilde{\rho}_E = \sum_0^\infty \rho_n \hbar^n$, thanks to eq. (5.11):

$$(\tilde{A} - E)\tilde{\rho}_E = \tilde{\rho}_E(\tilde{A} - E) = 0 \tag{6.3}$$

The idea is now to try to solve Eq. (6.3) directly for $\tilde{\rho}_E$. We call the solutions of (6.3) *asymptotic solutions* of (6.2), or *asymptotic eigenstates.* This notion generalizes the asymptotic solutions of Leray [*23*], which are defined only in the WKB case, and it has some analogy with Colin de Verdière's quasi-modes [*29*].

The advantage of the problem (6.3) is that it is defined, and sometimes it can be solved, entirely in the range of the asymptotic theory. But it can be very difficult to relate its solutions to those of the original problem (6.1); the difficulties are of various orders:

— summing the formal power series $\sum_0^\infty \rho_n \hbar^n$ in $\mathcal{S}'^{\mathbb{C}}(X)$ (one may have to account for quantum effects of order $\hbar^\infty$, which can notably change the eigenstates in quasi-degenerate situations [*57*]);

— check that $\rho_E(\hbar)$ is a projector of rank 1, and express $\psi_E(\hbar)$;

— in solvable cases, the asymptotic solutions $\tilde{\rho}_E(\hbar)$ depend smoothly on E (and on $\hbar$), with no manifest spectral selection rules. In the best case, such rules might exist *a posteriori*, with the sole effect of defining (*a*) subset (*s*) of values $\{ E_\alpha \} \subset \mathbb{R}$, for each of which the previously computed $\tilde{\rho}_E(\hbar)$ is really the expansion of an eigenstate $(|\psi_{E_\alpha}\rangle\langle\psi_{E_\alpha}|)^W$; each $\tilde{\rho}_E(\hbar)$ would thus describe a subfamily of eigenvectors. Some results in this direction are known only for completely integrable systems [*4*] [*23*] [*32*].

But here we shall stay in the formal asymptotic theory and not worry about those questions, which all concern the relevance of the asymptotic theory to the exact theory.

6.2. **The asymptotic equations of motion**

This question is examined here only as a preliminary to the eigenstate problem. Let $A \in \hat{\mathfrak{A}}$ be the self-adjoint operator of Eq. (6.1), with $A(x\,;\hbar) = \sum_0^\infty A_n(x)\hbar^n$. The time-dependent Schrödinger equation for A, describing the propagation of quantum waves, is:

$$i\hbar \frac{\partial\psi}{\partial t}(t\,;\hbar)(= i\hbar\dot{\psi}) = A(\hbar)\psi(t\,;\hbar)$$

The quantum state $\rho(t;\hbar) = |\psi(t;\hbar)\rangle\langle\psi(t;\hbar)|$ satisfies the Heisenberg equation:

$$i\hbar\dot{\rho} = [\mathrm{A}, \rho]_- \tag{6.4}$$

hence, if $\rho \in \mathscr{S}'^{\mathbb{C}}(\mathrm{X})$, the asymptotic equation:

$$i\hbar\dot{\tilde{\rho}} = [\tilde{\mathrm{A}}, \tilde{\rho}]_- \tag{6.5}$$

We restore the notations of theorem 3.4.4. as:

$$(\tilde{\mathrm{A}}\tilde{\rho})(x;\hbar) = \left[\tilde{\mathrm{A}}_{\mathrm{W}}(x;\hbar)\exp\frac{i\hbar\overleftrightarrow{\Lambda}}{2}\right]\tilde{\rho}^{\mathrm{W}}(x;\hbar) = \left(\sum_0^\infty \mathscr{A}_n(x,\partial_x)\hbar^n\right)\left(\sum_0^\infty \rho_n\hbar^n\right)$$

where the $\mathscr{A}_n$ are complex differential operators of order $\leq n$, linear in the coefficients $\mathrm{A}_{n'}(n' \leq n)$; in particular:

$$\mathscr{A}_0 = \mathrm{A}_0(x); \qquad \mathscr{A}_1 = \mathrm{A}_1(x) + \frac{i}{2}(\partial_q\mathrm{A}_0.\partial_p - \partial_p\mathrm{A}_0.\partial_q) = \mathrm{A}_1 - \frac{i}{2}\frac{d}{dt} \tag{6.6}$$

where d/dt is the total time derivative along the « classical » trajectories (of the hamiltonian $\mathrm{A}_0(x)$). Then Eq. (6.5) reads in expanded form, using Eq. (3.13″) and the property: $\mathrm{Im}\,\mathscr{A}_0 = 0$:

$$\sum_0^\infty \dot{\rho}_n\hbar^n = 2\left(\sum_1^\infty \mathrm{Im}\,\mathscr{A}_n\,.\,\hbar^{n-1}\right)\left(\sum_0^\infty \rho_n\hbar^n\right) \tag{6.7}$$

This leads to the recursive equations:

$$\begin{cases} \dot{\rho}_0 = \{\mathrm{A}_0, \rho_0\} : \text{(the classical equation of motion for the classical state } \rho_0). \\ \dot{\rho}_n = \{\mathrm{A}_0, \rho_n\} + \mathrm{V}_n[\rho_0, \ldots, \rho_{n-1}] \end{cases}$$

where V_n is a linear microlocal operator.

Assuming that the classical flow $\mathrm{U}_t^{\mathrm{A}_0}$ (for $0 \leqslant |t| < t_0 < \infty$) defines a regular map $x \to x_t$, we take the « interaction picture »:

$$\tilde{\rho}(t, x_t;\hbar) = \tilde{\rho}_{\mathrm{I}}(t, x;\hbar).$$

Then:

$$\dot{\tilde{\rho}}_{\mathrm{I}}(t, x;\hbar) = \hbar\mathrm{V}_{\mathrm{I}}(t, x;\hbar)\tilde{\rho}_{\mathrm{I}}(t, x;\hbar) \tag{6.8}$$

where V_{I} is a linear microlocal operator, regular as $\hbar \to 0$. The asymptotic solution of (6.8), say for $0 \leqslant t < t < t_0 < \infty$ with initial value at $t = 0$, is the Dyson series:

$$\tilde{\rho}_{\mathrm{I}}(t, x;\hbar) = \mathrm{T}\exp\left(\hbar\int_0^t \mathrm{V}_{\mathrm{I}}(t', x;\hbar)\right).\,\tilde{\rho}_{\mathrm{I}}(0, x;\hbar) \tag{6.9}$$

$$= \left[1 + \hbar\int_0^t \mathrm{V}_{\mathrm{I}}(t', x;\hbar)dt' + \hbar^2\int_0^t dt'\int_0^{t'} dt''\mathrm{V}_{\mathrm{I}}(t', x;\hbar)\mathrm{V}_{\mathrm{I}}(t'', x;\hbar) + \ldots\right]\tilde{\rho}_{\mathrm{I}}(0, x;\hbar)$$

This formula, although it appears complicated, has important simple consequences.

THEOREM 6.2.1. — *i)* $\tilde{\rho}_I(t, x; \hbar)$ depends microlocally on $\tilde{\rho}_I(0, x; \hbar)$ for $|t| < t_0 < \infty$.

ii) $\mathrm{ES}(\tilde{\rho}(t; \hbar)) = \mathrm{U}_t^{\mathrm{A}_0}[\mathrm{ES}(\tilde{\rho}(0; \hbar))]$ for $|t| < t_0 > \infty$:

the essential support is transported by the classical flow (of A_0).

Proof. — *i)* the bracket of (6.9) defines a microlocal operator at any order in $\hbar$ (its expansion has partial differential operator coefficients); *ii)* a microlocal operator preserves essential supports, hence

$$\mathrm{ES}(\tilde{\rho}_I(t)) \subseteq \mathrm{ES}(\tilde{\rho}_I(0)),$$

and by time reversal of the motion we get $\mathrm{ES}(\tilde{\rho}_I(t)) = \mathrm{ES}(\tilde{\rho}_I(0))$. By the definition of $\tilde{\rho}_I$, this proves the theorem.

6.3. The asymptotic stationary equations

The eigenstate equations (6.3) or equivalently: $[\tilde{\mathrm{A}} - \mathrm{E}, \tilde{\rho}_\mathrm{E}]_\pm = 0$, have the expanded form:

$$\left.\begin{aligned} 2\left(\sum_0^\infty \hbar^n \operatorname{Re} \mathscr{A}_n - \mathrm{E}\right)\left(\sum_0^\infty \rho_n \hbar^n\right) = 0 \\ 2\left(\sum_1^\infty \hbar^{n-1} \operatorname{Im} \mathscr{A}_n\right)\left(\sum \rho_n \hbar^n\right) = 0 \end{aligned}\right\} \tag{6.10}$$

leading to the recursive equations:

$$\begin{cases} (\mathrm{A}_0 - \mathrm{E})\rho_0 = 0 & (6.11^+) \\ \{\mathrm{A}_0, \rho_0\}\left[= -\dfrac{d\rho_0}{dt}\right] = 0 & (6.11^-) \end{cases}$$

(this means that ρ_0 is a *classical stationary state* of energy E), and:

$$\begin{cases} (\mathrm{A}_0 - \mathrm{E})\rho_n = -\mathrm{V}'_n[\rho_0, \ldots, \rho_{n-1}] & (6.12^+) \\ \{\mathrm{A}_0, \rho_n\}\left[= -\dfrac{d\rho_n}{dt}\right] = -\mathrm{V}_n[\rho_0, \ldots, \rho_{n-1}] & (6.12^-) \end{cases}$$

where V_n (introduced above) and V'_n are linear microlocal operators.

We see no direct method to compute the distributional solutions of these equations. We propose instead an indirect approach: first of all, to determine the family of all possible sets $\mathrm{ES}(\tilde{\rho}_\mathrm{E})$ for solutions $\tilde{\rho}_\mathrm{E}$; then for each such set Γ, to look for explicit solutions $\Sigma\rho_n\hbar^n$ such that $\mathrm{ES}(\tilde{\rho}_\mathrm{E}) = \Gamma$. For certain types of *submanifolds* Γ, this approach works — in ways quite dependent on the shape of Γ and especially on its *dimension.* This method might fail to yield all the solutions of (6.10), but in some cases it leads explicitly to large families of regular ones (cf. our forthcoming article, and [*58*] [*62*]).

The first step (finding all sets Γ) has a purely classical solution, analogous to the regularity theorems in [*7*]-[*10*].

THEOREM 6.3.1. — If $\tilde{\rho}_E \in \tilde{\mathcal{S}}'$ is a solution of (6.3):

i) $ES(\tilde{\rho}_E) \subset A_0^{-1}(E)$ $(= R\gamma(A_0 - E)$: the classical energy surface)

ii) if moreover the classical flow $U_t^{A_0}$ is regular at all points of $A_0^{-1}(E)$ (as we shall always assume), $ES(\tilde{\rho}_E)$ is invariant under $U_t^{A_0}$, hence it is a closed *union of classical trajectories.*

Proof. — *i)* on any open set of X where $(A_0(x) - E)$ does not vanish, all the ρ_n must vanish by Eqs. (6.11$^+$) and (6.12$^+$).

ii) $\tilde{\rho}(t, x) \equiv \tilde{\rho}_E(x)$ solves Eq. (6.5) and it suffices to apply theorem 6.2.1 *ii).*

DEFINITION 6.3.2. — We call an asymptotic eigenstate $\tilde{\rho}_E$ *regular* if $ES(\tilde{\rho}_E)$ is a submanifold of X (C^∞, without boundary...) depending smoothly on E (and possibly on other parameters), on which the flow $U_t^{A_0}$ is regular, and if the distributions ρ_n are continuous along $ES(\tilde{\rho}_E)$ (of the « multiple layer » type).

We shall only look at « well-posed » asymptotic problems admitting regular eigenstate solutions.

DEFINITION 6.3.3. — An invariant (under $U_t^{A_0}$), closed subset $M \subset X$ is called *minimal* if it contains (at least) one classical orbit dense in M.

A minimal set has the following properties: it lies on an energy surface, it is connected, and it cannot be further decomposed as a disjoint union of a family of closed invariant sets.

UNIQUENESS THEOREM 6.3.4. — A minimal submanifold $M \subset A_0^{-1}(E)$ is the support of at most one regular classical invariant state ρ_0. If moreover $M = A_0^{-1}(E)$, then it is the essential support of at most one regular asymptotic eigenstate $\tilde{\rho}$ [*23*] [*29*].

Proof. — Assume the existence of two continuous invariant measures ρ_0 and ρ'_0 on M. Then by Eq. (6.11$^-$), the Radon-Nikodym derivative $C(x) = d\rho'_0(x)/d\rho_0(x)$, a continuous function on M, satisfies $\frac{dC}{dt} = 0$ along a dense orbit, hence it is constant on M. We prove the second statement by recursion on n: assume $\tilde{\rho}$ is unique up to order $(n - 1)$, but that we have two solutions $\rho_n \neq \rho'_n$ of (6.12). Then $\sigma = \rho_n - \rho'_n$ satisfies: $(A_0 - E)\sigma = 0$, whose regular solutions on $A_0^{-1}(E)$ have the form $C(x)\delta(A_0(x) - E)$ (C continuous), and: $\frac{d\sigma}{dt} = 0$, which implies by the above argument: C = constant. Then $\sigma = C\rho_0$, and it can be absorbed in the overall normalization of $\tilde{\rho}$. Q. E. D.

Minimal essential supports play another interesting role (we only give a naive argument): the asymptotic eigenstates of a given $A \in \hat{\mathfrak{A}}$ form a convex set under mixture, and the extremal points are clearly the eigenstates with minimal essential supports. Any eigenstate has a unique barycentric decomposition on extremal eigenstates provided the family of all minimal essential supports forms a partition of phase space; this is very analogous to the spectral decomposition of the Hilbert space for the operator A. This suggests the following: write X as a disjoint (continuous) union of minimal sets: $X = \bigcup_\alpha M_\alpha$; if each M_α is a manifold and carries a regular eigenstate $\tilde{\rho}_\alpha$, we call the family $\{ \rho_\alpha \}$ the asymptotic spectral decomposition of A. We hope (this is a conjecture in general, which seems true for completely integrable systems [*29*]) that the family $\{ \rho_\alpha \}$ describes many of the eigenvectors $| \psi_n \rangle$ of the operator A, by virtue of a correspondence: $\widetilde{| \psi_n \rangle \langle \psi_n |} = \tilde{\rho}_{\alpha_n}$, where the relevant values α_n of the index α might be selected by appropriate quantization rules (depending on the shape and dimension of M_α).

EXISTENCE THEOREM 6.3.5. — The stationary equations (6.10) admit a regular solution $\tilde{\rho}_E$ with $ES(\tilde{\rho}_E) = A_0^{-1}(E)$ provided $A_0^{-1}(E) \subset X$ is a submanifold of codimension 1 on which the gradient form dA_0 does not vanish.

Proof. — We first compute by the parametrix method the expansion of the resolvent operator $G(z) = (A - z)^{-1}$, solution of: $(A - z)G(z) = \mathbb{1}$, for $z \in \mathbb{C}\backslash\mathbb{R}$ (actually: for $z \in \mathbb{C}\backslash\text{Range } (A_0)$), assuming that A satisfies condition (3.16). Then by theorem 3.4.4, $G(z) \in \hat{\mathfrak{A}}^{\mathbb{C}}$, and its expansion $\tilde{G}_W(z) = \sum_0^\infty G_n(z)\hbar^n$ is given by Eq. (3.17) with A_0 replaced by $(A_0 - z)$:

$$G_0(x, z) = \frac{1}{A_0(x) - z}$$

$$G_1(x, z) = \frac{- A_1(x)}{(A_0(x) - z)^2}$$

$$G_2(x, z) = \frac{- A_2(x)}{(A_0(x) - z)^2}$$

$$+ \frac{4A_1^2 + \sum_{j,k} (\partial_{q_j p_k} A_0 . \partial_{p_j q_k} A_0 - \partial_{q_j q_k} A_0 . \partial_{p_j p_k} A_0)}{4(A_0 - z)^3}$$

$$+ \frac{\sum_{j,k} (\partial_{q_j} A_0 . \partial_{q_k} A_0 . \partial_{p_j p_k} A_0 - 2\partial_{q_j} A_0 . \partial_{p_k} A_0 . \partial_{p_j q_k} A_0 + \partial_{p_j} A_0 . \partial_{p_k} A_0 . \partial_{p_j q_k} A_0)}{4(A_0 - z)^4}$$

$(\ldots)$

For general $n \geq 1$:

$$G_n(x, z) = -\frac{1}{A_0(x) - z}\left(\sum_{k=0}^{n-1} \mathscr{A}_{n-k}(x, \partial_x) G_k(x, z)\right) \qquad (6.14)$$

has the structure ([c]: integer part of c):

$$G_n(x, z) = \frac{G_n^1(x)}{(A_0(x) - z)^2} + \ldots + \frac{G_n^{[3n/2]}(x)}{(A_0(x) - z)^{[3n/2]+1}} \qquad (6.15)$$

where the $G_n^k(x)$ are polynomials of partial derivatives of order $\leq n$, taken at x, of the coefficients $A_{n'}(x)$ $(n' \leq n)$. This type of expansion is used in Thomas-Fermi computations in nuclear physics [*19*].

The proof can be done recursively using Eq. (6.14), where the $\mathscr{A}_k$ are, for $k \geq 1$, the same complex differential operators as in Eq. (3.17). And there is an interesting consistency check on Eqs. (6.14): from general operator theory, we know that $(A_0 - z)G(z) = \mathbb{1}$ implies $G(z)(A_0 - z) = \mathbb{1}$. In symbol calculus, this means: $\tilde{G}^*(z^*) = \tilde{G}(z)$, or: all the G_k^n in (6.15) must be *real*. This result is non-trivial since the $\mathscr{A}_k$ are complex operators. It can be checked on G_2 in Eq. (6.13).

The resolvent $G(z)$ thus defines an asymptotic operator

$$\tilde{G}(z) = \sum_0^\infty G_n(x, z)\hbar^n .$$

We now put:

$$\tilde{\rho}_E = \frac{1}{2\pi i} \lim_{\varepsilon \to 0^+} [\tilde{G}(E + i\varepsilon) - \tilde{G}(E - i\varepsilon)] = \sum_0^\infty \rho_n(x; E)\hbar^n \quad (6.16)$$

This limit exists in the sense of *asymptotic* functionals (i. e. order by order) because dA_0 does not vanish on $A_0^{-1}(E)$:

$$\left.\begin{aligned} \rho_0(x; E) &= \delta(A_0(x) - E) \text{ (the microcanonical measure)}: \\ \rho_n(x; E) &= \sum_{r=1}^{[3n/2]} \frac{(-1)^r}{r!} G_n^r(x) \times \delta^{(r)}(A_0(x) - E) (\in \mathscr{S}'(x)) \end{aligned}\right\} \quad (6.17)$$

so it defines an element of $\tilde{\mathscr{S}}'(X)$, which clearly solves (6.3). But each $\rho_n \in \mathscr{S}'(X)$ even if condition (3.16) is not assumed, so that eq. (6.17) defines $\tilde{\rho}_E \in \tilde{\mathscr{S}}'(X)$ in all cases. Q. E. D.

Note that the limit in $\hat{\mathscr{S}}'(X)$ for $\varepsilon \to 0^+$ of the admissible operator:

$$\frac{1}{2\pi i}(G(E + i\varepsilon) - G(E - i\varepsilon)) = \frac{1}{2\pi i}\sum_m \left(\frac{1}{E_m - E + i\varepsilon} - \frac{1}{E_m - E - i\varepsilon}\right)\rho_{E_m}$$

(assuming A has discrete spectrum $\{ E_m \}$ and eigenprojectors ρ_{E_m}) is not defined: we must let $\hbar \to 0$, i. e. go to the asymptotic theory, *before* letting $\varepsilon \to 0$. This means that we cannot write directly:

$$| \psi_{E_m} \rangle \langle \psi_{E_m} |^{W'} \sim \tilde{\rho}_{E|E=E_m}:$$

ρ_E is a (projector-valued) distribution in the variable E, and we only have the weaker relation [*21*]:

$$\tilde{\rho}_E = \lim_{\varepsilon \to 0^+} \left(\frac{\varepsilon}{2\pi(E^2 + \varepsilon^2)} * \left(\sum_m \delta(E - E_m) \, \widetilde{| \psi_{E_m} \rangle \langle \psi_{E_m} |^{W}} \right) \right)$$

so that $\tilde{\rho}_E$ is a regularization of ρ_E, and it will represent individual projectors $| \psi_E \rangle \langle \psi_E |$ only if these operators are restrictions of smooth functions of E: this will not happen, for instance, if the operator A has (quasi-) degeneracies in its spectrum.

Also, the asymptotic eigenstate (6.16) is not the only possible one, except if $A_0^{-1}(E)$ is a minimal set (i. e. if the flow $U_t^{A_0}$ is ergodic). For all these reasons, the solution (6.16), although easy to compute, may not be relevant for the asymptotic spectral decomposition of A. In Ref. [*58*], we define « controllable » systems for which the minimal asymptotic eigenstates can be constructed from solutions of the type (6.16): these include one-dimensional, also completely integrable, and possibly some ergodic, systems [*62*].

Therefore we are going to describe in some detail the applications of the theory to one-dimensional systems. The main result is that the *eigenvectors and the spectrum* can be obtained explicitly to all orders by establishing a connection with WKB theory. The extension of the results to completely integrable systems poses no theoretical difficulty.

7. ONE-DIMENSIONAL PROBLEMS

If $l = 1$, the results of section 6 lead to the *asymptotic eigenfunctions and eigenvalues* of the operator $A(\hbar)$ in certain regions of the spectrum $\sigma(A(\hbar))$ of the form $\sigma(A(\hbar)) \cap I$, where I is an open interval of $\mathbb{R}$ subjected to some conditions.

Essentially, for every $E \in I$, the energy curve $A_0^{-1}(E)$ must be regular, simple, *connected* (hence it is a *minimal* set, consisting of a single orbit of A_0). Since we are especially interested in the way the discrete spectrum of bound states is generated by quantization, we also ask $A_0^{-1}(E)$ to be a compact closed curve. Henceforth, $E \in I$ is chosen constant.

For simplicity, we also choose: $A(\hbar) = \hat{H}$: a quantized classical hamiltonian, i. e. $A_0(x) \equiv H(x)$ and $A_n(x) \equiv 0$ for $n \geq 1$: actually this is the most common case in quantum mechanics, and this choice involves no real loss of generality.

The methods described here will be independent of the form of H(x), and of the representation $\mathcal{R}$. A few simplifications will be mentioned however, for the special case of $H(x) = \frac{p^2}{2} + V(q)$ in a position representation (the computations will be shown in more detail in [*62*]).

7.1. The asymptotic eigenstate

In one dimension, the eigenstate $\tilde{\rho}_E$ has to be regular (it satisfies the transport equations (6.12$^-$)), it is unique because $H^{-1}(E)$ is a minimal set, so it is given by Eq. (6.16): when $l = 1$, $\tilde{\rho}_E$ can be deduced *directly from the resolvent* $\tilde{G}(z)$.

In the case [10] $A(\hbar) = \hat{H}$, there is a faster way to obtain $\tilde{G}(z)$ than Eqs. (6.14). We can write the resolvent equations $(H - z)\tilde{G}(z) = \tilde{G}(z)(H - z) = 1$ as: $[H - z, \tilde{G}(z)]_{\pm} = 1 \pm 1$, or:

$$\begin{cases} \left(H - z + \sum_1^\infty \mathcal{A}_{2n}(x, \partial_x)\hbar^{2n}\right)\left(\sum_0^\infty G_n(x ; z)\hbar^n\right) = 1 & (7.1^+) \\ \left(\sum_0^\infty \mathcal{A}_{2n+1}(x, \partial_x)\hbar^{2n+1}\right)\left(\sum_0^\infty G_n(x ; z)\hbar^n\right) = 0 & (7.1^-) \end{cases}$$

But Eqs. (7.1$^+$) alone imply, recursively:

$$\left.\begin{aligned} & G_0(x ; z) = \frac{1}{H(x) - z}; \qquad G_1(x ; z) = 0; \\ (n \geqslant 0) \quad & G_{2n+1}(x ; z) = \frac{-1}{H(x) - z} \left[\sum_{k=0}^{n-1} \mathcal{A}_{2(n-k)}(x, \partial_x).G_{2k+1}(x ; z)\right] \equiv 0 \\ (n \geqslant 1) \quad & G_{2n}(x ; z) = \frac{-1}{H(x) - z} \left[\sum_{k=0}^{n-1} \mathcal{A}_{2(n-k)}(x, \partial_x).G_{2k}(x ; z)\right] \end{aligned}\right\} \quad (7.2)$$

so the resolvent is an *even* function of $\hbar$. The G_{2n} are obtained without

[10] More generally, whenever $A_W(x, \hbar)$ is an *even* function of $\hbar$ (for any dimension l).

using Eqs. (7.1^-): these form an infinite set of non-trivial *identities* satisfied by the G_{2n}:

$$(\forall n \geqslant 1) \qquad \sum_{k=0}^{n-1} \mathscr{A}_{2(n-k)-1}(x, \partial_x).G_{2k}(x\,;z) \equiv 0 \tag{7.3}$$

Now $G_{2n}(x\,;z)$ has the general structure for $n \geq 1$:

$$G_{2n}(x\,;z) = \sum_{r=2}^{3n} \frac{G^r_{2n}(x)}{(H(x)-z)^{r+1}} \tag{7.4}$$

As compared with Eq. (6.15): $G^1_{2n}(x) \equiv 0$, and $G^r_{2n}(x)$ is a (real) polynomial of the form:

$$G^r_{2n}(x) = \sum_{\alpha,\beta\in\mathbb{N}^r} c_{\alpha\beta} \sum_{j=1}^{r} (\partial_q^{\alpha_j}\partial_p^{\beta_j}H(x)), \quad \text{with:} \quad \begin{cases} (\forall j) \quad \alpha_j + \beta_j \leqslant 2n \\ \displaystyle\sum_{j=1}^{r} \alpha_j = \sum_{j=1}^{r} \beta_j = 2n \end{cases} \tag{7.5}$$

(this results from dimensional analysis: $G_{2n}(x\,;z)$ must have the dimension $\dfrac{1}{(H)(\hbar)^{2n}} = \dfrac{1}{(H)(q)^{2n}(p)^{2n}}\Big)$. Thus, if $H(x) = \dfrac{p^2}{2} + V(q)$, $G^r_{2n}(q, p)$ is a polynomial in p of degree $k \leq r-2$ if $r \leq 2n$ and $k \leq 2n$ if $r \geq 2n+1$: otherwise a term of G^r_{2n} containing $(\partial_p H)^k$ cannot satisfy (7.5).

For instance:

$$G_2(x\,;z) = \frac{1}{4}\left[\frac{(\partial_{qp}H)^2 - \partial_{qq}H.\partial_{pp}H}{(H-z)^3} + \frac{(\partial_{qq}H)(\partial_p H)^2 - 2\partial_{qp}H.\partial_q H.\partial_p H + (\partial_{pp}H)(\partial_q H)^2}{(H-z)^4}\right] \tag{7.6}$$

The eigenstate (6.16) is then:

$$\tilde{\rho}_E = \sum_{n=0}^{\infty}\left(\sum_{r=2}^{3n} \frac{(-1)^r}{r!} G^r_{2n}(x) \times \delta^{(r)}(H(x)-E)\right)\hbar^{2n} \tag{7.7 a}$$

$$= \sum_{r=0}^{\infty} \frac{(-1)^r}{r!} \mathscr{G}_r(x\,;\hbar)\delta^{(r)}(H(x)-E) \tag{7.7 b}$$

where (7.7 *b*) is a finite reordering of (7.7 *a*) to every finite order in $\hbar$, and the $\mathscr{G}_r(x\,;\hbar)$ are formal power series given by:

$$\mathscr{G}_0(x\,;\hbar) = 1\,;\ \mathscr{G}_1(x\,;\hbar) = 0\,;\ (r \geqslant 2): \qquad \mathscr{G}_r(x\,;\hbar) = \sum_{n\geqslant r/3} G^r_{2n}(x)\hbar^{2n} \tag{7.8}$$

The identification between: $\tilde{G}(\hbar; x, z) = \sum_0^\infty \frac{\mathcal{G}_r(x; \hbar)}{(H(x) - z)^{r+1}}$ (defining the coefficients $\mathcal{G}_r$) and the operator Neumann series:

$$(\hat{H}(\hbar) - z)^{-1} \sim \sum_0^\infty \frac{(H(x).\mathbb{1} - \hat{H})^r}{(H_0(x) - z)^{r+1}}$$

(both considered at fixed $x \in X$, for $z \to \pm i\infty$) yields another explicit formula for $\mathcal{G}_r$: $(\forall r)$ $\mathcal{G}_r(x; \hbar) = [(H(x).\mathbb{1} - \hat{H})^r]_W(x; \hbar)$.

7.2. The « canonical operator »

The WKB theory [4] [23] asserts that the solutions of Eq. (6.1) in one dimension have local expansions of the form (5.12) on the lagrangian manifold $\Lambda_E = A_0^{-1}(E) = H^{-1}(E)$. We saw in theorem 5.4.2 that every WKB contribution $a^{\mathcal{R}}(q_R; \hbar)e^{\frac{i}{\hbar}S_\Lambda^R(q_R)}$ defines a local asymptotic functional in $\tilde{\mathcal{S}}'(\Omega)$, where $\Omega \subset X$ is an open set such that $\Omega \cap \Lambda$ is connected and the projection $\bar{\Omega} \cap \Lambda \overset{\pi_R}{\to} Q_R$ is one-to-one and has the inverse map

$$q_R \to X = \begin{pmatrix} q_R \\ p_R \end{pmatrix} = \begin{pmatrix} q_R \\ \partial_{q_R} S_\Lambda^R(q_R) \end{pmatrix}$$

The asymptotic functional resulting from patching together all these local functionals has to be the $\tilde{\rho}_E \in \tilde{\mathcal{S}}'(X)$ given by Eqs. (7.7), if our theory is consistent. We now show that $\tilde{\rho}_E$ is built up indeed from local WKB contributions, which moreover can be completely recovered from Eqs. (7.7) *to all orders in* $\hbar$, provided the coefficients ρ_{2n} satisfy a set of *nonlinear algebraic identities.* Our method will require a nonlinear adaptation of Maslov's « canonical operator »; it will be representation-independent, but we shall describe it in the position representation.

The WKB contributions will be easier to extract in the form:

$$\psi_{WKB}(q; E; \hbar) = a(q; E; \hbar)e^{\frac{i}{\hbar}S(q;E;\hbar)} \tag{7.9}$$

where $a(q; E; \hbar) = \sum_0^\infty a_n(q; E)\hbar^n$ and: $S(q; E; \hbar) = \sum_0^\infty S_n(q; E)\hbar^n$ are uniquely defined as *real* formal power series. The relation (5.5) between ψ_{WKB}

and the associated local functional $\tilde{\rho}^{\mathrm{WKB}}$ becomes explicitly (cf. the derivation of Eq. (5.13)):

$$\tilde{\rho}_{\Omega}^{\mathrm{WKB}}(q, p\,;\hbar) = \frac{1}{2\pi\hbar}\int_{\mathrm{Q}} a\left(q-\frac{r}{2}\,;\hbar\right)a\left(q+\frac{r}{2}\,;\hbar\right)e^{\frac{i}{\hbar}\left[\mathrm{S}\left(q-\frac{r}{2};\hbar\right)-\mathrm{S}\left(q+\frac{r}{2};\hbar\right)+pr\right]}d^{l}r$$

$$= \exp\left[\log a\left(q+\frac{i\hbar}{2}\partial_p\right)+\log a\left(q-\frac{i\hbar}{2}\partial_p\right)+\frac{i}{\hbar}\Sigma(q, i\hbar\partial_p)\right]\delta(p-p_{\mathrm{E}}(q))_{|\Omega}$$

where $q \rightarrow p_{\mathrm{E}}(q)$ is the function admitting $\Omega \cap \mathrm{H}^{-1}(\mathrm{E}) = \Omega_{\mathrm{E}}$ as graph, and $\Sigma(q, r\,;\hbar) = \mathrm{S}\left(q+\frac{r}{2}\,;\hbar\right) - \mathrm{S}\left(q-\frac{r}{2}\,;\hbar\right) - p_{\mathrm{E}}(q).r$. Finally:

$$\tilde{\rho}_{\Omega}^{\mathrm{WKB}}(q, p\,;\hbar) = \exp\left[p_{\mathrm{E}}(q).\partial_p + \sum_{k=0}^{\infty}\left(\frac{i\hbar}{2}\right)^{2k}\left(\frac{2\partial_q^{2k}(\log a).\partial_p^{2k}}{(2k)\,!} - \frac{\partial_q^{2k+1}\mathrm{S}.\partial_p^{2k+1}}{(2k+1)\,!}\right)\right].\delta(p-p_{\mathrm{E}}(q))_{|\Omega} \quad (7.10)$$

The identification $\tilde{\rho}_{\Omega}^{\mathrm{WKB}} = \tilde{\rho}_{\mathrm{E}|\Omega}$ will yield the power series a and S. It is convenient for this to rewrite Eq. (7.7 b) for $\tilde{\rho}_{\mathrm{E}|\Omega}$ as:

$$\tilde{\rho}_{\mathrm{E}|\Omega} = \sum_{s=0}^{\infty}\alpha_s(q\,;\mathrm{E}\,;\hbar)\delta^{(s)}(p-p_{\mathrm{E}}(q))_{|\Omega} \quad (7.11)$$

The coefficients α_s are computable by:

$$\alpha_s(q\,;\mathrm{E}\,;\hbar) = \int_{\mathrm{P}} dp\tilde{\rho}_{\mathrm{E}|\Omega}(q, p\,;\hbar)\frac{(p-p_{\mathrm{E}}(q))^s}{s\,!}$$

$$= \sum_{r=s}^{\infty}\frac{1}{r\,!}\left[\partial_{\mathrm{E}}^{r}\left(\frac{(p-p_{\mathrm{E}}(q))^s}{s\,!}.\left|\frac{\partial p_{\mathrm{E}}(q)}{\partial \mathrm{E}}\right|.\mathcal{G}_r(q, p_{\mathrm{E}}(q))\right)\right]_{p=p_{\mathrm{E}}(q)} \quad (7.12)$$

where $\partial_{\mathrm{E}} = \frac{\partial p_{\mathrm{E}}}{\partial \mathrm{E}}\frac{\partial}{\partial p_{\mathrm{E}}} = \left(\frac{1}{\partial_p \mathrm{H}}\right)_{|p=p_{\mathrm{E}}(q)}.\frac{\partial}{\partial p_{\mathrm{E}}}$. At any finite order $\mathcal{O}(\hbar^{2n})$, the sum (7.12) stops at $r = 3n$ and yields α_s as a finite expression, linear in the functions $\mathcal{G}_r(r \leqslant 3n)$. The $\hbar$-expansion of α_s has the general form:

$$\alpha_s(q\,;\mathrm{E}\,;\hbar) = \frac{\delta_{s0}}{\mathrm{H}_p} + \sum_{n\geqslant\frac{s}{3}}\left[\sum_{k=2}^{6n+1-s}\frac{\alpha_{snk}}{(\partial_p\mathrm{H})^k}(q, p = p_{\mathrm{E}}(q))\right]\hbar^{2n}$$

where the α_{snk} are polynomials of partial derivatives of H (fig. 5). The expression (7.11) is equivalent to (7.7 b) in Ω, but whereas (7.7 b) is globally regular in X, Eq. (7.12) becomes singular at the caustic points (or turning

$$
\begin{aligned}
\alpha_0 = {} & H(0,1)^{(-1)} + \hbar^2 * \Big(1/24*H(0,1)^{(-2)}*H(2,3) - 1/8*H(0,1)^{(-3)}*H(0,2)*H(2,2) - 1/6*H(0,1)^{(-3)}*H(0,3)*H(2,1) \\
& - 1/12*H(0,1)^{(-3)}*H(1,3)*H(1,1) - 1/12*H(0,1)^{(-3)}*H(2,0)*H(0,4) - 1/12*H(0,1)^{(-3)}*H(1,0)*H(1,4) \\
& + 1/4*H(0,1)^{(-4)}*H(0,2)^2*H(2,1) + 1/4*H(0,1)^{(-4)}*H(0,2)*H(1,2)*H(1,1) + 1/3*H(0,1)^{(-4)}*H(0,2)*H(0,3)*H(2,0) \\
& + 1/3*H(0,1)^{(-4)}*H(0,2)*H(1,3)*H(1,0) + 1/3*H(0,1)^{(-4)}*H(1,2)*H(0,3)*H(1,0) + 5/24*H(0,1)^{(-4)}*H(0,3)*H(1,1)^2 \\
& + 1/4*H(0,1)^{(-4)}*H(1,1)*H(0,4)*H(1,0) + 1/24*H(0,1)^{(-4)}*H(0,5)*H(1,0)^2 - 1/4*H(0,1)^{(-5)}*H(0,2)^3*H(2,0) \\
& - 3/4*H(0,1)^{(-5)}*H(0,2)^2*H(1,2)*H(1,0) - 3/8*H(0,1)^{(-5)}*H(0,2)^2*H(1,1)^2 - 4/3*H(0,1)^{(-5)}*H(0,2)*H(0,3)*H(1,1)*H(1,0) \\
& - 7/24*H(0,1)^{(-5)}*H(0,2)*H(0,4)*H(1,0)^2 - 1/6*H(0,1)^{(-5)}*H(0,3)^2*H(1,0)^2 + 5/4*H(0,1)^{(-6)}*H(0,2)^3*H(1,1)*H(1,0) \\
& + 25/24*H(0,1)^{(-6)}*H(0,2)^2*H(0,3)*H(1,0)^2 - 5/8*H(0,1)^{(-7)}*H(0,2)^4*H(1,0)^2 \Big)
\end{aligned}
$$

$$
\begin{aligned}
\alpha_1 = \hbar^2 * \Big(& - 1/8*H(0,1)^{(-2)}*H(2,2) + 1/4*H(0,1)^{(-3)}*H(0,2)*H(2,1) + 1/4*H(0,1)^{(-3)}*H(1,2)*H(1,1) \\
& + 1/6*H(0,1)^{(-3)}*H(0,3)*H(2,0) + 1/4*H(0,1)^{(-3)}*H(1,3)*H(1,0) - 1/4*H(0,1)^{(-4)}*H(0,2)^2*H(2,0) \\
& - 3/4*H(0,1)^{(-4)}*H(0,2)*H(1,2)*H(1,0) - 3/8*H(0,1)^{(-4)}*H(0,2)*H(1,1)^2 - 7/12*H(0,1)^{(-4)}*H(0,3)*H(1,1)*H(1,0) \\
& - 1/8*H(0,1)^{(-4)}*H(0,4)*H(1,0)^2 + 5/4*H(0,1)^{(-5)}*H(0,2)^2*H(1,1)*H(1,0) + 2/3*H(0,1)^{(-5)}*H(0,2)*H(0,3)*H(1,0)^2 \\
& - 5/8*H(0,1)^{(-6)}*H(0,2)^3*H(1,0)^2 \Big)
\end{aligned}
$$

$$
\begin{aligned}
\alpha_2 = \hbar^2 * \Big(& 1/8*H(0,1)^{(-2)}*H(2,1) - 1/8*H(0,1)^{(-3)}*H(0,2)*H(2,0) - 1/4*H(0,1)^{(-3)}*H(1,2)*H(1,0) - 1/8*H(0,1)^{(-3)}*H(1,1)^2 \\
& + 1/2*H(0,1)^{(-4)}*H(0,2)*H(1,1)*H(1,0) + 1/8*H(0,1)^{(-4)}*H(0,3)*H(1,0)^2 - 1/4*H(0,1)^{(-5)}*H(0,2)^2*H(1,0)^2 \Big)
\end{aligned}
$$

$$
\alpha_3 = \hbar^2 * \Big(- 1/24*H(0,1)^{(-2)}*H(2,0) + 1/12*H(0,1)^{(-3)}*H(1,1)*H(1,0) - 1/24*H(0,1)^{(-4)}*H(0,2)*H(1,0)^2 \Big)
$$

FIG. 5. — The coefficients $\alpha_s(q, \mathrm{E}; \hbar)$ to order $\hbar^2$; H(J, K) denotes $\partial_q^{\mathrm{J}}\partial_p^{\mathrm{K}}\mathrm{H}(q, p = p_{\mathrm{E}}(q))$; for $s \geq 4 : \alpha_s = \mathcal{O}(\hbar^4)$. The formal computer language Reduce [60] was used.

points) (11) where $\dfrac{\partial p_{\rm E}}{\partial {\rm E}} = \infty$. In $\Omega_{\rm E}$, $\partial_p {\rm H}$ cannot change sign or vanish; we may assume $\dfrac{\partial p_{\rm E}}{\partial {\rm E}} = \left(\dfrac{1}{\partial_p {\rm H}}\right)_{|\Omega_{\rm E}} > 0$.

We shall also need the expression:

$$\beta_0(q\,;{\rm E}\,;\hbar) = p_{\rm E}(q)\alpha_0(q\,;{\rm E}\,;\hbar) - \alpha_1(q\,;{\rm E}\,;\hbar)$$
$$= \sum_{r=0}^{\infty} \frac{1}{r!}\partial_{\rm E}^r \left[p_{\rm E}(q) \frac{\partial p_{\rm E}(q)}{\partial {\rm E}} \mathcal{G}_r(q,\, p_{\rm E}(q)) \right] \tag{7.13}$$

We now identify the coefficients of every $\delta^{(s)}(p - p_{\rm E}(q))$ in Eqs. (7.10) and (7.11):

$$(s=0):\quad a(q;{\rm E};\hbar)^2 = \alpha_0 \qquad \Rightarrow a(q;{\rm E};\hbar) = \alpha_0(q;{\rm E};\hbar)^{\frac{1}{2}} \tag{7.14}$$

$$(s=1):\quad a(q;{\rm E};\hbar)^2\left(-\frac{\partial {\rm S}}{\partial q} + p_{\rm E}(q)\right) = \alpha_1 \Rightarrow \frac{\partial {\rm S}}{\partial q}(q;{\rm E};\hbar) = \frac{\beta_0}{\alpha_0}(q;{\rm E};\hbar) \tag{7.15}$$

hence the wave function is determined up to an overall phase:

$$\psi_{\rm WKB}(q\,;{\rm E}\,;\hbar) = \alpha_0(q\,;{\rm E}\,;\hbar)^{\frac{1}{2}} e^{\frac{i}{\hbar}\left[\int^q \frac{\beta_0}{\alpha_0}(q'\,;{\rm E}\,;\hbar)dq' + {\rm C}\right]} \tag{7.16}$$

The remaining identities for $s \geq 2$ then result in *constraint relations* between the coefficients α_s in Eq. (7.11), for instance:

$$\left.\begin{aligned}
&(s = 2): \quad \alpha_2 = -\frac{\hbar^2}{8}\alpha_0\partial_q^2(\log\alpha_0) + \frac{\alpha_1^2}{2\alpha_0}\\
&(s = 3): \quad \alpha_3 = \frac{\hbar^2}{24}\alpha_0\partial_q^2\left(\frac{\beta_0}{\alpha_0}\right) - \frac{\hbar^2}{8}\alpha_1\partial_q^2(\log\alpha_0) + \frac{\alpha_1^3}{6\alpha_0^2}\\
&(s = 4): \quad \alpha_4 = \frac{\hbar^4}{384}\alpha_0\partial_q^4(\log\alpha_0) + \frac{\hbar^4}{128}\alpha_0(\partial_q^2\log\alpha_0)^2\\
&\qquad\qquad + \frac{\hbar^2}{24}\alpha_1\partial_q^2\left(\frac{\beta_0}{\alpha_0}\right) - \frac{\hbar^2}{16}\frac{\alpha_1^2}{\alpha_0}\partial_q^2(\log\alpha_0) + \frac{\alpha_1^4}{24\alpha_0^3}\\
&\text{etc.}
\end{aligned}\right\} \tag{7.17}$$

We have checked these identities up to $\mathcal{O}(\hbar^4)$: they are satisfied (they mean that the $\tilde{\rho}_{\rm E}$ of Eq. (7.7) is indeed a *rank 1* projector onto a WKB state). However Eqs. (7.17) are superfluous for the determination of $\psi_{\rm WKB}$: it is enough to know α_0 and α_1, and to use Eqs. (7.14)-(7.15).

(11) Such singularities are known to appear in the asymptotic form of the *wave function* in any particular representation.

In the case $H = \frac{p^2}{2} + V(q)$, Eqs. (7.11) and (7.12) yield:

$$\alpha_0(q\,;E\,;\hbar) = \sum_{r=0}^{\infty} \frac{1}{r!} \left[\frac{\partial^r}{\partial\left(\frac{p^2}{2}\right)^r} \frac{\mathcal{G}_r(q,p)}{p} \right]_{p=p_E(q)}$$

$$\beta_0(q\,;E\,;\hbar) = \sum_{r=0}^{\infty} \frac{1}{r!} \left[\frac{\partial^r}{\partial\left(\frac{p^2}{2}\right)^r} \mathcal{G}_r(q,p) \right]_{p=p_E(q)}$$

and by virtue of the remarks following Eq. (7.5), $\mathcal{G}_r$ is a polynomial in p of degree $\langle 2r$ if $r > 0$ (with even powers only, since H is even in p), hence we have exactly:

$$\left.\begin{aligned} &\beta_0 \equiv 1 \\ \text{and:}\quad &\psi_{\mathrm{WKB}}(q\,;E\,;\hbar) = \alpha_0(q\,;E\,;\hbar)^{\frac{1}{2}} e^{\frac{i}{\hbar}\int^q \frac{dq'}{\alpha_0(q'\,;E\,;\hbar)}} \end{aligned}\right\} \quad (7.18)$$

Eq. (7.15) then generalizes the well-known « continuity equation »: $a^2 \frac{\partial S}{\partial q} = \text{const}$ (= 1, here), valid only if $H = \frac{p^2}{2} + V(q)$, and which can be used to compute ψ_{WKB} to all orders in that case [*1*]. But Eqs. (7.18) are a special, nongeneric form of Eqs. (7.13)-(7.16).

We call « canonical operator in the representation $\mathcal{R}$ » the mapping:

$$\tilde{\rho}^{\mathrm{R}} \;\longrightarrow\; \psi^{\mathcal{R}}_{\mathrm{WKB}}(q_{\mathrm{R}}) = a^{\mathrm{R}} e^{\frac{iS^{\mathcal{R}}}{\hbar}} = (\alpha_0^{\mathrm{R}})^{\frac{1}{2}} e^{\frac{i}{\hbar}\left[\int^{q_{\mathrm{R}}} \frac{\beta_0^{\mathrm{R}}}{\alpha_0^{\mathrm{R}}} dq'_{\mathrm{R}} + C_{\mathcal{R}}\right]}$$

defined on every connected component of $H^{-1}(E)\backslash\Sigma_{\mathrm{R}}$ (Σ_{R} is the singular set for the projection $H^{-1}(E) \overset{\pi_{\mathrm{R}}}{\to} Q_{\mathrm{R}}$) by the Eqs. (7.12) to (7.16), which are valid in any representation ([12]). This mapping makes sense only if $\tilde{\rho}_E$ satisfies the constraints (7.17); it has all the asymptotic corrections to Maslov's canonical operator [*4*]; and it is local in the sense that $\psi^{\mathcal{R}}_{\mathrm{WKB}}(q_{\mathrm{R}})$ is determined by the germ of $\tilde{\rho}^{\mathrm{R}}$ at $\pi_{\mathrm{R}}^{-1}(q_{\mathrm{R}}) \subset H^{-1}(E)$; only the overall phase $e^{\frac{i}{\hbar}C_{\mathcal{R}}}$ of $\psi^{\mathcal{R}}_{\mathrm{WKB}}$ stays undetermined at this level.

The family $\{\psi^{\mathcal{R}}_{\mathrm{WKB}}\}_{\mathcal{R}\in\mathcal{F}}$ defines an asymptotic symplectic spinor $\psi(\hbar) \in \mathcal{S}'^{\mathbb{C}}(\mathcal{H})$ (mod $\sigma(\hbar^\infty)$) which can be considered as the tensor square root of the asymptotic functional $\tilde{\rho}$; each $\psi^{\mathcal{R}}_{\mathrm{WKB}}$ transforms like a half-form [*11*] under the group $GL(Q_{\mathrm{R}})$.

7.3. **Quantization conditions**

Assuming that the eigenvector $\psi(\hbar) \in \mathcal{S}'(\mathcal{H})$ is a WKB state vector, Eq. (4.7) implies for its WKB expansions:

$$\psi^{\mathcal{R}_1}_{\mathrm{WKB}} = \mathcal{V}\psi^{\mathcal{R}_2}_{\mathrm{WKB}} \qquad \text{if} \qquad \mathcal{R}_2 = \mathcal{R}_1\mathcal{V}, \qquad \mathcal{V} \in i\mathrm{Mp}(l)\,.$$

([12]) Because they express the relation (5.5), which is iMp(l)-covariant due to eq. (5.9).

This fixes completely the relative phase between any two expansions. But this procedure (the *asymptotic matching* of phases) appears to be consistent, when applied to expansions of the form (7.16), only for a *discrete subset* of eigenvalues: this is how the spectrum gets quantized.

It is better to do the matching, like Bouslaiev [46], along an interpolating curve of representations: $\{ \mathscr{R}(t) \}_0^T \subset \mathscr{F}$. For our present purpose (quantizing the spectrum). the curve can be rather arbitrary: there must only exist a map: $t \mapsto \Omega_E(t)$: where $\Omega_E(t)$ is a compact *connected* set $\Omega_E(t) \subset H^{-1}(E)\backslash\Sigma_{R(t)}$ (the frame $R(t) \in F$ corresponding to $\mathscr{R}(t)$), varying *continuously* with t, such that: $\bigcup_{0 \leq t \leq T} \Omega_E(t) = H^{-1}(E)$. (« *condition C* »).

We shall work here with a curve $\mathscr{R}(t)$ closely related to classical dynamics (and generalizable to higher dimensional problems), although in some cases simpler choices exist [58].

Let $\{ x_E(t) \}_0^{T(E)}$ be the closed curve $H^{-1}(E)$ parametrized by time: $T(E)$ is the period. Choose action-angle coordinates [59] (θ, I) on X:

$$\theta = \frac{2\pi t}{T(E)} + \text{const [mod } 2\pi]; \qquad I(E) = \int^E \frac{T(E')}{2\pi} dE' + \text{const.}$$

Let $R(\theta)$ be the tangent frame to the action-angle coordinates at $x(\theta, I) \in H^{-1}(E)$, with axes $\frac{\partial x}{\partial \theta}$ and $\frac{\partial x}{\partial I}$ (fig. 6); $R(\theta) \in F$ because $d\theta \wedge dI = dq \wedge dp$; the curve $\{ R(\theta) \}_0^{2\pi}$ is periodic; and the frame $R(\theta)$ is transported by the flow U_0 of the vectorfield $\left\{ \frac{dx}{d\theta} = \frac{T}{2\pi} \frac{dx}{dt} \right\}_{x \in X}$: the origin of $R(\theta)$ is $x(\theta)$, and any vector $e(\theta)$ attached to the frame satisfies: $e(\theta + \theta') = T_{x(\theta)}(U_{\theta'}) . e(\theta)$, hence by differentiation: $\frac{de}{d\theta} = T_{x(\theta)}\left(\frac{dx}{d\theta}\right) . e(\theta)$. In any frame, $T_{x(\theta)}\left(\frac{dx}{d\theta}\right)$ is the jacobian matrix at $x(\theta)$ of the map: $\begin{pmatrix} q \\ p \end{pmatrix} \to \frac{T}{2\pi}\begin{pmatrix} H_p \\ -H_q \end{pmatrix}$, i. e.:

$$T_{x(\theta)}\left(\frac{dx}{d\theta}\right) = \frac{T}{2\pi}\begin{pmatrix} H_{pq} & H_{p^2} \\ -H_q^2 & -H_{qp} \end{pmatrix} + \frac{1}{2\pi}\frac{dT}{dE}\begin{pmatrix} H_pH_q & H_p^2 \\ -H_q^2 & -H_qH_p \end{pmatrix} \in \mathrm{sp}(l)$$

Taking the motion of the origin into account, the apparent motion induced by $R(\theta)$ (q, p denoting $q_{R(\theta)}$, $p_{R(\theta)}$) is given by the equation:

$$\begin{aligned} \frac{d}{d\theta}\begin{pmatrix} q \\ p \end{pmatrix} &= -\frac{1}{2\pi}\left[T\begin{pmatrix} H_{pq} & H_{p^2} \\ -H_{q^2} & -H_{qp} \end{pmatrix} \right. \\ &\qquad \left. + \frac{dT}{dE}\begin{pmatrix} H_pH_q & H_p^2 \\ -H_q^2 & -H_qH_p \end{pmatrix} \right]\begin{pmatrix} q \\ p \end{pmatrix} - \frac{T}{2\pi}\begin{pmatrix} H_p \\ -H_q \end{pmatrix} \\ &= -v(\theta)\begin{pmatrix} q \\ p \end{pmatrix} \end{aligned}$$

with $v(\theta) \in i\mathrm{sp}(l)$; then $\mathscr{q}(\theta) = \mathscr{q}^{h}(v(\theta))$ is given by:

$$\mathscr{q}(\theta) = \frac{1}{2\pi}\left[\frac{T}{2}(H_{pp}p^2 + 2H_{qp}qp + H_{qq}q^2) + \frac{1}{2}\frac{dT}{dE}(H_p^2p^2 + 2H_qH_pqp + H_q^2q^2) + T(H_pp + H_qq)\right] \quad (7.19)$$

all coefficients being evaluated at $x(\theta)$, i. e. at $q = p = 0$; if $[f]_k(\theta)$ is the kth order Taylor expansion of the function $f(x)$ at $x(\theta)$, then:

$$\mathscr{q}(\theta) = \frac{1}{2\pi}\left(T[H - E]_2(\theta) + \frac{1}{2}\frac{dT}{dE}([H - E]_1(\theta))^2\right)$$

We now take for $\{\mathscr{R}(\theta)\}_0^{2\pi}$ a horizontal lift-up to $i\mathrm{Mp}(l)$ of $\{R(\theta)\}_0^{2\pi}$; the infinitesimal matching condition for $\psi_{\mathrm{WKB}}^{\mathscr{R}(\theta)}$ is given by Eq. (4.24):

$$i\hbar\frac{\partial}{\partial\theta}\psi_{\mathrm{WKB}}^{\mathscr{R}(\theta)} = -\hat{\mathscr{q}}(\theta).\psi_{\mathrm{WKB}}^{\mathscr{R}(\theta)} \quad (7.20)$$

Substituting (7.9) and (7.19) into (7.20), we get the coupled WKB equations in the moving frame $R(\theta)$ for a and S:

$$\left\{\begin{aligned} \frac{\partial S^{\mathscr{R}(\theta)}}{\partial\theta} = \frac{1}{2\pi}\Bigg[&\left(TH_{pp} + \frac{dT}{dE}H_p^2\right)\left(\frac{(\nabla S)^2}{2} - \frac{\hbar^2}{2}\frac{\Delta a}{a}\right) \\ &+ \left(TH_{qp} + \frac{dT}{dE}H_qH_p\right)(q.\nabla S) + \left(TH_{qq} + \frac{dT}{dE}H_q^2\right)\frac{q^2}{2} \\ &+ T(H_p.\nabla S + H_qq)\Bigg]_{R(\theta)} \\ \frac{\partial(a^2)}{\partial\theta} + \nabla(a^2w) = 0, &\qquad \text{where:} \quad w(q) = -\frac{\partial\mathscr{q}}{\partial p}(q, p = \nabla S) \end{aligned}\right\} \quad (7.21)$$

is the classical velocity flow of $(-\mathscr{q})$.

But the solution to Eqs. (7.21) is given by the canonical operator acting on $\tilde{\rho}_E$ in the representation $\mathscr{R}(\theta)$, except for an unknown overall phase which we can take as $S^{\mathscr{R}(\theta)}(q = 0)$ ($q = 0$ is always a *regular* point, for all θ). At $q = 0$: $H_q = 0$ and $p_E(q) = 0$ because of the position of the frame R: hence by (7.15): $\nabla S = -\frac{\alpha_1}{\alpha_0}$; also $H_p(q = 0, p = 0) = \frac{\partial H}{\partial I} = \frac{2\pi}{T}$, and:

$$\frac{\partial S^{\mathscr{R}(\theta)}}{\partial\theta}(q=0) = \frac{1}{2\pi}\left[\frac{1}{2}\left(TH_{pp} + \frac{dT}{dE}\frac{4\pi^2}{T^2}\right)\left(\frac{\alpha_1^2}{\alpha_0^2} - \hbar^2\frac{\Delta(\alpha_0^{1/2})}{\alpha_0^{1/2}}\right) - 2\pi\frac{\alpha_1}{\alpha_0}\right]_{R(\theta)} (q = p = 0)\ ([13]) \quad (7.22)$$

$(= \mathcal{O}(\hbar^2))$.

([13]) The point here is that the RHS depends on $\psi_{\mathrm{WKB}}^{\mathscr{R}(\theta)}$ *only through* $\tilde{\rho}^{R(\theta)}$.

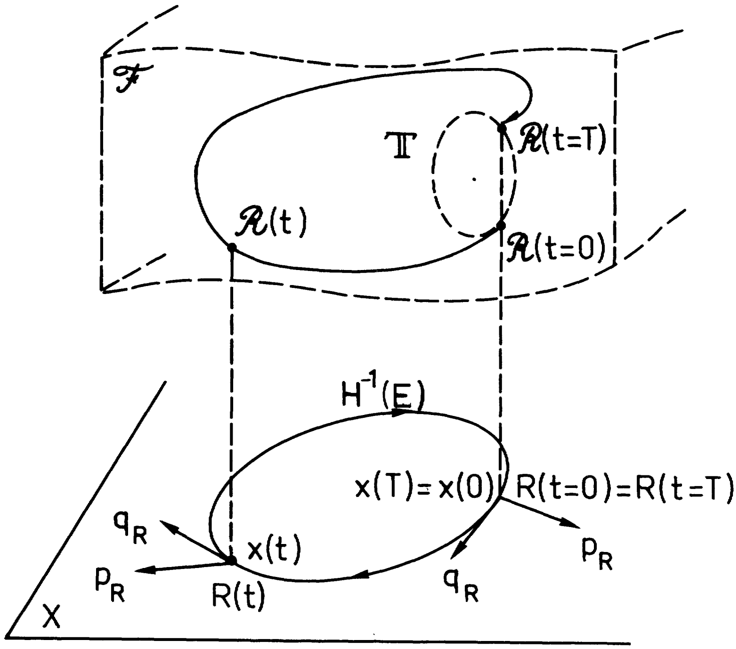

FIG. 6.

But by theorem (4.8.1): $\mathscr{R}(2\pi)=\mathscr{R}(0).(-1)^{n(\gamma)}e^{\frac{1}{i\hbar}\int_S \omega}$ $(S=\{H<E\}\subset X)$
so that $\psi^{\mathscr{R}(2\pi)} = (-1)^{n(\gamma)}e^{\frac{i}{\hbar}\int_S \omega}\psi^{\mathscr{R}(0)}$. Comparing $S(2\pi) = S(0)$ with Eq. (7.22), we obtain:

$$\int_S \omega + (2k + n(\gamma))\pi\hbar$$

$$= \int_0^{2\pi} d\theta\left[\left(\frac{1}{4\pi}\mathrm{TH}_{pp} + \frac{d\mathrm{T}}{d\mathrm{E}}\frac{\pi}{\mathrm{T}^2}\right)\left(\frac{\alpha_1^2}{\alpha_0^2} - \hbar^2\frac{\Delta(\alpha_0^{1/2})}{\alpha_0^{1/2}}\right) - \frac{\alpha_1}{\alpha_0}\right]_{\mathrm{R}(\theta)} \quad (7.23)$$

(in the RHS all quantities are evaluated in the frame $R(\theta)$ at $q = p = 0$).

This is an *asymptotic quantization condition.* It has the form:

$$\mathscr{S}(\mathrm{E}\,;\hbar^2) = (2k + n(\gamma))\pi\hbar \qquad (k\in\mathbb{Z})$$

where $\mathscr{S}$ is an *even* power series in $\hbar$ with coefficients regular in E.
Since $\mathscr{S}(\mathrm{E}, 0) = \oint_{\mathrm{H}^{-1}(\mathrm{E})} pdq = 2\pi\mathrm{I}(\mathrm{E})$ and $\frac{\partial \mathrm{I}}{\partial \mathrm{E}} = \frac{\mathrm{T}(\mathrm{E})}{2\pi} > 0$, eq. (7.23) can be formally inverted to yield E as a function of $\hbar$ and of k: $\mathrm{E}_k(\hbar)$ is the kth eigenvalue.

We can clarify somewhat the relation of Eq. (7.23) to the spectrum of $\hat{\mathrm{H}}$. Eq. (7.23) expresses the consistency of the metaplectic representation:

it *must* hold if E is in the spectrum of $\hat{H}$, because then $\psi \in \mathcal{S}'^{\mathbb{C}}(\mathcal{H})$ (on the other hand if E is not in the spectrum, any solution of $\hat{H}\psi = E\psi$ in one dimension will have an exponentially increasing branch at infinity, hence $\psi \notin \mathcal{S}'^{\mathbb{C}}(\mathcal{H})$: so ψ lies outside of the domain of $i\mathrm{Mp}(\mathcal{H})$, in which case the whole § 4.9 is irrelevant). Conversely, if the spectrum of $\hat{H}$ is simple and if all eigenvectors are WKB vectors, then the spectrum spacing is $\mathcal{O}(\hbar)$ by (7.23), and in that case each semi-classical eigenvalue approximates a true eigenvalue [*4*] [*56*] modulo $\mathcal{O}(\hbar^2)$; then each solution of (7.23) must be an eigenvalue, modulo $\sigma(\hbar^\infty)$.

More generally, a quantization condition along a curve $\{ \mathcal{R}(t) \}$ (satisfying the condition C) is needed when this curve is *closed*, to ensure that the 1-form $(- \hat{\varphi}(t)\psi^{\mathcal{R}(t)}_{\mathrm{WKB}})\,dt\,(= i\hbar\, d\psi^{\mathcal{R}(t)}_{\mathrm{WKB}})$ is exact on $\{ \mathcal{R}(t) \}$; such a condition depends only on the homotopy class of the curve in $\mathcal{F}$; and it will only concern the phase of ψ, since the modulus $|\psi^{\mathcal{R}(t)}| = \sqrt{\alpha_0^{\mathrm{R}(t)}}$ automatically returns to its initial value $(\alpha_0^{\mathrm{R}(2\pi)} = \alpha_0^{\mathrm{R}(0)})$ because the curve $\{ \mathrm{R}(t) \}$ is closed). The explicit quantization condition (7.23) is thus obtained from the closed curve formed by the horizontal lift-up $\{ \mathcal{R}(\theta) \}_0^{2\pi}$ closed by an arc from $\mathcal{R}(2\pi)$ to $\mathcal{R}(0)$ in the fiber $\mathbb{T}$ above R(0) (fig. 6). If all closed curves $\{ \mathcal{R}(t) \}$ satisfying condition C are homotopic to a point in $\mathcal{F}$, there is no quantization condition (case of the continuous spectrum).

In conclusion, the use of admissible functionals and of the metaplectic representation allows to solve completely, by quadratures, the most general one-dimensional Schrödinger equation, in regular power series of $\hbar$ (we only had to impose some global restrictions to avoid degeneracies and tunneling). All the arguments can also be translated back to the homogeneous theory of section 2 for mathematical applications. Finally, our methods have extensions to multi-dimensional problems, which will be given in a forthcoming article [*62*].

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