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Section A :
Physique théorique.

Semi-classical approximations

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ABSTRACT. — We give a unified presentation of the most common semi-classical approximations to non-relativistic quantum mechanics: the Wigner representation, the WKB-Maslov method and quantization à la Bohr along closed classical paths (Balian-Bloch, Gutzwiller). We start from a simplified, physically oriented version of the symbolic calculus developed by Hörmander, Duistermaat, Leray, ...: it leads to the Wigner method and to a definition of those operators (quantum observables or density matrices) for which the classical limit makes sense. The WKB method applies when the semi-classical density in phase space is supported by a Lagrangian submanifold: for the levels of a separable system this leads to the Bohr-Sommerfeld rules corrected by the Maslov index. We then show that non-separable systems can also be treated in the neighborhood of closed, stable classical, physical paths (or invariant, involutive manifolds more generally): non trivial corrections to the Bohr rules arise, corresponding to quantized transverse fluctuations (as in the rotational spectrum of a nucleus). Each path yields a multiple series of levels which fixes the local structure of the spectrum.

1. INTRODUCTION

In physics a method of solving a quantum problem is usually called semi-classical if it produces the result as a power series in $\hbar$. Empirically,

(1) Attaché de Recherches au C. N. R. S.

the term of lowest order turns out to be related to the trajectories of the classical system and the next power in $\hbar$ is related to the invariant density on the trajectories; higher powers are often too complicated to be computed or interpreted. In spite of their family likeness, these semi-classical expansions are arrived at through very different methods depending on the object considered: geometrical optics, stationary phases, harmonic approximations to the potential, etc. The mathematical theory of differential operators has more unity but it is very abstract and remote from physical considerations. The purpose of this paper is partly to give a unified formulation of various existing methods, and partly to show the physical relevance of the recent mathematical developments, in particular for the quantization of non-separable systems. Thus a part of the paper has to be in review form but it does not claim to completeness nor to full mathematical rigor (the latter can be found in the references of section 3): we have rather stressed the geometrical structure common to all methods and its physical consequences. We begin here by a brief survey.

1) The standard semi-classical equations

Let $\psi \in L^2(\mathbb{R}^l)$ be a solution of the Schrödinger equation in a regular, semi-bounded $(-\infty < c < V(q))$ potential:

$$\left[i\hbar \frac{\partial \psi}{\partial t} + \frac{\hbar^2}{2m} \Delta_q - V(q) \right] \psi(t, q) = 0 \tag{1}$$

If we explicit the modulus and phase as $\psi = ae^{iS/\hbar}$, eq. (1) is equivalent to the system (2):

$$\frac{\partial S}{\partial t} + \frac{(\vec{\nabla} S)^2}{2m} + V = \frac{\hbar^2}{2m} \frac{\Delta a}{a} \tag{2'}$$

$$\frac{\partial(a^2)}{\partial t} + \operatorname{div}\left(a^2 \frac{\vec{\nabla} S}{m} \right) = 0 \tag{2''}$$

Physically (2″) is the continuity equation for the probability density $a^2 = \psi^* \psi$ and its current $a^2 \frac{\vec{\nabla} S}{m} = \frac{\hbar}{2im} \psi^* \vec{\nabla} \psi$, and $\frac{\vec{\nabla} S}{m}(t, q)$ is interpreted as the local velocity field of the flow [1] [2].

2) The semi-classical approximation

If terms of order $\hbar^2$ and higher are neglected, system (2) describes a classical flow of particles without mutual interactions, in the potential V, with action $S = S_0$, invariant density $a^2 = \chi$ and velocity field $v = \dfrac{\overrightarrow{\nabla S_0}}{m}$, satisfying:

$$\frac{\partial S_0}{\partial t} + \frac{(\overrightarrow{\nabla S_0})^2}{2m} + V = 0 \qquad \text{(Hamilton-Jacobi equation [3])} \tag{3'}$$

$$\frac{\partial \chi}{\partial t} + \operatorname{div}\left(\chi \frac{\overrightarrow{\nabla S_0}}{m}\right) = \frac{d\chi}{dt} + \frac{\Delta S_0}{m}\chi = 0\,, \tag{3''}$$

where $\dfrac{d}{dt} = \dfrac{\partial}{\partial t} + v.\nabla$ is the total derivative along the classical path. The « semi-classical » expression $\psi_{\text{cl}} = \sqrt{\chi}e^{iS_0/\hbar}$ solves (1) modulo $\mathcal{O}(\hbar^2)$: e. g. for Cauchy data $\psi(t_0) = \sqrt{\chi^0(q)}\exp\left(\dfrac{iS_0}{\hbar}(t_0, q)\right)$

$$\chi(t, q_t) = \chi^0(q_{t_0})\exp\left(-\int_{t_0}^{t}\frac{\Delta S_0}{m}(t', q_{t'})dt'\right) \tag{4}$$

solves (3″) in terms of the *explicit* classical action S_0 and paths q_t.

The right hand side (RHS) of (2′) can be *exactly* interpreted as an elastic force between the particles of the flow [4]. But we shall use a different, recursive approach.

3) The WKB expansion (2)

Assume that $S = S_0$ but that a is a formal power series (FPS):

$$a \sim \sum_0^{\infty} a_n(i\hbar)^n$$

with $a_0 = \sqrt{\chi}$. The correction terms a_n $(n \geq 1)$ satisfy a recursive set of ordinary differential equations along the classical paths [5]:

$$\left[\frac{\partial a_n}{\partial t} + \frac{\nabla S}{m}.\nabla a_n + \frac{\Delta S}{2m}a_n\right] \equiv \frac{da_n}{dt} + \frac{\Delta S}{2m}a_n = \frac{i\hbar}{2m}\Delta a_{n-1}\,. \tag{5}$$

THEOREM 1. — Assuming the initial data:

$$\psi(t_0, q) \sim \sum_{j\in J}\left(\sum_0^{\infty} a_{jn}^0(q)(i\hbar)^n\right)e^{i\frac{S_j}{\hbar}(t_0,q)}\text{(FPS)} \tag{6'}$$

(2) It is the analog of the « eikonal » in optics, named after Wentzel, Kramers, Brillouin.

where the S_j are *distinct* solutions of (3′) for $j \in J$ (a *finite* set): the Cauchy problem for (1) has the solution:

$$\psi(t, q) \sim \sum_{j \in J} \left(\sum_{0}^{\infty} a_{jn}(t, q)(i\hbar)^n \right) e^{i\frac{S_j}{\hbar}(t,q)} \text{(FPS)} \qquad (6'')$$

where for each j, a_{jn} is obtained by integrating (5) *along the classical paths* corresponding to the action S_j: in short, writing $\chi_j \equiv a_{j0}$:

$$a_{jn}(t) = \sqrt{\frac{\chi_j(t)}{\chi_j(t_0)}}\, a_{jn}^0 + \sqrt{\chi_j(t)} \int_{t_0}^{t} dt' \frac{\Delta a_{j,n-1}(t')}{2m\sqrt{\chi_j(t')}} \qquad (7)$$

(thus the distinct S_j do not interfere).

COROLLARY. — If (6′) holds in the sense of asymptotic series, so does (6″) provided that for all $t' \in [t_0, t]$, and for all j, the $S_j(t')$ remain disconnected solutions of (3′) and all integrands in (7) remain finite, in particular $\chi_j(t') \neq 0$.

Analogous expansions exist for systems [*6*] like the Dirac equation [*7*].

4) The caustic surfaces

They are the envelopes of the classical paths of S. A simple caustic is locally the boundary between a region where S has two branches S_1, S_2 (which join on the caustic) and a region where S is not defined as a real function (forbidden region); and $\frac{1}{\chi}$ has a simple zero at each focal point [*5*] (i. e. a contact point of a path with the caustic). Thus the WKB method breaks down and the semi-classical wave is infinite on the caustic; this follows from high quantum interference between waves with the almost equal phases S_1 and S_2 (Figure 1 shows a caustic of straight paths in two

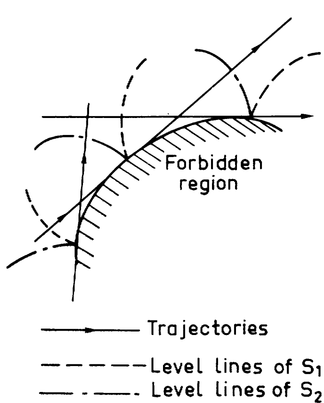

FIG. 1.

dimensions: caustic singularities are *not* related to singularities of the potential).

However the semi-classical wave can be continued beyond the (simple) caustic in the form $\psi_{cl} = \sqrt{|\chi|}\, e^{iS_0/\hbar} e^{-i\pi/2}$. Along a classical path the discrete phase jumps add up to $e^{-in\pi/2}$ where n is the number of focal points encountered (for a geodesic flow, n is the Morse index of the path [8]).

5) Uniform semi-classical methods (3)

Uniform semi-classical methods are those which are also applicable *on* and *beyond* caustics. They are necessary whenever the difficulties due to caustics must be overcome (e. g. to compute energy levels and eigenstates). All uniform methods are obtainable by representing the quantum problem in classical *phase space*, where the classical flow, being incompressible, cannot have caustics (cf. section 4). Such a realization, in a form invariant by canonical transformations of phase space, exhibits the unity of all methods.

The *Wigner* method [9] (section 4) approximates, in an « algebra of observables » framework, quantum observables (resp. states) by classical observables (resp. states), with weak convergence (of expectation values) as $\hbar \to 0$.

The *Maslov* method [*10*] [*11*] [*12*] (section 5) defines Hilbert spaces in which wave functions of the WKB type can be followed as $\hbar \to 0$. The Hilbert space structure allows us to look for semi-classical eigenstates and energy levels: the latter are given by Bohr-Sommerfeld rules corrected by the « Maslov index ». But practically only separable systems can be treated in this way. The representation in phase space makes a crucial use of the invariant Lagrangian submanifolds of phase space.

In section 6 we take a look at geometric quantization from a similar point of view.

For a non-separable system admitting closed stable paths (or invariant manifold of higher dimensions), we show in section 7 how the Maslov method can be explicitly applied to yield energy levels and eigenfunctions, provided the transverse fluctuations of the system are approximated by their quadratic (harmonic) parts. Each closed path yields a multiple series of levels involving the angles of rotation (or characteristic exponents [*14*]) and a generalization of the Maslov index. These results extend previous results relating quantization and closed paths (refs. [*15*] to [*19*]).

Since the completion of this article, we have in addition obtained the

(3) We shall not look at higher powers of $\hbar$ which are not determined by classical dynamics alone.

full $\hbar$-expansions of the quantum bound states described herein (articles in preparation, and [*54*]).

We have omitted several important topics such as the Feynman path integral [*19*], the stochastic methods [*20*], analytic function methods [*21*] and the hydrodynamical picture [*4*]. For an extensive review with a complete bibliography, see ref. [*22*].

2. CLASSICAL MECHANICS

We give a short summary of canonical mechanics in the framework of a cartesian phase space with a Hamiltonian flow [*23*] [*24*] [*25*], assuming C^∞ smoothness everywhere. More general phase spaces (symplectic manifolds) are sometimes useful [*24*] but they pose global problems, mostly unsolved, for quantization (examples in section 6).

1) Notations

We often follow ref. [*22*].

Configuration space $\mathscr{Q} = \mathbb{R}^l$; momentum (dual) space $\mathscr{P} = \mathscr{Q}^*$.

Phase space $M = \mathscr{Q} \oplus \mathscr{P}$ with points $x = (q, p)$. We let:

$C^\infty(M)$ = algebra of real-valued functions on M (called *observables*),

$\mathscr{X}(M)$ = space of vector fields on M (a vector field X defines a Lie derivative L_X and a 1-parameter semi-group of mappings U_t^X),

$\Omega^p(M)$ = space of differential forms on M of degree p (p-forms).

2) The canonical form

$\omega = \sum_1^l dp_i \wedge dq^i$ (in short, $dp \wedge dq$). Derived notions:

a) *Define*: $\mathscr{X}(M) \xrightarrow{b} \Omega^1(M)$ by $(b(X_1))(X_2) \equiv \omega(X_1, X_2)$.

In coordinates $x = \begin{pmatrix} q \\ p \end{pmatrix}$, b has the matrix $J = \begin{pmatrix} 0 & 1_l \\ -1_l & 0 \end{pmatrix}$; ω is non-degenerate (i. e. $\sharp = b^{-1}$ exists) and closed ($d\omega = 0$): it is a *symplectic form.*

b) *Canonical transformation*: a mapping $M \xrightarrow{U} M$ preserving ω.

For $X \in \mathscr{X}(M)$, U_t^X is canonical ($\forall t$) iff $L_X\omega \equiv 0$.

Linear canonical maps on M form a sub-group $Sp(l)$ of $GL(2l)$ called the symplectic group [*11*] [*13*]. In matrix form $U \in Sp(l)$ iff ${}^tUJU = J$; the eigenvalues of U come in pairs $(\lambda, \lambda^{-1})_{\lambda\in\mathbb{R}}$ or $(e^{i\theta}, e^{-i\theta})_{\theta\in\mathbb{R}}$, or in quadruples $(\lambda, \bar\lambda, \lambda^{-1}, \bar\lambda^{-1})_{\lambda\in\mathbb{C}}$. The Lie algebra $sp(l)$ is the set of matrices A such that ${}^tAJ + JA = 0$ [*23*]. It has dimension $l(2l + 1)$.

c) *Canonical orientation:* every space $\mathbb{R}_k^2$ (spanned by q^k and p_k) is oriented by the volume $\omega_k = dp_k \wedge dq^k$.

d) *Symplectic gradient:* for $f \in C^\infty(M)$ let:

$$\nabla_\omega f = \sharp(df) \qquad (= (\nabla_p f, - \nabla_q f)).$$

e) *Poisson brackets:* $C^\infty(M)$ is a Lie algebra for:

$$\{ f, g \} = L_{\nabla\omega g} f = - L_{\nabla\omega f} g = \sum_1^l \left(\frac{\partial f}{\partial q^k} \frac{\partial g}{\partial p_k} - \frac{\partial f}{\partial p_k} \frac{\partial g}{\partial q^k} \right). \tag{8}$$

3) The canonical volume

$$\Omega = \frac{(-1)^{[l/2]}}{l!} \omega^{\wedge l} = \left(\bigwedge_1^l dp_i \right) \wedge \left(\bigwedge_1^l dq^i \right).$$

where $[l/2]$ = integer part of $l/2$. Derived notions:

a) *Determinant* (jacobian) of a mapping $M \xrightarrow{U} M$: the scalar function defined by $U^*\Omega = (\det_\Omega U)\Omega$.

b) *Divergence* (trace) of $X \in \mathscr{X}(M)$: the scalar function defined by: $L_X\Omega \equiv (\operatorname{div}_\Omega X)\Omega$; the identity:

$$\frac{d}{dt}(\det_\Omega U_t^X)_{t=0} = \operatorname{div}_\Omega X \tag{9}$$

implies that U_t^X is volume-preserving *(incompressible)* iff $\operatorname{div}_\Omega X \equiv 0$. A canonical transformation is always volume-preserving.

4) A special class of canonical transformations

We introduce the following notations for subsets K, H, ... of $Q = \{ 1, 2, \ldots, l \}$: $P = \emptyset$; $|K| = \operatorname{card} K$; $K' = \complement K$; $K - H = K \cap H'$; $K \,\Delta\, H = (K - H) \cup (H - K)$ (a group operation). Following Leray [12]; we introduce canonical transformations exchanging the configuration and momentum coordinates in some spaces $\mathbb{R}_k^2$; for any mapping U of $\mathbb{R}^2$, let U_K be the product of U on all spaces $\mathbb{R}_k^2$ ($k \in K$) and of the identity on all spaces $\mathbb{R}_{k'}^2$ ($k' \in K'$).

If now U is the rotation by $\left(+\frac{\pi}{2}\right) : \begin{pmatrix} q \\ p \end{pmatrix} \to \begin{pmatrix} +p \\ -q \end{pmatrix}$: $(\forall K)\ U_K \in Sp(l)$, and:

$$U_K U_L = U_L U_K = (-1)_{K \cap L} U_{K \Delta L}. \tag{10}$$

Denote by $\begin{pmatrix} t_K \\ s_K \end{pmatrix}$ the *ordered* set of coordinates obtained by the action of $U_{K'}$ on the original coordinates $\begin{pmatrix} q \\ p \end{pmatrix}$:

$$t^j_K = q^j \quad \text{if} \quad j \in K, \qquad t^j_K = p_j \quad \text{if} \quad j \in K'.$$
$$s^j_K = p_j \quad \text{if} \quad j \in K, \qquad s^j_K = -q^j \quad \text{if} \quad j \in K'.$$

The 1-forms $\theta_K = \sum_1^l s^j_K dt^j_K$ satisfy $d\theta_K = \sum ds^j_K \wedge dt^j_K = \omega$ and:

$$\theta_K - \theta_H = d\Big(\sum_{K-H} p_j q^j - \sum_{H-K} p_j q^j\Big) \tag{11}$$

5) **Lagrangian manifolds** [*10*]

A Lagrangian subspace is a vector subspace of M, isotropic for ω, maximal (i. e. of rank l); a submanifold $\Lambda \subset M$ is called Lagrangian if its tangent space at any $x \in \Lambda$, $T_x(\Lambda)$ is Lagrangian; or equivalently: $\dim \Lambda = l$ and:

$$\omega|_\Lambda \equiv 0$$

A Lagrangian manifold is stable by canonical transformations. We now provide two descriptions of connected Lagrangian manifolds.

a) *The* K-*charts* : define the projections $x = \begin{pmatrix} q \\ p \end{pmatrix} \in \Lambda \begin{smallmatrix} \xrightarrow{\pi_Q} q \in \mathcal{Q} \\ \xrightarrow{\pi_P} p \in \mathcal{P} \end{smallmatrix}$; π_Q is locally 1-1 except on the *singular set* $\Sigma_Q \subset \Lambda$ (fig. 2):

$$\Sigma_Q = \{ x \in \Lambda \mid \dim (T_x(\Lambda) \cap \mathcal{P}) > 0 \} = \{ x \in \Lambda \mid (dq^1 \wedge \dots \wedge dq^l)|_\Lambda = 0 \}.$$

On any connected open set $V \subset \Lambda - \Sigma_Q$, Π_Q defines a local chart which we call Q-chart; V is the graph of the vector field $q \in \Pi_Q(V) \xrightarrow{\Pi_P \Pi_Q^{-1}} p$

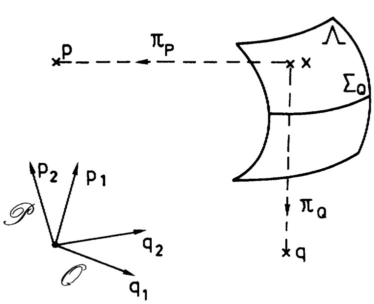

FIG. 2. — $l = 2$; it is impossible to show graphically the Lagrangian property $\omega|_\Lambda = 0$.

and (12) is equivalent to: curl $p \equiv 0$. Define the *Q-generating function of* Λ, $S_Q(q)$, by: $p = \nabla_q S_Q$, i. e. $S_Q(q) = \int_{x_0}^{x \in \Pi_Q^{-1}(q)} \sum p_i dq^i$ integrated along any curve on Λ of arbitrary fixed origin x_0. The integral is one-valued on the universal covering $\tilde{\Lambda}$ of Λ; we assume the homotopy group $\Pi_1(\Lambda) = \tilde{\Lambda}/\Lambda$ to be free and we choose independent generating cycles γ_i: then the integral is defined on Λ, modulo the set of constants $\left\{ \sum n_i \alpha_i \right\}_{n_i \in \mathbb{Z}}$ where $\alpha_i = \oint_{\gamma_i} pdq$ (changing x_0 adds an irrelevant overall constant); moreover S_Q has several branches (their number will always be assumed *finite*) according to the choice of $x \in \Pi_Q^{-1}(q)$: those branches connect two by two on $\Pi_Q(\Sigma_Q)$.

Similarly, for any $K \subset \{ 1, \ldots, l \}$ we define the K-chart by:

$$x \in \begin{pmatrix} t_K \\ s_K \end{pmatrix} \in (\Lambda - \Sigma_K) \overset{\Pi_K}{\rightarrow} t_K$$

($\in$ « K-space ») and the *K-generating function*:

$$S_K(t_K) = \int_{x_0}^{x \in \Pi_K^{-1}(t_K)} \theta_K \tag{13}$$

which has the same ambiguity as S_Q since $\oint_{\gamma_i} \theta_K = \alpha_i$.

The K-charts form an atlas of Λ (proof in ref. [*10*]). The coordinate transformation from the K-chart to the H-chart is:

$$t_H = \Pi_H \Pi_K^{-1} t_K \,. \tag{14}$$

(11) and (13) imply:

$$S_H(t_H) = S_K(t_K) - \left(\sum_{K-H} p_j q^j - \sum_{H-K} p_k q^k \right) = S_K(t_K) - \sum_{K \Delta H} s_K^j t_K^j \,. \tag{15}$$

In terms of S_K and S_H, (14) is equivalent to:

$$\begin{array}{lll} \text{if } j \notin K \,\Delta\, H & t_H^j = t_K^j & \\ \text{if } j \in K - H & \dfrac{\partial S_K}{\partial t_K^j} = t_H^j & \left(\Leftrightarrow \dfrac{\partial S_H}{\partial t_H^j} = - t_K^j \right) \\ \text{if } j \in H - K & \dfrac{\partial S_K}{\partial t_K^j} = - t_H^j & \left(\Leftrightarrow \dfrac{\partial S_H}{\partial t_H^j} = t_K^j \right). \end{array} \tag{16}$$

(15) and (16) describe a partial *Legendre transformation* noted: $S_H(t_H) = \mathscr{L}_H^K S_K(t_K)$. The symbols $\mathscr{L}_H^K$ satisfy:

$$\mathscr{L}_L^K \mathscr{L}_K^H = \mathscr{L}_L^H, \qquad \mathscr{L}_K^K = \text{identity} \,. \tag{17}$$

Conversely to any family $\{ S_K \}$ with $S_H = \mathscr{L}_H^K S_K$ we can associate *one* Lagrangian manifold Λ of equations $\partial S_K/\partial t_K = s_K$ for all K-charts.

b) *Phase equations:* if Λ is defined by l equations $\{ F_j(x) = 0 \}$ in M (with independent $dF_j's$ in a neighborhood of Λ) then (12) holds iff: $\forall j, k$, $\forall x \in \Lambda$ $\{ F_j, F_k \} = 0$. If moreover the $F_j's$ are l observables in *involution*, i. e.

$$\forall j, k, \quad \forall x \in M : \{ F_j, F_k \} (x) = 0 \tag{18}$$

the equations $\{ F_j = \alpha_j \text{ (constant)} \}$ define an l-parameter family of Lagrangian manifolds $\{ \Lambda_\alpha \}$ which fill (a domain of) phase space; this is called a polarization, or Lagrangian foliation, of M. Each Λ_α admits a canonical volume η_α which is the pull-back of Ω, normalizable to 1 if Λ_α is compact: $\eta_\alpha = C\delta(F_1 - \alpha_1) \ldots \delta(F_l - \alpha_l).\Omega$, i. e.

$$(dF_1 \wedge \ldots \wedge dF_l) \wedge \eta_\alpha = C.\Omega . \tag{19}$$

By projection on any K-chart we obtain η_α in the t_K coordinates:

$$(\Pi_K)_* \eta_\alpha = C \frac{D(s_K^1 \ldots s_K^l)}{D(F_1, \ldots, F_l)} (dt_K^1 \wedge \ldots \wedge dt_K^l) \tag{19'}$$

and the Jacobian vanishes on $\Pi_K(\Sigma_K)$.

6) Hamiltonian mechanics

An energy function $H(x)$ is given over M (or a domain of M). The *classical* paths are the integral curves of the *Hamiltonian vector field* $X = \nabla_\omega H$, i. e. the *Hamiltonian flow* U_t^X satisfies:

$$\frac{dU_t^X}{dt} = \sharp dH \qquad (\Leftrightarrow \dot{q} = \nabla_p H \text{ and } \dot{p} = - \nabla_q H) \tag{20}$$

For any observable f, (8) implies:

$$\dot{f} \text{ (i. e. } L_X f) = \{ f, H \} \tag{21}$$

The flow U_t^X is *canonical* (proof: (20) implies $\dot{\omega} = d\dot{p} \wedge dq + dp \wedge d\dot{q} \equiv 0$) therefore *incompressible* (Liouville's theorem).

7) The time-independent Hamilton-Jacobi theory

Let Λ be a Lagrangian manifold contained in the energy shell $\hat{\Sigma}_E = H^{-1}(E) \subset M$. We consider such Λ as *generalized solutions* of the time-independent Hamilton-Jacobi equation, since in the Q-chart, wherever S_Q is defined it does satisfy:

$$H(q, \nabla_q S_Q) = E \tag{22}$$

THEOREM 2. — *a*) Any classical trajectory intersecting Λ lies in it; thus Λ

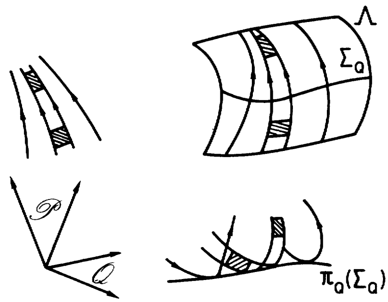

FIG. 3. — Striped areas represent invariant volume elements in tubes of paths.

is generated by classical trajectories, on the energy shell $\hat{\Sigma}_E$, of a stationary flow (fig. 3).

b) If γ is a classical path in Λ, then for variations $\tilde{\gamma}$ of γ in $\hat{\Sigma}_E$, with fixed endpoints, the integral $\int_{\tilde{\gamma}} \sum p_i dq^i$ is stationary at $\tilde{\gamma} = \gamma$ and equal to S_Q (+ const).

Proof. — *a*) It suffices to prove that if a trajectory $\gamma(t)$ meets Λ at x, then $d\gamma/dt\,|_x \in T_x(\Lambda)$. In the Q-chart (but this is chart-independent), (22) implies

$$0 = \nabla_q H + \nabla^2_{q^2} S_Q . \nabla_p H \quad \text{but by (20) the RHS is} \quad \left(- \frac{dp}{dt} + \nabla^2_{q^2} S_Q \frac{dq}{dt} \right),$$

proving the result. Every $x \in \Lambda$ is the initial point of a classical path, and all these paths, travelled along according to (20), form a stationary flow on Λ. If the flow is ergodic on Λ, any single dense trajectory generates Λ (by taking the closure).

b) is in all textbooks [*3*] (the Maupertuis principle); S_Q is known as the time-independent (« reduced ») action.

8) The time-dependent Hamilton-Jacobi theory

To investigate non stationary problems in a similar framework, we add time and energy coordinates to M to obtain an extended phase space $\tilde{M} \sim \mathbb{R}^{2l+2}$ with the symplectic form $\tilde{\omega} = - dE \wedge dt + \sum_1^l dp_i \wedge dq^i$.

Let $\tilde{\Lambda}$ be a Lagrangian manifold in $\tilde{M}$ ($\Leftrightarrow$ dim $\tilde{\Lambda} = l + 1$ and $\tilde{\omega}\,|_\Lambda \equiv 0$), contained in the hypersurface $\{ H(q, p) - E = 0 \}$. In the (t, Q)-chart $S(t, q) = \int pdq - Edt$ satisfies the Hamilton-Jacobi equation:

$$\frac{\partial S}{\partial t} + H(q, \nabla_q S) = 0 \tag{23}$$

As before, Λ is generated by classical trajectories, along which the action is extremal and equal to $S(t, q)$ (+ const.). Moreover, time evolution is given by:

THEOREM 3. — The projection on M of $\tilde{\Lambda} \cap \{ t = t_0 \}$ is a Lagrangian manifold $\Lambda_{t_0} \subset M$ which is transported (with time t_0) by the flow U_{t_0} satisfying the laws of motion (20).

The same $\tilde{\Lambda}$ seen in the (E, Q)-chart has the generating function:

$$S(E, q) = [S(t, q) + Et]_{\frac{\partial S}{\partial t} = -E}$$

This is the reduced action for all values of E, and indeed the time-independent theory can be entirely recovered by this change of chart (which is a Legendre transformation).

9) Explicit examples

The ultimate (but generally hopeless) solution of a Hamilton-Jacobi equation is a *complete integral* [*3*] [*26*], i. e. some subfamily of solutions $\{ S_\alpha \}_{\alpha \in \mathbb{R}^l}$ for which any other solution is one of its envelopes ([4]). The time-independent theory is completely integrable if there exist l observables $F_1 = H, \ldots, F_l$ in involution (eq. (18)): on $\Lambda_\alpha = \{ F_j(q, p) = \alpha_j \}_{\alpha \in \mathbb{R}^l}$ (cf. § 5 *b*) we can express p as a function of q and α; then the Q-generating function of Λ_α:

$$S_\alpha = \int_{\Lambda_\alpha} p dq = \int p(q\,; \alpha) dq \tag{24}$$

can be computed by quadratures and is a suitable complete integral. Examples:

a) free particle ($l = 3$) with spherical wave fronts:

$$(t > t_0) \qquad S(t, q) = \frac{m(q - q_0)^2}{2(t - t_0)} \qquad S(E, q) = \sqrt{2mE}\,|\,q - q_0\,| \tag{25}$$

b) The same with plane wave fronts:

$$S(t, q) = p.q - \frac{p^2}{2m} t \qquad S(E, q) = p.q\left(\frac{p^2}{2m} = E\right) \tag{26}$$

c) 1-dimensional harmonic oscillator of frequency $\frac{\omega}{2\pi}$:

$$S(t, q) = \frac{m\omega}{2 \sin \omega(t - t_0)} \left[\cos \omega(t - t_0)(q^2 + q_0^2) - 2q.q_0\right]$$

$$\left(0 < t - t_0 < \frac{\pi}{\omega}\right) \tag{27}$$

([4]) Ref. [*26*] stresses the importance for partial differential equations of envelope techniques (such as the Legendre transformation).

It is worth mentioning that the mapping U_t is the elliptic rotation around the origin by the angle $+\omega t$; this rotation is uniform with angular velocity ω. Conversely any elliptic symplectic map in $\mathbb{R}^{2l}$ (see section 7) can be interpreted as the action during a finite time of a harmonic oscillator; each normal mode gives an independent rotation in a 2-dimensional plane [*13*].

The reduced action is:

$$S(E, q) = \frac{E}{\omega} \operatorname{Arcsin}\left(\sqrt{\frac{m}{2E}}\,\omega q\right) + \sqrt{\frac{mE}{2}}\, q \sqrt{1 - \frac{m\omega^2 q^2}{2E}} \tag{28}$$

d) In general we can solve (22) or (23) in powers of the coupling constant, with $S = \sum_0^\infty S_n$: S_0 is a given solution of the free equation: the S_n's are then obtained by successive integrations along the *unperturbed* paths.

3. SYMBOLIC CALCULUS ON DIFFERENTIAL OPERATORS

1) Introduction

Let P be a linear differential operator (LDO); in multi-index notation:

$$P(q, D) = \sum_{|\alpha| \leq m} A_\alpha(q) D^\alpha \tag{29}$$

where $q \in \mathbb{R}^l$, $D^\alpha = \dfrac{i^{|\alpha|}\, \partial^{|\alpha|}}{\partial q_1^{\alpha_1} \ldots \partial q_l^{\alpha_l}}$, and the A_α are real and C^∞.

The highest order terms form the principal symbol [*28*] of P:

$$P_m(q, p) = \sum_{|\alpha| = m} A_\alpha(q) p^\alpha, \qquad (p \in \mathbb{R}^l). \tag{30}$$

Possible discontinuities of solutions of $Pu = 0$ are studied with the ansatz [*6*]

$$u \sim \sum_0^\infty a_j(q) f_j(\varphi(q)), \tag{31}$$

where $f_0(\varphi)$ is arbitrary, and for $j \geq 1$: $\dfrac{df_j}{d\varphi} \equiv f_{j-1}$ (the f_j's form a sequence of increasingly smoother functions). For instance $f_j = \dfrac{e^{i\omega\varphi}}{(i\omega)^j}$ will describe high frequency waves and (31) will then define u up to terms of rapid decrease in ω ; another choice: $f_j = \frac{(\varphi - s)_+^j}{j!} \left(= \theta(\varphi - s) \frac{(\varphi - s)^j}{j!} \right)$ will describe waves discontinuous across the hypersurface $\{ q \in \varphi^{-1}(s) \}$, and then (31) will describe u up to terms C^∞ across that hypersurface; in all cases the algebra is the same.

Substitution of (31) into $Pu = 0$ and identification in the f_j's yields:

$$P_m(q, \nabla_q \varphi) = 0 \tag{32'}$$

$$\nabla_p P_m(q, \nabla_q \varphi) . \nabla_q a_j + C a_j = K_j(a_0, \ldots, a_{j-1}) \tag{32''}$$

where the scalar function C and the LDO's K_j depend on the A_α's and on the function φ chosen among the solutions of (32').

Eq. (32') expresses the fact [26] that in Q-space the surfaces $\{ \varphi = \text{const.} \}$ must be *characteristic*. Then, by the Euler equation:

$$\nabla_q \varphi . \nabla_p P_m(q, \nabla_q \varphi) = m P(q, \nabla_q \varphi) \qquad (= 0 \text{ by eq. } (32'))$$

the so-called *characteristic curves* $q(t)$, solutions of

$$\frac{dq}{dt} = \nabla_p P_m(q, \nabla_q \varphi) \tag{33}$$

lie in the surfaces $\{ \varphi = \text{const.} \}$, which they generate thereby.

A solution φ of (32') is also the Q-generating function of a Lagrangian manifold in phase space $\Lambda \subset P_m^{-1}(0)$. The curves in phase space, solutions of

$$\frac{dq}{dt} = \nabla_p P_m(q, p) \qquad \frac{dp}{dt} = - \nabla_q P_m(q, p) \tag{34}$$

are called *bicharacteristic*; their projections on $\mathcal{Q}$ are characteristic curves; and moreover they generate Λ (cf. theorem 2 and fig. 3).

We recognize in (32') the Hamilton-Jacobi equation of the « hamiltonian » P_m; (34) defines the classical trajectories; eq. (32'') just states that the amplitude of a discontinuity is *transported along the classical paths* by some formula like (7).

2) The Wigner symbol

In order to generalize the preceding results, it is convenient to compute the action of an operator like $P(q, D)$ by means of an associated scalar function called its *symbol*.

Given an integral operator A:

$$(A\psi)(q) = \int_{\mathbb{R}^l} a(q, q')\psi(q')dq' \tag{35}$$

we formally define its *Wigner symbol* [9] $A_w(q, p)$ by any one of the equivalent formulae:

$$A_w(q, p) = \int dr e^{ipr} a\left(q - \frac{r}{2}, q + \frac{r}{2}\right) = \int \frac{dk}{(2\pi)^l} e^{-ikq} \tilde{a}\left(p - \frac{k}{2}, p + \frac{k}{2}\right) \quad (36')$$

$$a(q, q') = \int \frac{dp}{(2\pi)^l} A_w\left(\frac{q + q'}{2}, p\right) e^{i(q-q')p} \quad (36'')$$

$$A = \int d\xi d\eta e^{i(\xi Q + \eta P)} \tilde{A}_w(\xi, \eta) \quad (37)$$

where

$$\tilde{a}(p, p') = \int e^{-i(pq - p'q')} a(q, q') dq dq' \quad (38)$$

$$A_w(q, p) = \int e^{i(\xi q + \eta p)} \tilde{A}_w(\xi, \eta) d\xi d\eta \quad (39)$$

and Q and P are operators with kernels:

$$Q(q, q') = q\delta(q - q') ; \qquad P(q, q') = -i\delta'(q - q')$$

satisfying the Heisenberg commutation rules: $[Q^j, P_k] = i\delta^j_k \mathbb{1}$; (37) holds in the weak topology (equality of matrix elements).

The reciprocal operation $A_w \to A$, or the passage from (39), where q and p commute, to (37), is called the *Weyl quantization.* It is reality-preserving since it associates hermitian operators to real symbols [27].

To begin with, we define (36) for $\psi \in L^2(\mathbb{R}^l)$ and $A \in HS(\mathbb{R}^l)$ (the Hilbert space of Hilbert-Schmidt operators) with the scalar product:

$$\langle B, A \rangle_{HS} = \operatorname{Tr} B^\dagger A = \int b^*(q, q') a(q, q') dq dq' .$$

The Plancherel theorem tells us that $(A \to A_w)$ is a *unitary isomorphism* of $HS(\mathbb{R}^l)$ onto $L^2\left(\mathbb{R}^{2l}, \frac{dqdp}{(2\pi)^l}\right)$, so that for $A, B \in HS(\mathbb{R}^l)$:

$$\operatorname{Tr} B^\dagger A = \int \frac{dqdp}{(2\pi)^l} B^*_w(q, p) A_w(q, p) . \quad (40)$$

But Fourier transformation works for other spaces too. In quantum theory using algebras of observables, B is restricted to be of trace class and A runs over the dual space of bounded operators; then :

$$\operatorname{Tr} B = \int \frac{dqdp}{(2\pi)^l} B_w(q, p') \quad (41)$$

but otherwise symbolic calculus is very difficult in this frame [29]: the author knows no necessary and sufficient condition ensuring that a symbol belongs to a trace-class (resp. bounded; resp. positive ([5])) operator. A convenient framework for symbolic calculus and classical limits is obtained by restricting the symbols of observables A_w to certain spaces of test functions (with some freedom of choice for the space) and letting B_w run over the dual space of distributions. Thus, the symbol of an LDO like P in (29) is a polynomial in p, and eqs. (32) to (34) show that the principal symbol (30) governs the propagation of discontinuities for distributions u such that $Pu = 0$ (or similarly $Pu \in C^\infty$). Mathematically, the computation of discontinuities for such problems amounts to solving equations like

$$Au = f. \tag{42}$$

(A: integral operator; u, f: distributions) « modulo C^∞ », i. e. writing off all smooth ($= C^\infty$) contributions to u, f, and to the kernel of A, i. e. omitting all rapidly decreasing (as $|p| \to \infty$) terms in the symbol of A (for a consistent and rigorous exposition, see ref. [*28*]). Having considerably relaxed the problem as compared to solving (42) exactly, we can enlarge the class of A in (42) from LDO's to linear *pseudo-differential operators* (PDO), characterized (modulo terms of rapid decrease in p, which *escape investigation* in the present approach) by a C^∞ symbol asymptotic to a sum of the form:

$$A_w(q, p) \sim \sum_{n=0}^{\infty} a_{m-n}(q, p) \tag{43}$$

where a_r is homogeneous of degree r in p, a_m (called *principal symbol*) is not identically 0; m (a real number) is the order of A.

The product of two operators *formally* satisfies Groenewold's rule, where $\overleftrightarrow{\Lambda}$ stands for the two-sided differential operator $(\overleftarrow{\nabla}_q \overrightarrow{\nabla}_p - \overleftarrow{\nabla}_p \overrightarrow{\nabla}_q)$:

$$(AA')_w = A_w \exp\left(\frac{i}{2}\overleftrightarrow{\Lambda}\right)A'_w = A_w A'_w + \frac{i}{2}\{ A_w, A'_w \} + \dots . \tag{44}$$

If A and A′ are PDO's of principal symbols a_m and $a'_{m'}$, (44) gives an asymptotic expansion of the type (43), so that AA′ is a PDO (modulo C^∞), of principal symbol $a_m a'_{m'}$ if $a_m a'_{m'} \not\equiv 0$. Moreover, if A is *elliptic* (i. e. $a_m(q, p) \neq 0$ $\forall p \neq 0$), it has a PDO inverse A^{-1} : $AA^{-1} = 1$ [mod C^∞] $= A^{-1}A$ with:

$$(A^{-1}) = E\left(\sum_0^\infty (1 - AE)^n\right) \qquad \text{[FPS]}$$

where $E_w = \dfrac{1}{a_m}$ so that:

$$(A^{-1})_w = \frac{1}{a_m(q, p)} + 0(|p|^{-m-1})$$

([5]) Positive operators of trace 1 are used as quantum density matrices.

3) Other symbols

We just mention that other orderings are possible in eq. (37), changing the correspondance (operator $\leftrightarrow$ symbol). For instance Hormander's symbols [28] have the (non-hermitian) definition:

$$A = \int \frac{d\xi d\eta}{(2\pi)^l} e^{i\xi Q} e^{i\eta P} A_w(\xi, \eta) \tag{37'}$$

while Wick ordering in suitable units $\left(\alpha = \dfrac{Q + iP}{2}, \alpha^{\dagger} = \dfrac{Q - iP}{2}\right)$ uses

$$A = \int \frac{d\xi d\eta}{(2\pi)^l} e^{i(\xi + \eta)\alpha^{\dagger}} e^{i(\xi - i\eta)\alpha} A_w(\xi, \eta) \tag{37''}$$

Wick ordering always refers to some fondamental mode whose frequency fixes the scale between Q and P. For a general non-relativistic problem there is no preferred mode; we shall use the more intrinsic Weyl quantization. We note that under changes of ordering, symbols obey transformation rules which leave principal symbols *invariant.*

4) The characteristic set

The characteristic set of a PDO A of order m is defined as the subset $\gamma(A) = a_m^{-1}\{0\} \subset M - \{p = 0\}$; it is closed and conical in the p variables (in physics $\gamma(A)$ is the union over points $q \in \mathcal{Q}$ of the « momentum light cones » at q).

5) The C^∞ singular spectrum

The C^∞ singular spectrum of a distribution $f \in \mathcal{D}'$ is the closed, conical (in p) subset $SS(f) \subset M - \{p = 0\}$, defined ([6]) as follows. We call $\mathcal{D}_{q_0}$ the set of functions in $C_0^\infty(\mathcal{Q})$ equal to 1 in a neighborhood of q_0, and we write $(f \otimes \mu)(q, q') = f(q)\mu(q')$. Then:

$$(q_0, p_0) \notin SS(f) \Leftrightarrow (f \otimes \mu)_w(q_0, \lambda p) = o\left(\frac{1}{\lambda^N}\right) \qquad \forall N$$

when $\lambda \to +\infty$, for some $\mu \in \mathcal{D}_{q_0}$ and for all p in some neighborhood of p_0. An equivalent definition is [28]:

$$SS(f) = \bigcap_{A | Af \in C^\infty} \gamma(A) \qquad (A \text{ is any PDO such that } Af \in C^\infty).$$

The set $SS(f)$ describes how f deviates from C^∞ smoothness; outside of

([6]) Also called « wave front set of f », in short $WF(f)$.

the projected set Π_Q (SS(f)) = sing supp $f \subset \mathcal{Q}$ (*singular support* of f), the distribution f is actually C^∞.

THEOREM 4 (regularity theorem). — If P is a real PDO of order m with a *simple* characteristic set (i. e. $\forall x \in \gamma(P) : dp_m(x) \neq 0$), then for all $u \in \mathcal{D}'$, $f \in \mathcal{D}'$ with $Pu = f$: $SS(u) \subset SS(f) \cup \gamma(P)$, and $SS(u) - SS(f)$ is *invariant by the Hamiltonian flow in* M *of the principal symbol* p_m.

A very special case of singular spectrum occurs when f is only singular across an isolated hypersurface of equation $\varphi(q) = s$ (all this: locally); then: $SS(f) \subset \{ (q, \lambda.\nabla\varphi) \in M \mid q \in \varphi^{-1}(s), \lambda \neq 0 \}$; such a singular spectrum belongs for instance to a function u given by (31) with $f_j = (\varphi - s)^j_+/j\,!$, or to a WKB wave of quantum mechanics (in the homogeneous variables of eq. (45)); eq. (32) provide a quantitative description of theorem 4. Unfortunately we shall see in 5, § 9 that if f is a solution in a bounded domain of a Helmholtz-type equation, we cannot expect in general SS(f) to have such a simple structure.

4. THE WIGNER CLASSICAL LIMIT

The formalism of section 3 can be applied without change to Maxwell's equation in an inhomogeneous medium (wave optics) and yields geometrical optics: bicharacteristics (light rays) satisfying the Fermat principle.

1) For quantum mechanics,

however, we must first change the form of the differential operator, to ensure that all terms will have the same weight in the classical limit, irrespective of their order as derivatives. The equation (whichever it is) is homogeneized by the substitution $\frac{1}{\hbar} = i\frac{\partial}{\partial s}$; for instance (1) becomes:

$$\left[\frac{\partial^2}{\partial s \partial t} - \frac{\Delta}{2m} - V(q)\frac{\partial^2}{\partial s^2}\right]\psi(s, t, q) = 0 \tag{45}$$

the classical limit is then the high frequency (in « proper time » s) limit, or the limit of geometrical optics in $(l + 2)$ dimensions: we have there an extended phase space $\check{M} = \{ (s, t, q, \lambda, \check{E} = \lambda E, \check{p} = \lambda p) \}$ with the form: $\omega = - d\lambda \wedge ds - d\check{E} \wedge dt + d\check{p} \wedge dq$: $(\lambda, \check{E}, \check{p})$ are homogeneous coordinates for the physical quantities E and p ; s is conjugate to the *variable* λ $\left(\text{physically } \lambda = \frac{1}{\hbar}\right)$; s is analogous to (in the absence of interactions: proportional to) the proper time (which is conjugate to the mass).

The fact that (1) becomes homogeneous under $\frac{1}{\hbar} \to i\frac{\partial}{\partial s}$ seems to be an essential property of quantization in the sense that if terms of lower order were present in (45), they could not be canonically determined by classical dynamics alone.

If we parametrize the characteristic surfaces $\Phi(s, t, q) = \text{const.}$ of (45), which satisfy

$$\frac{\partial\Phi}{\partial s}\frac{\partial\Phi}{\partial t} - \frac{1}{2m}(\nabla\Phi)^2 - V(q)\left(\frac{\partial\Phi}{\partial s}\right)^2 = 0$$

in the form $s = S(t, q) + \text{const.}$, we recover the classical action of eq. (23); the physical characteristic surfaces $S(t, q) = \text{const.}$ are no longer generated by classical trajectories (this was true only for homogeneous systems) but we recall that the bicharacteristics still generate the Lagrangian manifold of S in the phase space $\tilde{M}$ (cf. 2, § 8). This reduction of phase space $\check{M} \to \tilde{M}$ corresponds to the choice of λ as scaling variable, $\frac{\check{E}}{\lambda}$ and $\frac{\check{p}}{\lambda}$ remaining fixed when $\lambda \to \infty$; we could take other scaling variables, each yielding a different reduced phase space with a different dynamics, but they all correspond to different parametrizations of the *same* surfaces $\Phi(s, t, q) = \text{const.}$ We could thus describe the high energy limit ($E \to \infty$). On the free equations, the $s \leftrightarrow t$ symmetry of (45) shows that the asymptotics for $\lambda \to \infty$ and $E \to \infty$ is the same, while for the Klein-Gordon equation $\left(\frac{\partial^2}{\partial t^2} - \Delta - m^2\frac{\partial^2}{\partial s^2}\right)\psi = 0$ making $\lambda \to \infty$ gives the *euclidean* high energy limit.

We recall that semi-classical methods can be used for various other problems involving scaling, such as thermodynamics (volume $V \to \infty$, the intensive variables remaining fixed), statistical mechanics (expansions around mean field theory viewed as a « classical limit », e. g. ref. [*30*]); or (Appendix 1) quantum field theory expanded around the sum of tree graphs [*48*].

2) The Wigner method [*9*]

The choice of parametrization: $\Phi(s, t, q) = S(t, q) - s$ and the restriction in M to the hyperplane $\lambda = \frac{1}{\hbar}$ correspond to some changes in the formulae of section 3 when viewed in M.

Wigner symbols are given not by (36′) but by:

$$A_w(\hbar\,; q, p) = \int dr e^{ipr/\hbar} a\left(q - \frac{r}{2}, q + \frac{r}{2}\right) = \int \frac{dk}{(2\pi\hbar)^l} e^{-ikq/\hbar} \tilde{a}\left(p - \frac{k}{2}, p + \frac{k}{2}\right) \quad (46)$$

where

$$\tilde{a}(p, p') = \int e^{-\frac{i}{\hbar}(pq - p'q')} a(q, q')dqdq' \quad (47)$$

so that

$$\operatorname{Tr} B^{\dagger}A = \int \frac{dqdp}{(2\pi\hbar)^l} B_w^*(q, p)A_w(q, p) \tag{48}$$

and

$$\operatorname{Tr} B = \int \frac{dqdp}{(2\pi\hbar)^l} B_w(q, p). \tag{49}$$

We shall restrict observables to have the form $\frac{1}{\lambda^m}\check{A}$ where $\check{A}$ is a PDO of arbitrary order m in the homogeneous variables and independent of s. Expressed in the physical variables, eq. (43) means:

$$A_w(\hbar\,; q, p) \sim \sum_0^{\infty} a_{-n}(q, p)\hbar^n \qquad (\hbar \to 0^+) \tag{50}$$

where $A_w(q, p)$ and $(\forall n)\ a_{-n}(q, p) \in C^{\infty}(\mathbb{R}^{2l})$; moreover, as $|p| \to \infty$:

$$a_{-n}(q, p) \sim \sum_{r=0}^{\infty} a_{-n,m-n-r}(q\,; p),$$

where $a_{-n,n'}$ is homogeneous of degree n' in the p variables.

Neither classical mechanics nor Weyl quantization distinguish between q and p. We are thus led to define a quantum observable as *admissible* if A_w satisfies analogous relations in both variables $(q, p) = x$, that is: eq. (50) with:

$$a_{-n}(x) \sim \sum_{r=0}^{\infty} a_{-n,m-2n-r}(x)\,;$$

$a_{-n,n'}$ homogeneous of degree n' in x. All usual non-singular hamiltonians are admissible observables.

If A and A′ are admissible observables, eq. (44) implies that:

$$(AA')_w = A_w\big(e^{\frac{i\hbar}{2}\overleftrightarrow{\Lambda}}\big)A'_w = A_wA'_w + \frac{i\hbar}{2}\{A_w, A'_w\} + 0(\hbar^2) \tag{51}$$

and that $[A, A']_{\pm}$ are admissible observables.

As *admissible states* we then take the positive linear functionals B such that:

$$\frac{1}{(2\pi\hbar)^l} B_w(\hbar\,; q, p) \sim \sum_0^{\infty} b_n\hbar^n, \tag{52}$$

with $B_w(q, p)$ and $b_n(q, p) \in \mathcal{S}'(\mathbb{R}^{2l})$ (tempered distributions [*31*]).

The expansion (52) is uniquely characterized as weakly asymptotic: the expectation value of any admissible observable A in the admissible state B satisfies, provided all the brackets make sense:

$$\mathrm{Tr}\, \mathrm{B}^{\dagger}\mathrm{A} \sim \sum_{n=0}^{\infty}\left(\sum_{m=0} \langle b_m^*, a_{m-n} \rangle\right)\hbar^n \tag{53}$$

so that:

$$\lim_{\hbar\to 0} \mathrm{Tr}\, \mathrm{B}^{\dagger}\mathrm{A} = \langle b_0^*, a_0 \rangle \qquad \text{(the \textit{classical limit})}. \tag{54}$$

3) The quantum expectation values

The quantum expectation values have the form Tr ρA, where ρ is a density matrix (a positive operator of trace 1) and A is a hermitian operator [*51*]. We know no criterion on ρ_w ensuring the positivity of ρ. However, if we want ρ to be a positive operator *for all values* $\lambda \to \infty$ it is necessary that ρ_0 as given by (54) should be a positive distribution (i. e. a measure); moreover $\langle \rho_0, 1 \rangle = 1$ therefore ρ_0 is a classical density on M: the classical limit of the quantum density ρ; eq. (54) implies:

$$\lim_{\hbar\to 0} \mathrm{Tr}\, \rho \mathrm{A} = \langle \rho_0, a_0 \rangle = \int \rho_0(q, p)\mathrm{A}_{\mathrm{cl}}(q, p)dqdp\,.$$

For instance the quantum density of a coherent state (a minimal wave packet) satisfies all requirements, moreover:

$$\rho_w(q, p) = 2^l \exp\left(-\frac{1}{\hbar}\left[m\omega(q - q_0)^2 + \frac{(p - p_0)^2}{m\omega}\right]\right)$$
$$\sim (2\pi\hbar)^l . \sum_0^{\infty}\left[\frac{(m\omega\Delta_p + (m\omega)^{-1}\Delta_q)^n}{4^n n\,!}\delta(q - q_0)\delta(p - p_0)\right]\hbar^n$$

so that the classical limit is the state localized [7] at $(q_0, p_0) \in \mathrm{M}$: for any observable A:

$$\lim_{\hbar\to 0} \mathrm{Tr}\, \rho \mathrm{A} = \mathrm{A}_{\mathrm{cl}}(q_0, p_0)\,.$$

4) The equations of motion

We use the Heisenberg picture in order to exploit Groenewold's formula (51). Heisenberg's equation $\dot{\mathrm{A}} = \frac{i}{\hbar}[\mathrm{H}, \mathrm{A}]$ is equivalent to:

$$\dot{\mathrm{A}}_w = -\frac{2}{\hbar}\mathrm{H}_w\left(\sin\frac{\hbar\overleftrightarrow{\Lambda}}{2}\right)\mathrm{A}_w \qquad (= \{ \mathrm{A}_w, \mathrm{H}_w \} + 0(\hbar^2))$$

[7] Simultaneous localization in q and p occurs because both

$$\langle \Delta q^2 \rangle^{1/2} \sim \langle \Delta p^2 \rangle^{1/2} = 0(\hbar^{1/2})\,.$$

This makes the coherent state densities useful as convolution kernels to study classical limits (ref. [*29*]).

and at lowest order this implies the classical equation (21): $\dot{A}_{cl} = \{ A_{cl}, H_{cl} \}$ meaning that time evolution is generated by the Liouville operator [51].

In this approximation it is equivalent to keep observables fixed and transport the states by the reversed flow.

It follows from ref. [28] that the quantum evolution operator for a finite time is not a PDO but a « Fourier integral operator » whose symbol is roughly an expansion like (50) multiplied by an overall phase $e^{\frac{i}{\hbar}\Sigma(q,p)}$. Their calculus yields [28] rigorous properties of quantum vs. classical time evolution (ref. [15] is another approach to this problem).

5) The scope of the Wigner method

A description by algebras of observables is possible for both quantum [51] and classical systems. Clearly the Wigner method provides a smooth transition when $\hbar \to 0$ from the (quantum) operator algebra to the (classical) function algebra. We could not have expected such smoothness for any scheme involving Hilbert space explicitly, since the Hilbert space is expected to somehow vanish in the classical limit. So the Wigner limit is weakly, not strongly continuous at $\hbar = 0$. It will not provide reliable information on the spectrum, nor on the eigenstates of operators. For instance the semi-classical spectrum $\sigma_{cl}(H)$ naively defined as the set of singularities of $\left(\frac{1}{z - H}\right)_{cl} = \frac{1}{z - H_{cl}}$, is a continuous spectrum if $H_{cl}(q, p)$ is a continuous function:

$$\sigma_{cl}(H) = \{ \lambda \mid \lambda = H_{cl}(x) \text{ for some } x \in M \}.$$

6) The Thomas-Fermi spectrum

There exists a roundabont way to quantize the spectrum according to the Wigner approach. Define: $V_E = H_{cl}^{-1}(-\infty, E]$ (V_E has boundary $\hat{\Sigma}_E$) and $\mathscr{V}(E) = \text{volume}(V_E) = \int_{V_E} |\Omega|$. The « region of bound states » is defined as $\mathscr{B} = \{ x \in M \mid \mathscr{V}(H(x)) < \infty \}$. If ψ_E is an eigenvector of energy E, a reasonable classical limit for $\rho^E = |\psi_E\rangle\langle\psi_E|$ must be an invariant measure on $\hat{\Sigma}_E$ of total mass $(2\pi\hbar)^l$ because of (49); for instance $\rho_{cl}^E = \frac{(2\pi\hbar)^l}{d\mathscr{V}/dE}\delta(H_{cl} - E)$, which is the only candidate if the motion is ergodic. When we fill the region $\mathscr{B}$ so that $\sum_n \rho_{cl}^{E_n} \sim 1|_{\mathscr{B}}$ we obtain the quantization « rule »:

$$\mathscr{V}(E_n) \sim \left(n + \frac{1}{2}\right)(2\pi\hbar)^l, \tag{55}$$

which has only a heuristic value but predicts the correct Weyl [16] or Thomas-Fermi [17] asymptotic density of levels $\rho(\mathrm{E})d\mathrm{E}$

$$\rho(\mathrm{E}) \sim (2\pi\hbar)^{-l}\frac{d\mathscr{V}}{d\mathrm{E}} \tag{56}$$

Eq. (55) will at best hold for ergodic systems. On the contrary, for the many quantum systems (like nuclei) which are degenerate or quasi-degenerate (i. e. the density $\rho(\mathrm{E})$ has sharp peaks) more adapted and precise methods are given in section 5 and 7.

5. THE MASLOV-WKB METHOD

We shall work here with time-independent wave functions; later we can choose them to be stationary states, or else introduce time as a parameter. We shall show that the Lagrangian manifold, whose generating function is the phase of a WKB wave, is an intrinsic object in phase space, independent of the quantum representation of the wave.

1) Quantum change of representation

In 1 dimension we go from the coordinate to the momentum representation of wave functions by a Fourier transformation. The natural generalization to $\mathbb{R}^l$ is to introduce [12] for each state vector ψ and each set of coordinates $\{ t_{\mathrm{K}} \}$ of K-space (cf. 2, § 4) a wave function $\psi_{\mathrm{K}}(t_{\mathrm{K}}) \in \mathrm{L}^2(\mathbb{R}^l)$ such that:

$$\psi_{\mathrm{H}}(t_{\mathrm{H}}) = \int \prod_{j\in\mathrm{K}-\mathrm{H}} \left(\frac{\lambda}{2\pi i}\right)^{1/2} dq^j \prod_{k\in\mathrm{H}-\mathrm{K}} \left(\frac{-\lambda}{2\pi i}\right)^{1/2} dp_k$$
$$\exp\left\{ -i\lambda\left(\sum_{\mathrm{K}-\mathrm{H}} p_j q^j - \sum_{\mathrm{H}-\mathrm{K}} p_k q^k\right)\right\}\psi_{\mathrm{K}}(t_{\mathrm{K}}) \tag{56}$$

where $\lambda = \frac{1}{\hbar}$ and $\mathrm{Arg}\,(\pm\, i)^{1/2} = \pm\,\frac{\pi}{4}$. This partial Fourier transformations $\mathscr{F}_{\mathrm{H}}^{\mathrm{K}}$ is unitary and satisfies

$$\mathscr{F}_{\mathrm{L}}^{\mathrm{K}}\mathscr{F}_{\mathrm{K}}^{\mathrm{H}} = \mathscr{F}_{\mathrm{L}}^{\mathrm{H}}\,; \qquad \mathscr{F}_{\mathrm{K}}^{\mathrm{K}} = \text{identity}. \tag{57}$$

For observables: $\mathrm{A}_{\mathrm{H}}\left(t_{\mathrm{H}}, -\frac{i}{\lambda}\frac{\partial}{\partial t_{\mathrm{H}}}\right) = \mathscr{F}_{\mathrm{H}}^{\mathrm{K}}\mathrm{A}_{\mathrm{K}}\left(t_{\mathrm{K}}, -\frac{i}{\lambda}\frac{\partial}{\partial t_{\mathrm{K}}}\right)\mathscr{F}_{\mathrm{K}}^{\mathrm{H}}$: this is simply realized by the formal substitutions (without changing the ordering!):

$$\text{if } j \in \mathrm{K} - \mathrm{H}: \quad t_{\mathrm{K}}^{j} \to \frac{i}{\lambda}\frac{\partial}{\partial t_{\mathrm{H}}^{j}}, \qquad -\frac{i}{\lambda}\frac{\partial}{\partial t_{\mathrm{K}}^{j}} \to t_{\mathrm{H}}^{j}$$

$$\text{if } j \in \mathrm{H} - \mathrm{K}: \quad t_{\mathrm{K}}^{j} \to -\frac{i}{\lambda}\frac{\partial}{\partial t_{\mathrm{H}}^{j}}, \qquad \frac{i}{\lambda}\frac{\partial}{\partial t_{\mathrm{K}}^{j}} \to t_{\mathrm{H}}^{j}$$

$$\text{if } j \notin \mathrm{K} \,\Delta\, \mathrm{H}: \quad \text{no change.}$$

Equivalently: $\mathrm{A_K}$ and $\mathrm{A_H}$ describe the *same* invariant Wigner symbol $\mathrm{A}_w(q, p)$ in the two sets of coordinates $\begin{pmatrix} t_\mathrm{K} \\ s_\mathrm{K} \end{pmatrix}$ and $\begin{pmatrix} t_\mathrm{H} \\ s_\mathrm{H} \end{pmatrix} = \mathrm{U_{H'}U_{K'}^{-1}}\begin{pmatrix} t_\mathrm{K} \\ s_\mathrm{K} \end{pmatrix}$:

$$(\mathrm{A_K})_w(t_\mathrm{K}, s_\mathrm{K}) = (\mathrm{A_H})_w\left(\mathrm{U_{H'}U_{K'}^{-1}}\begin{pmatrix} t_\mathrm{K} \\ s_\mathrm{K} \end{pmatrix}\right) \tag{58}$$

2) The asymptotic Fourier transformation

If in some K-representation ψ_K has the form $a^\mathrm{K}(t_\mathrm{K})e^{i\lambda \mathrm{S_K}(t_\mathrm{K})}$, we associate to it the Lagrangian submanifold $\Lambda \subset \mathrm{M}$ of K-generating function $\mathrm{S_K}$ (notations of section 2); to allow for a *finite* number of branches of $\mathrm{S_K}$ we shall conside. more general waves which we denote « WKB waves »:

$$\psi_\mathrm{K}(t_\mathrm{K}) \sim \sum_{x \in \Pi_\mathrm{K}^{-1}(t_\mathrm{K})} a^\mathrm{K}(x) \exp\left(i\lambda \int_{x_0}^{x} \theta_\mathrm{K}\right). \tag{59}$$

We call the (possibly complex) function a^K the amplitude and $\lambda \int \theta_\mathrm{K}$ the phase; a^K is only given as an *asymptotic series* (cf. (6)):

$$a^\mathrm{K}(x) = \sum_{n=0}^{\infty} \frac{a_n^\mathrm{K}(x)}{(i\lambda)^n}, \qquad a_n^\mathrm{K} \in \mathrm{C}^\infty;$$

let $\operatorname{supp} a^\mathrm{K} = \overline{\bigcup_{n=0}^{\infty} \operatorname{supp} a_n^\mathrm{K}}$ (it is not the support of the *function* a^K) and assume it is a compact subset of Λ. If the series a^K is reduced to one term, say a_0^K, we call ψ_K a *semi-classical wave.* It is a crucial fact that the WKB form (and, as seen later, the semi-classical form) is covariant under the change of representation (K) $\xrightarrow{\mathscr{F}_\mathrm{H}^\mathrm{K}}$ (H); Λ is invariant and $\mathscr{F}_\mathrm{H}^\mathrm{K}$ acts locally in x on $a^\mathrm{K}(x)$ at every order in λ. This follows from the stationary phase expansion of $\psi_\mathrm{H}(t_\mathrm{H})$ in (56) (Appendix 1) which holds provided:

$$\forall x \in \Pi_\mathrm{H}^{-1}(t_\mathrm{H}) \qquad \mathrm{D_H^K}(x) = \det\left(\frac{\partial^2 \mathrm{S_K}(x)}{\partial t_\mathrm{K}^j \partial t_\mathrm{K}^k}\right)_{j,k \in \mathrm{K}\Delta\mathrm{H}} \neq 0$$

The result is (the overall phase γ can and will be disregarded):

$$\psi_{\mathrm{H}}(t_{\mathrm{H}}) \sim e^{i\gamma} \sum_{x \in \Pi_{\mathrm{H}}^{-1}(t_{\mathrm{H}})} a_{\mathrm{H}}(x) \exp\left(i\lambda \int_{x_0}^{x} \theta_{\mathrm{H}}\right) \tag{59'}$$

$$a^{\mathrm{H}}(x) = \sum_{0}^{\infty} \frac{a_n^{\mathrm{H}}(x)}{(i\lambda)^n} = \frac{1}{\mathrm{D}_{\mathrm{H}}^{\mathrm{K}}(x)^{1/2}} \sum_{0}^{\infty} \frac{a_n^{\mathrm{H}}(x)}{\mathrm{D}_{\mathrm{H}}^{\mathrm{K}}(x)^{3n}(i\lambda)^n} \tag{60}$$

where a_n^{H} is a polynomial of the derivatives *at* x:

$$\partial^\alpha \mathrm{S}_{\mathrm{K}}(2 \leq |\alpha| \leq 2n+2) \quad \text{and} \quad \partial^\beta a_{n'}^{\mathrm{K}}(n' \leq n, |\beta| \leq 2(n-n'))$$

and $(\mathrm{D}_{\mathrm{H}}^{\mathrm{K}})^{1/2}$ has the complex determination

$$(\mathrm{D}_{\mathrm{H}}^{\mathrm{K}}(x))^{1/2} = i^{\mathrm{I}_{\mathrm{H}}^{\mathrm{K}}(x) - |\mathrm{H}-\mathrm{K}|} \, |\mathrm{D}_{\mathrm{H}}^{\mathrm{K}}(x)|^{1/2} \tag{60}$$

where $\mathrm{I}_{\mathrm{H}}^{\mathrm{K}}(x)$ is the inertia of the quadratic form $\left(\dfrac{\partial^2 \mathrm{S}_{\mathrm{K}}(x)}{\partial t_{\mathrm{K}}^j \partial t_{\mathrm{K}}^k}\right)_{j,k \in \mathrm{K}\Delta\mathrm{H}}$ i. e. the number of negative terms in any diagonal form; this number will jump by integer values when $\mathrm{D}_{\mathrm{H}}^{\mathrm{K}}(x)$ goes through the value 0. In particular

$$a_0^{\mathrm{H}}(x) = \frac{i^{|\mathrm{H}-\mathrm{K}| - \mathrm{I}_{\mathrm{H}}^{\mathrm{K}}(x)}}{|\mathrm{D}_{\mathrm{H}}^{\mathrm{K}}(x)|^{1/2}} a_0^{\mathrm{K}}(x) \tag{61}$$

so that the semi-classical approximation is also covariant (and consistent). Eq. (16) implies $\dfrac{\partial t_{\mathrm{H}}^j}{\partial t_{\mathrm{K}}^k} = \Bigg(\underbrace{\dfrac{\partial^2 \mathrm{S}_{\mathrm{K}}}{\partial t_{\mathrm{K}}^j \partial t_{\mathrm{K}}^k}}_{j \in \mathrm{K}-\mathrm{H}} \Bigg| - \underbrace{\dfrac{\partial^2 \mathrm{S}_{\mathrm{K}}}{\partial t_{\mathrm{K}}^j \partial t_{\mathrm{K}}^k}}_{j \in \mathrm{H}-\mathrm{K}} \Bigg| \underbrace{\delta_{jk}}_{j \notin \mathrm{K}\Delta\mathrm{H}}\Bigg)$ so that, using (14):

$$\begin{aligned}(-1)^{|\mathrm{H}-\mathrm{K}|} \mathrm{D}_{\mathrm{H}}^{\mathrm{K}} &= (-1)^{|\mathrm{H}-\mathrm{K}|} \det \left(\frac{\partial^2 \mathrm{S}_{\mathrm{K}}}{\partial t_{\mathrm{K}}^j \partial t_{\mathrm{K}}^k}\right)_{j,k \in \mathrm{K}\Delta\mathrm{H}} \\ &= \det \left(\frac{\partial t_{\mathrm{H}}^j}{\partial t_{\mathrm{K}}^k}\right)_{j,k=1,\dots,l} = \frac{\mathrm{D}(t_{\mathrm{H}})}{\mathrm{D}(t_{\mathrm{K}})} = \det(\Pi_{\mathrm{H}}\Pi_{\mathrm{K}}^{-1}).\end{aligned}$$

Thus $\mathrm{D}_{\mathrm{H}}^{\mathrm{K}} = 0$ on Σ_{H}; the expansion of ψ_{H} is regular only if supp $a \cap \Sigma_{\mathrm{H}} = \varnothing$ (where we write supp a for the chart-independent set supp a^{H}). Now any arbitrary amplitude a can be decomposed, by a partition of unity subordinate to the covering $\Lambda = \bigcup_{\mathrm{K}} (\Lambda - \Sigma_{\mathrm{K}})$, into a sum of terms $a(\mathrm{K})$ each expandable in the K-chart. This gives a singularity-free WKB expansion [*10*] [*12*] [*32*] indeed, but very cumbersome! It is clearly desirable to somehow attach the WKB expansion to the manifold Λ since all the trouble seems to come from the projection operators Π_{K} being singular on Σ_{K}.

Assume now $x \in (\text{supp } a \cap \Sigma_{\mathrm{H}}) \neq \varnothing$; formulae (59) and (60) indicate that ψ_{H} has the phase $\lambda \mathrm{S}_{\mathrm{H}}$ (which is the Legendre transform $\lambda \mathscr{L}_{\mathrm{H}}^{\mathrm{K}} \mathrm{S}_{\mathrm{K}}$) plus a term discontinuous across Σ_H like $I_K^H(x)$; and the amplitude is infinite ([8]) like $|D(t_H)/D(t_K)|^{-1/2}$. To show that these singularities are caused by Π_H it is necessary to show that they have an expression independent of K; the real difficulty is for the phase and is solved by the Maslov index theory of Keller, Maslov, Arnold [*10*] [*12*] [*38*].

3) The Maslov index

The function $n_H^K(x) = I_H^K(x) - |H - K|$ is locally constant on $\Lambda - (\Sigma_K \cup \Sigma_H)$; its jumps are those of the phase of ψ_K across Σ_K, and of minus the phase of ψ_H across Σ_H (moreover $n_H^K \equiv -n_K^H$). Maslov [*10*] proves the following generic properties (we omit details): for all H, Σ_H is a submanifold of Λ of dimension $(l-1)$ on which $D_H^K(x)$ has a *simple* zero (apart from exceptional points $x \in \Sigma_H$); Σ_H has a positive and negative side on Λ, such that for any K, $I_H^K(x)$ jumps by $+1$ (-1) when x crosses Σ_H from the negative to the positive (resp. positive to negative) side. See fig. 4.

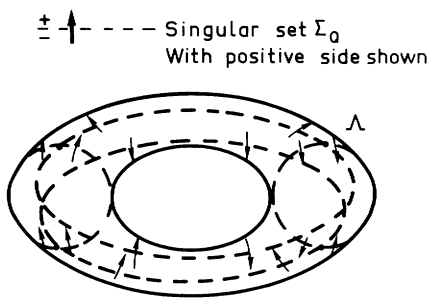

FIG. 4. — A typical $l = 2$ toric Lagrangian manifold.

The Maslov index $n_H(x)$ is defined as the *Kronecker index* with respect to Σ_H of any oriented curve γ on Λ, with arbitrary fixed origin x_0 and extremity x, i. e. it is obtained by adding $+1$ (-1) every time the curve crosses Σ_H from the negative to positive (resp. positive to negative) side. This quantity is unchanged by continuous deformation of γ with x_0 and x fixed; therefore $n_H(x)$ is a single-valued function on the covering $\tilde{\Lambda}$, defined up to an overall additive integer (x_0 being arbitrary). But there exists a choice for the indices $n_K(x)$ $\forall$K, such that $\forall$K, H : $n_H(x) - n_K(x)$ is single-valued *on* Λ and equal to $n_H^K(x)$.

The most important property of the Maslov index is the following: for a closed oriented curve (a cycle) γ, the index $n_H(\gamma)$, which counts the inter-

([8]) These singularities belong not to the ψ_H's but only to their expansions.

sections with Σ_H, only depends on the homology class of the cycle γ, and has the same value *for all* H : thus the index is the value of an (integer) cohomology class $n \in H^1(\Lambda, \mathbb{Z})$. The rigorous proofs (Arnold [11]) use a coordinate-free definition of n in the cohomology of the manifold of all Lagrangian vector spaces in M.

Thus we have on Λ two intrinsic cohomology classes of degree 1, a real-valued one: $\gamma \to \int_\gamma \theta_K$ and an integer-valued one: $\gamma \to n_K(\gamma)$, both independent of K, when γ is a *cycle.*

4) The semi-classical approximation

Eq. (61), which proves the consistency of the semi-classical approximation, allows us to define the semi-classical Fourier transformations $\tilde{\mathscr{F}}_H^K$ by:

$$\mathscr{F}_H^K\left(a_0^K \exp\left(i\lambda\int\theta_K\right)\right) = a_0^H \exp\left(i\lambda\int\theta_K\right).$$

Clearly: $\tilde{\mathscr{F}}_L^K\mathscr{F}_K^H = \tilde{\mathscr{F}}_L^H$; $\tilde{\mathscr{F}}_K^K = id$: $\tilde{\mathscr{F}}_H^K$ is local, unitary since

$$|a_0^H(t_H)|^2 dt_H = |a_0^K(t_K)|^2 dt_K,$$

and regular at x if $0 < |D_H^K(x)| < \infty$.

Under reasonable assumptions, the error term $\delta\psi_H = (\mathscr{F}_H^K - \tilde{\mathscr{F}}_H^K)\psi_K$ can be bounded in Hilbert space locally in $x \notin \Sigma_K \cup \Sigma_H$. Following Appendix 1, we must assume S_K and $S_H \in C^\infty$ on supp a, and $\psi_K \in$ domain $(-h^2\Delta_{t_K} + t_K^2)$, to get H-chart estimates of the form: $\forall K\ \exists C_H^K$ (depending on derivatives of S_K):

$$\|\delta\psi_H\|_{L^2(dt_H)} < \frac{C_K^H}{\lambda}\left\|\left(-\frac{1}{\lambda^2}\Delta_{t_K} + t_K^2\right)\psi_K\right\|_{L^2(dt_K)}$$

Thus the approximation is uniform in each H-chart away from Σ_H.

5) The canonical operators

Assume Λ to be orientable, i. e. there exists a global volume element $\eta \in \Omega^l(\Lambda)$, $\eta(x) \neq 0\ \forall x$. If $\psi \in L^2(\Lambda, \eta)$ we let:

$$(\tilde{\Pi}_{K,x_0}^{\Lambda\eta}\psi)(t_K) = \sum_{x\in\Pi^{-1}(t_K)} \left|\frac{D\eta}{Dt_K}(x)\right|^{1/2} i^{-n_K(\gamma_x)} \exp\left(i\lambda\int_{\gamma_x}\theta_K\right)\psi(x) \qquad (62)$$

where $\frac{D\eta}{Dt_K}$ stands for det Π_K, and γ_x is any curve on Λ from x_0 to x; the choice of x_0 fixes the global phase and the choice of η is irrelevant, so we omit the subscripts x_0 and η. By construction $\tilde{\Pi}_K^\Lambda$ is local, isometric, of domain $\{\psi \mid \operatorname{Supp}\psi \cap \Sigma_K \neq \emptyset\}$, and $\mathscr{F}_H^K = \tilde{\Pi}_H^\Lambda(\tilde{\Pi}_K^\Lambda)^{-1}$ with properly adjusted phases.

Physically, if ψ is regular on Λ and has a constant phase, $\tilde{\Pi}_K^\Lambda\psi$ will have the right semi-classical phase (with the jumps at Σ_K) and the right semi-classical singularity in the amplitude. Conversely the action of $(\tilde{\Pi}_K^\Lambda)^{-1}$ on any WKB wave $\psi_K(t_K) \sim \sum_x a^K(x) \exp\left(i\lambda \int \theta_K\right)$ kills the phase and singularities:

$$\| (\tilde{\Pi}_K^\Lambda)^{-1}\psi_K(x) - a_0^\Lambda(x) \|_{L^2(\Lambda,\eta)} = 0\left(\frac{1}{\lambda}\right), \tag{63}$$

where $a_0^\Lambda(x) = \left|\dfrac{Dt_K}{D\eta}\right| i^{n_K} a_0^K(x)$ is independent of K and regular on Λ.

The scheme is consistent only if the semi-classical phase can be defined as a single-valued function, i. e. if the RHS of (62) is single-valued. But γ_x is defined modulo cycles, so that the phase is unique iff any cycle γ of a homotopy basis for Λ satisfies the *Bohr-Sommerfeld-Maslov quantization rule* (where the LHS is independent of K):

$$(\forall\gamma) \qquad \frac{\lambda}{2\pi}\int_\gamma \theta_K - \frac{n_K(\gamma)}{4} \in \mathbb{Z}\,. \tag{64}$$

Eq. (64) select the manifolds Λ on which the semi-classical approximation is consistent. Then (63) shows that the representation on $L^2(\Lambda)$, which Maslov calls the *semi-classical representation*, is regular for the classical limit. We remark that the superposition principle disappears when $\lambda \to \infty$, since waves with different phases will « live » on different Λ's and cannot be combined.

It is a crucial but open problem to extend the scheme to higher orders on $\frac{1}{\lambda}$ and obtain a uniform WKB expansion defined on Λ; this requires the explicit construction of *full* canonical operators Π_K^Λ (depending on a quantization procedure, and satisfying $\mathscr{F}_H^K \equiv \Pi_H^\Lambda(\Pi_K^\Lambda)^{-1}$). The answer is known only for very special cases (e. g. if Λ = a Lagrangian subspace, the Π_K^Λ are the evolution operators of certain harmonic oscillators). The only known method is then to work out a standard WKB expansion in any K-chart, away from $\Pi_K(\Sigma_K)$.

6) Comparison with the Wigner method

If in the Q-chart:

$$\psi_Q(q) \sim \sum_0^\infty \frac{a_n^Q(q)}{(i\lambda)^n} \exp\left(i\lambda \int \theta_Q\right) = a^Q e^{i\lambda S_Q}$$

then we have the following expansion for the symbol of $\rho = \psi \otimes \psi$ (the density):

$$\rho_w(q, p)$$
$$= \int a^Q\left(q - \frac{r}{2}\right)a^{Q*}\left(q + \frac{r}{2}\right) \exp\left(i\lambda\left[S_Q\left(q - \frac{r}{2}\right) - S_Q\left(q + \frac{r}{2}\right) + pr\right]\right)dr$$
$$\sim (2\pi\hbar)^l\left[a^Q\left(q + \frac{i\hbar}{2}\nabla_p\right)a^{Q*}\left(q - \frac{i\hbar}{2}\nabla_p\right)\exp\left(\frac{i}{\hbar}\Sigma_Q(q, i\hbar\nabla_p)\right)\right]\delta(p - \nabla_q S_Q)$$

where

$$\Sigma_Q(q, r) = S_Q\left(q + \frac{r}{2}\right) - S_Q\left(q - \frac{r}{2}\right) - r\nabla_q S_Q(q) = 0(r^3)$$

which is meaningful (and chart-independent) when applied to admissible observables. The expansion is concentrated ([9]) on Λ, in particular:

$$\rho_w(q, p) = (2\pi\hbar)^l[\,|\,a_0^Q(q)\,|^2\delta(p - \nabla_p S_Q) + 0(\hbar)] \tag{65}$$

(and if a_0^Q and a_1^Q are *real* $0(\hbar)$ becomes $0(\hbar^2)$), thereby showing that the wave in the semi-classical representation is the square root of the classical density. Obviously this gives a 1-1 correspondence between classical densities concentrated on Lagrangian manifolds and semi-classical waves. We may call those densities « pure-classical states » and think of all other densities as continuous mixtures of pure-classical states, a case for which we have no canonical method to obtain the wave functions as power expansions in $\hbar$.

For pure-classical states we can write (65) as:

$$\rho_w(q, p) = (2\pi\hbar)^l[a_0^\Lambda(x)^2\delta_{\Lambda,\eta}(x) + 0(\hbar)]$$

where $\delta_\eta(\Lambda)$ is defined as:

$$\int \delta_{\Lambda,\eta}(x)u(x)dqdp = \int_\Lambda u(x)\eta\,.$$

The action of an observable A, given by (51), involves derivation operators transversal to Λ. The Maslov method is interesting when the semi-classical term of (51), namely $\frac{i\hbar}{2}(\nabla_q A_w . \nabla_p - \nabla_p A_w . A_q)$ acts along Λ; for simplicity we assume that in (50) $a_{-1} \equiv 0$ (this is true in usual cases). So we shall suppose that Λ *lies in a hypersurface* $A_{cl} = c$; this implies (cf. theorem 2) that Λ is invariant by the flow V_s of $\nabla_\omega A$; but

$$\frac{i\hbar}{2}(\nabla_q A_{cl} . \nabla_p - \nabla_p A_{cl} . \nabla_q) = -\frac{i\hbar}{2}\frac{d}{ds}$$

([9]) But coefficients of $\hbar^n$ ($n \neq 0$) are not measures and have no intrinsic interpretation on $L^2(\Lambda, \eta)$.

along the flow. Formally then:

$$A = c - \frac{i\hbar}{2}\frac{d}{ds} + 0(\hbar^2).$$

Applying this to a real semi-classical wave $\psi(x) = a_0^\Lambda(x)$ in the semi-classical representation we obtain:

$$(A\psi)(x) = ca_0^\Lambda(x) - i\hbar\frac{d}{ds}(a_0^\Lambda . \sqrt{\eta}) + 0(\hbar^2) \tag{66}$$

(compare to eqs. (3) and (5)). The simplest choice for η is a measure *invariant by the flow* V_s. The residual term contains second order derivatives of $a_0^\Lambda(x)$; if these are bounded and if Λ is compact we get L^2 estimates:

$$\left\| \left(A - c + i\hbar\frac{ds}{ds}\right)\psi \right\|_{L^2(\Lambda,\eta)} = \| (A - A_{s.c.})\psi \|_{L^2(\Lambda,\eta)} = 0(\hbar^2).$$

It is much harder but essential to show *[10]* *[32]* the analogous result in the Q-chart (for instance) for the uniform WKB wave ψ_Q:

$$\| (A - A_{s.c.})\psi_Q \|_{L^2(\mathscr{Q},dq)} = 0(\hbar^2). \tag{67}$$

In the semi-classical approximation: $A_{s.c.} = c - i\hbar\frac{d}{ds}$ is the sum of the scalar value of A_{cl} and of the *linear* translation generator $T_A = -i\hbar\frac{d}{ds}$, which is self-adjoint since η is invariant. The system (Λ, η, V_s) is a classical dynamical system in the sense of ref. *[13]*.

We now apply the foregoing considerations to specific cases.

7) The initial value problem

Given a semi-classical wave $\psi(t = 0; x)$ there corresponds to it an initial Lagrangian manifold Λ_0 of M. We already know that the corresponding solution of the classical equation (23) is the Lagrangian manifold $\tilde{\Lambda} \subset \tilde{M}$ generated by the classical paths starting from Λ_0. There is an obvious invariant volume element η associated to any volume $\tilde{\eta}_0$ on Λ: $\tilde{\eta}(t, x_t) = dt \wedge \tilde{U}^*_{-t}\eta(x_0) = dt \wedge \eta_t$ (x_t = classical path; $\tilde{U}_t$ = flow, on $\tilde{M}$).

We can apply eq. (66) with $A = i\hbar\frac{\partial}{\partial t} - H$; since $A_{cl} = E - H_{cl}(q, p) = 0$ on $\tilde{\Lambda}$, we get:

$$0 = \left(i\hbar\frac{\partial}{\partial t} - H\right)\psi(x) = -i\hbar\frac{da_0^{\tilde{\Lambda}}}{dt} + 0(\hbar^2),$$

i. e. a_0^Λ is *constant along the classical paths.*

The semi-classical wave at time t is thus defined on the section $\Lambda_t \subset M$ of $\tilde{\Lambda}$ (cf. 2, § 8) by: $a_0^{\Lambda_t}(x_t) = a_0^{\Lambda_0}(x_0)$; the K-chart wave is obtained by applying the canonical operator $\tilde{\Pi}_K^{\Lambda_t}$: only at this step are the possible caustic singularities introduced: the caustics are the hypersurfaces of K-space $\left\{ t_K \,\middle|\, \frac{Dt_K}{D\eta_t} = 0 \right\}$; under time evolution they move and a connected component may even appear or vanish at some instant.

The connection with the usual treatment of caustics [5] is established via the following result [10] [11]: if $\left(\frac{\partial^2 H_{cl}}{\partial p_j \partial p_k}\right)$ is a positive definite form, the Maslov index n_Q along a classical trajectory is equal to the Morse index [8]: this is true for the time-dependent (in $\tilde{M}$) or time-independent (in M) problems $\left(\text{but only in the Q-chart for } H_{cl} = \frac{p^2}{2m} + V, \text{ V arbitrary}\right)$. Since the canonical operator $\tilde{\Pi}_Q^{\Lambda}$ has a phase i^{-n_Q} it introduces a phase loss of $\pi/4$ per focal point encountered.

It also follows from Hormander's theory [28] that the time-dependent Green's function $G_t(q, q')$ $(0 < t < \infty)$ has a WKB form, with $\tilde{\Lambda}$ generated by the trajectories in $\tilde{M}$ radiating at time $t = 0$ from the source point q' (this will not be true in the time-independent case). So the time dependent problem admits a uniform semi-classical approximation.

Under reasonable conditions (the flow $\tilde{U}_t$ must be continuous and proper) the approximation will be uniform for finite times. We assert nothing about the $t \to \infty$ behaviour of the method.

8) Time-independent problems

Time-independent problems could in principle be treated along the same lines. To any WKB wave ψ^E such that $H\psi^E = E\psi^E$ corresponds an invariant Lagrangian manifold $\Lambda \subset \hat{\Sigma}_E$ (cf., 2, § 7) such that

$$\psi_Q^E(q) \sim a_0^Q \exp\left(i\lambda \int_\Lambda \theta_Q\right).$$

If η is a volume on Λ, the semi-classical amplitude $a_0^{\Lambda,\eta}$ is such that the density (= positive l-form) $|a_0^{\Lambda,\eta}|^2\eta$ on Λ must be invariant by the flow. Solutions ψ_E are thus described by the invariant densities on Λ.

If Λ is not compact we expect in general $\psi_Q^E \notin L^2$ (a generalized eigenvector of the continuous spectrum). For instance, Λ defined by (22) and by the $(q_l = -\infty)$ boundary conditions: $p_1 = \ldots = p_{l-1} = 0$, $p_l = \sqrt{2mE}$ describes the scattering of an incident wave $\exp\left(\frac{i}{\hbar} p_l q_l\right)$ (cf. the eikonal method [22] [33]).

If Λ *is compact* $\psi^{E} \in L^2(\Lambda, \eta)$ describes an eigenstate, but we suggest in § 9 that if E is a bound energy, ψ^{E} will often not have a WKB form and no $\Lambda \subset \hat{\Sigma}_E$ will exist. Here we assume that ψ^{E} is a WKB wave for all E. Then the quantization of the spectrum is concretely realized by the rules (64). Since there are in general l independent cycles on Λ ($\Rightarrow l$ equations (64)), and since Λ is determined by l parameters, among which the energy E, only a discrete subset $\{ E_n \}$ will satisfy the Bohr rules. We now make a digression on their meaning in this framework.

a) On the one hand, the Bohr spectrum is related to the discrete spectrum of the *classical system* [*13*] $\left(\Lambda, \eta, -i\dfrac{d}{dt}\right)$, i. e. the spectrum of the time-translation generator on $L^2(\Lambda, \eta)$, or « Liouville operator ». This appears clearly in one dimension, where Λ is a closed curve (an energy shell $\hat{\Sigma}_E$ in $M = \mathbb{R}^2$); if T_E is the period of the curve, the classical spectrum is $\left\{ \dfrac{2\pi n}{T_E} \right\}_{n\in\mathbb{Z}}$; the spectrum of the semi-classical Hamiltonian $\left(E - i\hbar\dfrac{d}{dt}\right)$ (acting on $\Lambda = \hat{\Sigma}_E$) is $\left\{ E - \dfrac{2\pi n\hbar}{T_E} \right\}$. The Bohr rule (64) says:

$$S(E_n) = \int_{\hat{\Sigma}_{En}} p\,dq = 2\pi\left(n + \frac{n_Q}{4}\right)\hbar \qquad (n_Q = \text{Maslov index of } \hat{\Sigma}_E)$$

but (cf. ref. [*2*]) $\dfrac{\partial S}{\partial E} = T_E$, implying that for energies near E, the spacing of the Bohr eigenvalues has the Taylor expansion:

$$E_{n+1} - E_n = \frac{2\pi\hbar}{T_{E_n}}\left(1 - \pi\hbar\frac{1}{T_{E_n}^2}\frac{dT}{dE} + 0(\hbar^2)\right).$$

The first term gives the semi-classical spacing; the second term becomes negligible in the limit $T \to \infty$ (which often coincides with the large quantum number limit) or $\dfrac{dT}{dE} \to 0$ (where one keeps only the quadratic fluctuations only around the classical path). For the harmonic oscillator the semi-classical spacing is exact everywhere (and uniform). In several dimensions we expect the same results but since the spacing of levels has several generators the picture is more complicated (see section 7).

b) On the other hand, the Bohr rule gives not only the spacing but also an absolute position to the eigenvalues; in particular the Maslov indices play a non-trivial role in fixing the zero-point energy of the system. The relation of the Bohr spectrum to the *exact* discrete spectrum results from the L^2 estimate (67): it implies that if the exact spectrum is simple, with a spacing of order $0(\hbar)$, then the Bohr spectrum approximates it at order $0(\hbar^2)$. Heuristically, one writes (66) as:

$$H = H_{s.c.} + \hbar^2 . \delta H$$

and one applies standard perturbation theory to the (unperturbed) Bohr spectrum and Maslov-WKB eigenvectors. In principle it should work if the Maslov WKB solutions belong to the domain of δH (δH is essentially a PDO of degree 2) and if in some sense the unperturbed level spacing is large with respect to the size of δH. Meaningful perturbative calculations require the use of the semi-classical representation, which however is extremely unpractical at higher orders.

9) **Recurrence problems**

Little notice seems to have been paid in the literature to a difficulty which concerns the time-independent Maslov method, and restricts its theoretical and practical use to a limited class of dynamical systems (see § 10). On a formal level the time-dependent and time-independent WKB problems are solved alike, by finding a Lagrangian manifold $\tilde{\Lambda} \subset \tilde{M}$ (resp. $\Lambda \subset M$) satisfying the Hamilton-Jacobi eq. (23) (resp. (22)), and by loading it with an invariant density. We shall now view $\tilde{\Lambda}$ or Λ as generated by classical paths (theorems 2, 3). Indeed $\tilde{\Lambda}$ was generated (§ 7) by the trajectories through an initial l-manifold [10] Λ_0^l, and the density $\tilde{\eta}$ was the pullback along the same paths of an initial density. Locally, we can also realize Λ as the union of the paths through an initial manifold $\Gamma^{l-1} \subset \hat{\Sigma}_E^{2l-1}$ but *globally* we cannot ensure that the union of the full-length $(-\infty < t < +\infty)$ paths through Γ^{l-1} will form an *l-submanifold* of M: if just one path is recurrent it may alone « fill » (by closure) a manifold of dimension up to $(2l - 1)$. For regular scattering problems this trouble will not occur, so the WKB (or eikonal) theory is possible. But recurrent paths are a fairly general feature of *bound state* problems.

For the worst case of an *ergodic* system, Birkhoff's theorem [*34*] [*35*] implies that almost every path fills $\hat{\Sigma}_E$, and that the pullback of any initial density given on (almost any) Γ^{l-1} is the invariant measure $\Omega_E = C\delta(H_{cl} - E)\Omega$ obtained in (55) by the Wigner method and concentrated on $\hat{\Sigma}_E^{2l-1}$ (while the WKB density (65) is concentrated on an l-manifold). For $l > 1$, this means that the eigenstates of H are not « pure-classical » and do not have WKB expansions. Only the weaker Wigner method seems available for them. The argument does not quite exclude the existence of some Lagrangian manifolds generated by exceptional non-ergodic paths, but with such implicit objects the examples of § 12 suggest that no calculation is manageable. We conclude that for all practical purposes, the Maslov method is then useless.

([10]) We shall sometimes exhibit the dimension as an upper index.

10) Completely integrable systems

There exists an amount of degeneracy which is exactly sufficient (and practically necessary, by arguments as in § 9) to make the Maslov-WKB method work smoothly: it is the completely integrable situation.

Assume that the quantum system admits l commuting observables F_j, with $F_1 = H$, where every F_j is an *admissible* observable quantized à la Weyl and the relations: $[F_j, F_k] = 0$ are meant as *identities* in the parameter λ. Then (50) and (51) imply : $\{ (F_j)_{cl}, (F_k)_{cl} \} = 0$, thus making the classical system completely integrable. We have introduced in section 2, § 5*b*, the Lagrangian foliation $\{ \Lambda_\alpha \}_{\alpha \in \mathbb{R}^l}$ defined by the equations $\{ F_j^{cl}(x) = \alpha_j \}$: each Λ_α is a good candidate for the time-independent WKB method since $\Lambda_\alpha \subset \hat{\Sigma}_{E(=\alpha_1)}$; it carries a natural invariant density (19); using (19'), (24) and (62) we find the semi-classical wave in the Q-chart:

$$\psi_Q(q) = \sum_{x \in \Pi_Q^{-1}(q)} \left| \frac{D(p_1, \ldots, p_l)}{D(F_1, \ldots, F_l)}(x) \right|^{1/2} i^{-n_Q(\gamma_x)} e^{i\lambda S_Q(x)} . \qquad (68)$$

Since $F_1, \ldots, F_l$ play the same role, ψ_Q will be a joint eigenstate of all F_j provided Λ_α satisfies the Bohr rules; the solutions $\{ \alpha_j \}$ represent the *joint spectrum* of the commuting set $\{ F_j \}$ (all that in the semi-classical approximation). If Λ_α is compact and connected, it is homeomorphic [*13*] to a torus T^l (the direct product of l circles) therefore it has exactly l independent cycles, each giving rise to a Bohr quantization condition.

We remark that for a cycle, the Maslov index is *always even*, since it jumps by ± 1 every time the jacobian changes sign along the cycle ([11]).

There is also a natural picture using paths: if the motion is ergodic on the Λ_α then almost every classical trajectory fills a Λ_α, and its measure dt (t = time) generates in the sense of averages precisely the unique invariant measure η_α (by Lewis's ergodic theorem [*35*]). That trick solves (22) without referring to any initial conditions (which would involve a degree of arbitrariness not present in the solution). Unfortunately if the quantum system has more degeneracy than strictly needed (i. e. more than l commuting admissible observables), the ergodicity of the classical system is correspondingly reduced and the path picture collapses. The Maslov method works anyway, but the explicitly constructible family $\{ \Lambda_\alpha \}$ is not unique, moreover on each Λ_α there is an infinity of invariant densities. That is the way quantum degeneracy shows up in a semi-classical representation.

The problem is much worse if the additional degeneracy is caused by a *non-admissible* commuting observable, for instance by a discrete symmetry operator. Arnold [*36*] provides the example of a plane cavity having the

([11]) This is true on any orientable Lagrangian manifold.

symmetry group of the equilateral triangle: semi-classical waves are 3-fold degenerate by geometrical arguments, but it is possible to show that the exact modes have multiplicity ≤ 2. The three semi-classical waves behave like three resonators of the same frequency weakly coupled through the quantum perturbation $\hbar^2 . \delta H$: this term mixes the states and splits the levels (partially or totally): the latter effect is small but the first one is not (and depends crucially on δH). The situation of Λ having several connected components presents the same problems.

More generally we expect the WKB formulæ for eigenstates to be inaccurate whenever the corresponding semi-classical levels are degenerate or almost degenerate, since the necessary information to approximate the states is missing at the semi-classical level.

11) Explicit examples of completely integrable systems

a) *1-dimensional systems* ($l = 1$): the family $\{ \Lambda_\alpha \}$ coincides with the energy shells $\{ \Sigma_E \}$, the singular set on each Λ is the set of turning points; (68) becomes:

$$\psi_Q(q) = \sum_{x \in \Pi_Q^{-1}(q)} | p(x) |^{-1/2} i^{-n_Q(x)} \exp \left(i\lambda \int_{x_0}^{x} pdq \right). \qquad (69)$$

The 1-dimensional case is exceptional in many respects; all curves are trivially Lagrangian; the energy shells coincide with the classical paths, they are either unbounded or periodic: in the latter case, provided a path is homotopic to a circle, its Maslov index is just $2 \times$ (number of turns) so that formulae (55) and (64) coincide.

A remarkable example is the harmonic oscillator (fig. 5): $\{ \hat{\Sigma}_E \}$ is a

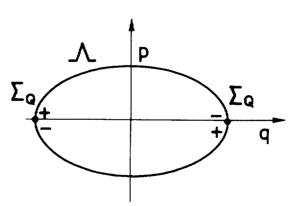

FIG. 5.

family of concentric ellipses and the Bohr (or Thomas-Fermi) rule gives

$$2\pi\left(n + \frac{1}{2}\right)\hbar = \oint_{\Sigma_E} pdq = \iint_{H<E} dpdq = 2\pi E. \qquad (70)$$

b) *Separable systems*: when separation of variables is possible, it leads to a complete integral [3] of the classical system, therefore a family $\{ \Lambda_\alpha \}$ and a semi-classical solution can be computed; but the same result would have been obtained by applying the 1-dimensional WKB method to each variable of the quantum equation separately. For example, 3-dimensional potentials are treated in Appendix 2.

12) Examples of non-integrable systems

For such systems one cannot fill the region of bound states $\mathscr{B}$ by a family $\{ \Lambda_\alpha \}$ of Lagrangian manifolds. However in a few cases one can almost do it.

a) For the *billiard ball problem* in a finite domain of $\mathbb{R}^2$ with a convex regular boundary, Lazutkin [37] has shown the existence, in a neighborhood of the boundary, of (closed) « caustic » curves such that a classical path remains tangent to it after an arbitrary number of reflections on the boundary. The tangents to a caustic curve generate an invariant Lagrangian manifold Λ (for the singularity at the boundary, see § 13) homeomorphic to a torus T^2. Unfortunately the caustic curves do not fill even a neighborhood of the boundary in $\mathscr{Q}$, only their relative density tends to 1 as we approach the boundary (itself a limiting caustic curve); the paths enveloping the caustics must satisfy conditions of an *irrational* nature and the caustics cannot be constructed explicitly. Not to speak of the difficulties of practical computations using those Lagrangian manifolds, it is impossible to determine which of them, if any, satisfy the Bohr rules (64) which are of a rational nature. There is an exception: for the elliptic boundary, the caustics are *all* the cofocal ellipses and the WKB method works throughout [38].

b) For a system differing from a completely integrable system by a *small perturbation* the Kolmogorov-Arnold-Moser implicit function theorem asserts the existence of invariant Lagrangian manifolds. Let $\{ \Lambda_\alpha \}$ be the Lagrangian foliation of the unperturbed system; fix $\Lambda \subset \{ \Lambda_\alpha \}$, Λ is homeomorphic to a torus T^l and we can define mod 1 the rotation numbers $(v'_1, \ldots, v'_l)$ of the classical flow: $v' = (v'_1, \ldots, v'_l)$ is the velocity of a linear flow on T^l which averages the classical flow in time. If v' satisfies some condition of *irrationality* there exists an invariant Lagrangian manifold of the perturbed system which goes to Λ as some norm ε of the perturbation tends to 0; moreover the manifolds obtained in this way fill a subset of M of relative measure tending to 1 as $\varepsilon \to 0$ (there exist various precise statements of this according to the regularity requirements on the data, see refs. [13] and [39] for details). On the other hand, it is known since Poincaré [14] that a Λ with rationally dependent rotation numbers is unstable and breaks up into a very complicated pattern of closed paths. The situation is as bad as in the preceding case for explicit computations.

13) Discontinuous potentials

It is standard to apply the WKB method in the case of discontinuous potentials. The classical trajectories are then reflected by the singularities of the potential. But these turning points are essentially different from caustic turning points, which have nothing to do with any singularities of the potential (fig. 1); accordingly, the phase discontinuity depends on the dynamics and is no longer a Maslov index. For reflection on a wall with Dirichlet boundary conditions, the incident and reflected waves have opposite phases, so the semi-classical phase shift is taken to be π (cf. section 7, § 9 and Appendix 2, *c*). But the mathematical theory is less advanced, so we take this only as a heuristic extension of the WKB method.

14) The scope of the Maslov-WKB method

The value of the method is that it yields the classical limit in a Hilbert space framework: the limiting « classical » Hilbert space is $L^2(\Lambda, \eta)$ (depending on ψ, of course) and many observables reduce to translation operators induced by flows on Λ; this scheme serves as a skeleton to non-euclidean quantization (see section 6). But there are serious conceptual and practical obstacles against extending the method to all powers in $\hbar$.

For bound states, the method applies well to completely integrable systems (in practice this means separable systems, so that the computing power is the same as for the 1-dimensional WKB method); moreover no discrete degeneracy must be present. Then the Bohr-Sommerfeld-Maslov levels are exact at $0(\hbar^2)$ if the spacing is $0(\hbar)$, and the normalized eigenvectors are strongly approximated at $0(\hbar)$.

For non-separable systems, classically ergodic on manifolds of dimension $> l$, the Maslov method does not apply. On the other hand we show in section 7 that a non-separable system for which there exist *stable closed trajectories* (a non-ergodic property) can be approximated by a linearized system for which the Maslov-WKB method is *fully applicable.*

6. GEOMETRIC QUANTIZATION

For classical systems such as rotators, constrained systems ... the formalism of section 2 is too restrictive. The phase space is then a general symplectic manifold (M, ω), i. e. a $2l$-manifold M with a non degenerate, closed ($d\omega = 0$) differential form ω of degree 2 (refs. [*23*] to [*25*]). The search for a canonical quantization of such systems, generalizing the Weyl rule (46), has a long history. *Geometric quantization* attempts to define a general procedure solely in terms of the symplectic structure (with possible applications to relativistic spinning particles [*40*] [*41*], systems in curved space-time, non-trivial field theories, ...). We shall not treat the subject here (refs. [*24*] [*42*] [*43*]), only give a few remarks in close connection with section 5 and suggest why the method does not seem to solve physical problems.

1) The semi-classical structure and the integrality condition

A reasonably quantized system should give the same semi-classical structure as in section 5, inasmuch as the cartesian nature of M does not come into play. The quantum Hilbert space $\mathscr{H}$ should contain semi-classical vectors to which are associated constant densities on Lagrangian manifolds of M. Therefore to any Lagrangian foliation $\{\Lambda_\alpha\}$ we can associate a « semi-classical Hilbert space » $\mathscr{H}_{\{\Lambda_\alpha\}} = \int_\alpha^\oplus \mathbb{C}_\alpha$ where $\mathbb{C}_\alpha$ is the 1-dimensional Hilbert space spanned by the invariant half-density $\sqrt{\eta_\alpha(x)}$, η_α being the invariant volume on Λ_α.

Any non-trivial cycle $\gamma \subset \Lambda_\alpha$ must satisfy some quantization rule analogous to (64). But whereas in (64) $\oint_\gamma \theta_K$ could be replaced by $\oint_\gamma \theta$ with θ: any 1-form such that $\omega = d\theta$, here no such θ will exist if the closed form ω is not exact, i. e. if its class $[\omega]$ in the (de Rham) cohomology $H^2(M, \mathbb{R})$ is $\neq 0$; θ can always be defined *locally* so we can define $\oint_\gamma \theta$ by addition of pieces but this value has a *global* ambiguity ([12]): if γ is moved around and back to itself so as to generate a closed 2-surface σ without boundary (a 2-cycle: we note $\sigma \in Z_2(M)$), $\oint_\gamma \theta$ is shifted by the value $\int_\sigma \omega$ (using the Stokes theorem). So the Bohr rules (64) are consistent *iff* M *satisfies the integrality condition* [*24*] [*43*]:

$$\forall \sigma \in Z_2(M) \qquad \frac{1}{2\pi\hbar}\int_\sigma \omega \qquad \in \mathbb{Z}. \tag{71}$$

If non-trivial cycles (i. e. not homotopic to 0) exist, eq. (71) impose « *pre-quantization* » conditions on M; then we can quantize the manifolds Λ_α using (64), if we assume the existence of the Maslov index.

2) Example : the non-relativistic spin

Let $\vec{s} = s\hat{u}$ be a spin of fixed length s. The phase space is $(M, \omega) = (S^2, s\Omega)$ where S^2 is the unit sphere and Ω is the euclidean area (this ω leads to the

([12]) Physically: the action function is not globally defined, only its variation is.

correct Larmor equation [24] [40]). Eq. (71) yields for the only non-trivial 2-cycle $\sigma = \mathrm{M}$:

$$\int_{\mathrm{M}} s\Omega = 4\pi s = 2\pi n\hbar \quad \text{or} \quad s = \frac{n\hbar}{2} \qquad \textit{(integer or half-integer spins)}$$

Semi-classically (cf. (55)) the volume of M in units $2\pi\hbar$ gives the dimension of the Hilbert space $d = 2j + 1$; here $d = \frac{2s}{\hbar} \Rightarrow s = \left(j + \frac{1}{2}\right)\hbar$ (compare to the Langer shift of Appendix 2).

3) The Kostant-Souriau quantization

(Very roughly speaking) takes the desired semi-classical structure as an input, e. g. defines the quantum Hilbert space as $\mathscr{H}_{\Lambda_\alpha}$ for some $\{ \Lambda_\alpha \}$ provided M satisfies (71). Unfortunately, two different foliations give in general unitarily inequivalent Hilbert spaces. We think this is related to the fact that the canonical structure alone cannot predict the higher powers of $\hbar$ which are inevitably present in a quantum theory (in the euclidean theory, cf. eqs. (52), (60), (65), etc.). Higher powers of $\hbar$ can be consistently discarded only if there exists some large symmetry group. Then quantization is related to the important classification by Kostant [42] of the representations of the group (with the Poincaré group it leads to the usual description of free relativistic spinning particles).

For the reasons given here it seems that the method as it stands cannot deal consistently [43] with interacting systems (apart from exceptional potentials with high symmetry).

7. QUANTIZATION ALONG CLOSED PATHS

For a general non-separable, non-ergodic system, all the previous methods fail. We are going to show that the periodic, Poincaré stable, classical trajectories can be used to construct a semi-classical approximation. Generically there are (infinitely) many closed paths; all we need is to find a « simple » (explained later) *stable* one and to compute its linearized Poincaré map; this is much simpler than to compute Lagrangian manifolds. The price to pay is some loss of accuracy.

1) Previous results

We recall the study of closed paths by Poincaré [14], and their quantization by the Bohr-Sommerfeld rule. More recently, Balian and Bloch [16] have shown that the quantum density of modes in a cavity

$$\rho(k) = \frac{1}{\pi} \int dq \, [\mathrm{Im}\, \mathrm{G}_{k^2 + i0}(q, q')]_{q' = q}$$

can be expanded by the stationary phase method if the time-independent Green's function is given a semi-classical form

$$\mathrm{G_E}(q, q') = \mathrm{A}(q, q') \exp\left(\frac{i\mathrm{S}(q, q')}{\hbar}\right).$$

Each stationary phase corresponds to a closed path of energy E and yields an oscillatory contribution $\sin \frac{\mathrm{L}k}{\hbar}$ to $\rho(k)$, L being the length of the path; $\mathrm{L} = 0$ gives the monoscillating Thomas-Fermi contribution (56); analogous results hold for the Schrödinger equation [*17*]. They have found moreover that for the spherical cavity the sum of a few first oscillating terms (corresponding to the shortest paths) is already sharply peaked near the exact levels; this looks like a miracle.

Gutzwiller [*18*] uses a slightly different approach: since one closed path gives a contribution $\exp(i\mathrm{S_E}/\hbar)$ to $\int \mathrm{G_E}(q, q)dq \left(\text{where } \mathrm{S_E} = \oint pdq\right)$ then the same path repeated m times contributes $\exp(im\mathrm{S_E}/\hbar)$ and the sum contributes $\sum_m \exp(im\mathrm{S_E}/\hbar) = \sum_n \delta(\mathrm{S_E} - 2\pi n\hbar)$, i. e. a series of sharp levels. He finds moreover that the stability exponents and the focal points act to shift all the levels together, but his proof works only for $l = 2$. Besides, in a neighborhood of a simple closed path there will in general exist paths which close up after a considerable number M of turns, and it is not clear whether these should be treated separately in the same way or counted together with the « simple » path repeated M times. Finally we need to understand the relation between the Balian-Bloch and the Gutzwiller methods of building the quantized levels; at first sight they seem orthogonal to each other.

2) The Fourier transform of the spectrum

The semi-classical form for $\mathrm{G_E}(q, q')$, used by Balian and Bloch, is not justified (see section 5, § 9). To get mathematically rigorous results we must use the time-dependent formalism. The corresponding result holds under mild assumptions [*44*]:

THEOREM 5. — If

$$\rho(t) = \int \rho(\mathrm{E}) \exp(i\mathrm{E}t/\underline{\hbar})d\mathrm{E} = \sum_n \exp(\pm\, i\mathrm{E}_n t/\underline{\hbar})$$

(for $\{\mathrm{E}_n\}$ = the spectrum of a positive elliptic PDO of order 2, assuming the spectrum discrete) then $\rho \in \mathscr{D}'$ and sing supp $\rho = \{\pm \mathrm{T}, 0\}$, where T runs over the set of periods of *all* closed bicharacteristics.

The proof uses the stationary phase expansion of $\rho(t) = \int G_t(q, q)dq$ where the time dependent Green's function can rigorously be written [28] $G_t = A_t(q, q') \exp\left(\frac{iS_t(q, q')}{\hbar}\right)$. Since a singularity of $\tilde{\rho}(t)$ at $t = T$ describes an oscillation of $\rho(E)$ of period $\Delta E = \frac{2\pi\hbar}{T}$, the theorem corresponds to the Balian-Bloch results.

3) The converse problem

Theorem 5 gives the discrete classical periods, knowing the oscillations of the quantum spectrum. But the problem of quantization goes in reverse: find discrete levels in the quantum spectrum, knowing the classical closed paths. Unfortunately we have no inverse Fourier transformation yielding $\rho(E)$ in terms of the singular part of $\tilde{\rho}(t)$ only, given by the closed paths. There is an exception however: for the linear flow on the unit circle $E_n = n\hbar$; theorem 5 reduces to the Poisson formula:

$$\rho(t) = \sum_{n \in \mathbb{Z}} e^{int} = \sum_{m \in \mathbb{Z}} \delta(t - 2m\pi).$$

The converse problem is solved by the dual Poisson formula:

$$\sum_{m \in \mathbb{Z}} \exp\left(\frac{2\pi m i E}{\hbar}\right) = \sum_{n \in \mathbb{Z}} \delta(E - n\hbar)$$

(and similarly for a linear flow on a torus T^l); the spectrum is thus generated by summation over repeated paths. The dual Poisson formula will now be applicable to an arbitrary system if we can linearize its flow by action-angle coordinates on invariant tori T^l: this will be performed by the Maslov method in the neighborhood of a closed stable path.

4) The linearized system

Let: $t \in [0, T] \to \gamma(t) \in M = \mathbb{R}^{2l}$ be a closed classical path of energy E and of period $0 < T < \infty$: $x_0 = \gamma(0) = \gamma(T)$. The case $l = 1$ is exceptional and has been treated in section 5, § 12; we assume $l > 1$. We suppose γ « simple » meaning that for all x_1 in a neighborhood of x_0 (of volume $= 0(\hbar^l)$), the classical trajectory $t \in [0, T] \to x(t)$ such that $x(0) = x_1$ is smooth and has *no multiple points*; the idea is that quantities like T, the size of the path, the radius of curvature, etc. should be *macroscopic*, i. e. finite and continuous when $\hbar \to 0$, even if quantum fluctuations are present. We shall also suppose (this is less important) that the projection on $\mathcal{Q}$, $\Pi_Q(\gamma)$, should be simple.

The Poincaré map [13] $x(0) \to x(T)$ has the fixed point x_0; the tangent map P at x_0 is the linear part of $(x_0 + \delta x(0)) \to (x_0 + \delta x(T))$ where

$$\frac{d}{dt}(\delta x(t)) = \sharp d(\delta H(t)) = \begin{pmatrix} \dfrac{\partial^2 H(x)}{\partial p \partial q} & \dfrac{\partial^2 H(x)}{\partial p^2} \\ \dfrac{\partial^2 H(x)}{\partial q^2} & -\dfrac{\partial^2 H(x)}{\partial p \partial q} \end{pmatrix}_{x=\gamma(t)} \times \begin{pmatrix} \delta q \\ \delta p \end{pmatrix} \tag{72}$$

In terms of the reduced action $S_E(q', q'')$, P is given in matrix form by:

$$\begin{pmatrix} \delta q'' \\ \delta p'' \end{pmatrix} = \begin{pmatrix} -\left(\dfrac{\partial^2 S_E}{\partial q' \partial q''}\right)^{-1} \left(\dfrac{\partial^2 S_E}{\partial q'^2}\right) & -\left(\dfrac{\partial^2 S_E}{\partial q' \partial q''}\right)^{-1} \\ \left(\dfrac{\partial^2 S_E}{\partial q'' \partial q'}\right) - \left(\dfrac{\partial^2 S_E}{\partial q''^2}\right)\left(\dfrac{\partial^2 S_E}{\partial q' \partial q''}\right)^{-1} & -\left(\dfrac{\partial^2 S_E}{\partial q''^2}\right)\left(\dfrac{\partial^2 S_E}{\partial q' \partial q''}\right)^{-1} \end{pmatrix}_{q=q'=\Pi_Q(x_0)} \times \begin{pmatrix} \delta q' \\ \delta p' \end{pmatrix} \tag{73}$$

We know that $P \in \mathrm{Sp}(2l)$ and that if we change $x_0 = \gamma(0)$ to $\gamma(t_0)$, P is only changed by a symplectic equivalence $P \to S_{t_0} P S_{t_0}^{-1}$; $S_{t_0} \in \mathrm{Sp}(2l)$: $T_{\gamma(0)}(M) \to T_{\gamma(t_0)}(M)$, and $S_{t_0} = TU_{t_0}$, where U_t is the classical flow.

By standard results [23]: the eigenvalues of P come in quadruples $\left(\lambda, \dfrac{1}{\lambda}, \bar{\lambda}, \dfrac{1}{\bar{\lambda}}\right)$ or pairs $\left(\lambda, \dfrac{1}{\lambda}\right)_{\lambda \in \mathbb{R} - \{0\}}$ or pairs $(e^{iv}, e^{-iv})_{v \in \mathbb{R}}$: we assume that only the last case occurs, i. e. γ is a *stable path.* There exist canonical coordinates $\delta x = \begin{pmatrix} \delta y \\ \delta z \end{pmatrix}$ in which $P = \prod_{j=1}^{l} P_j$ where P_j is the rotation by v_j in the 2-plane $\mathbb{R}_j^2$ spanned by $\{\delta y^j, \delta z_j\}$ and oriented by the symplectic form $\omega\left(= \sum dz_j \wedge dy^j\right)$.

The v_j are called the *angles of rotation* (they are functions of E); at least one, say v_1, is equal to 0. To avoid difficulties, we moreover assume $v_1, \ldots, v_l$ *all distinct and* $\neq \pi$ mod 2π (and we select the determination $|v_j| < \pi$). Then γ is *parametrically stable* [13] (a property preserved under small perturbations); also, γ actually belongs to a *continuous family* $\{\gamma_{E'}\}$ of closed orbits of the exact system [23], of energies E′ (for E′ near E), of periods $T_{E'}$; and $\gamma_E = \gamma$. The reduced action $S(E') = \oint_{\gamma_{E'}} p dq$ is the Legendre transform of the time-dependent action (cf. section 2, § 8) for $t = t_{E'}$; so, at $E' = E$ for instance [3]:

$$\frac{dS(E)}{dE} = T \tag{74}$$

The invariant eigenspace $\mathbb{R}_1^2$ (for $v_1 = 0$) is spanned by the directions of time translation along γ and of energy increase in the family $\{ \gamma_{E'} \}$; so we can choose $\delta y^1 = \delta t$ and $\delta z_1 = \delta E$: the latter follows from the independence relations and eq. (72):

$$\delta_1^j = \frac{d(\delta y^j)}{d(\delta y^1)} = \frac{d(\delta y^j)}{d(\delta t)} = \frac{\partial(\delta H)}{\partial(\delta z_j)} \quad \text{and} \quad 0 = \frac{d(\delta z_j)}{d(\delta y^1)} = \frac{d(\delta z_j)}{d(\delta t)} = \frac{-\partial(\delta H)}{\partial(\delta y^j)}$$

which imply that the direction δz_1 is the normal to the energy shell $\hat{\Sigma}_E$. We shall now remain in $\hat{\Sigma}_E$ and fix $\delta E = 0$. The remaining planes $\mathbb{R}_j^2$ ($j = 2, \ldots, l$) are called *transversal*. Any vector $\delta x // \Sigma_E$ can be decomposed as $\delta x = (\delta t, \delta x')$, $\delta x'$ denoting the transversal part. Also, primed (resp. unprimed) indices will run from 2 to l (resp. 1 to l). All transversal tori $\Gamma_{\delta E_2} \times \ldots \times \Gamma_{\delta E_l}$ are preserved by P, where $\Gamma_{\delta E_{j'}}$ is the circle in $\mathbb{R}_{j'}^1$:

$$\Gamma_{E_{j'}} = \left\{ \delta x_{j'} \in \mathbb{R}_{j'}^2 \,\middle|\, \frac{1}{2}(\delta y^{j'2} + \delta z_{j'}^2) = \delta E_{j'} \text{ (const)} \right\} \tag{75}$$

The linearized system (72) is *completely integrable* because $\{ \delta E, \delta E_{j'} \}$ are in involution. The invariant foliation $\{ \Lambda_\alpha \}$ is given by the equations: $\{ \delta E = \alpha_1, \delta E_{j'} = \alpha_{j'} \}$; We now fix $\Lambda_\alpha \subset \hat{\Sigma}_E$ (α_j fixed, $\alpha_1 = 0$: now we shall omit the subscript α everywhere). Each constant time section Λ^t of Λ is an image of the torus $T^{l-1} = \Gamma_{\alpha_2} \times \ldots \times \Gamma_{\alpha_l}$ (see eq. (75)); the image in Λ^t of the circle $\Gamma_{\alpha_{j'}}$, denoted $\Gamma_{j'}^t$, carries a natural angular coordinate $\theta_{j'}^t$. The dynamical behaviour of Λ^t is that of an $(l - 1)$-dimensional harmonic oscillator representing transversal fluctuations around the path; taking them *small* makes the linear approximation reasonable (fig. 6).

The linearized flow $\tilde{U}_{t'}$ carries Λ^t onto $\Lambda^{t+t'}$; moreover $\Lambda^{t+T} = \Lambda^t$ and

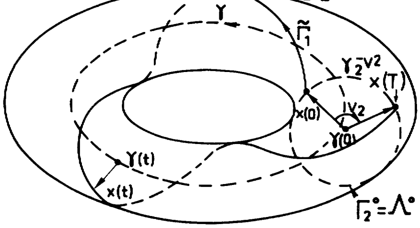

FIG. 6.

$\Gamma_{j'}^{t+T} = \Gamma_{j'}^{t}$ $\left(\text{thus } \Lambda = \bigcup_{0 \leq t < T} \Lambda^t \text{ is a torus } T^l\right)$ but each $\Gamma_{j'}$ has rotated by an angle $v_{j'}$ (mod. 2π) under the flow. This « twist » prevents the separation of variables, and there are no nice angular coordinates $\theta_{j'}$ global in t.

The invariant volume on Λ is, using eqs. (19) and (75):

$$\eta = C\delta(\delta E)\delta^{(l-1)}(\delta E_{j'} - \alpha_{j'}).\Omega = Cdt \wedge d\theta_2^t \wedge \ldots \wedge d\theta_l^t .$$

5) The semi-classical formalism

We now apply the Maslov method to the *linearized problem*. To compute the Maslov index we need a basis of the homology of Λ, represented by l independent cycles. Of these, $(l-1)$ can be taken as the circles $\Gamma_{j'}^t$ at some arbitrary t (transversal cycles); we need a longitudinal cycle Γ_1 running once along to complete the basis; such a Γ_1 is only defined up to the addition of any number of transversal cycles, but this will not affect the final results. We propose:

a) To choose Γ_1 not intersecting the singular set $\Sigma_Q \subset \Lambda_\alpha$ of the projector Π_Q; unfortunately Γ_1 might not exist if the geometry of Λ_α is too twisted (Γ_1 does exist if the problem is separable, or if $l = 2$). *If Γ_1 exists*, it defines a unique homotopy class, which moreover stays unchanged under a continuous canonical displacement of the coordinate frame of M (redefining Q and Π_Q) as long as $\Pi_Q(\gamma)$ remains *simple* (the proof relies on the fact that if $\Pi_Q(\gamma)$ is simple the structure of the transversal sections Λ_α^t *and* Σ_Q^t is the same as for an $(l-1)$ dimensional harmonic oscillator). Clearly Γ_1 winds up *minimally* around γ with respect to cartesian coordinates, therefore the basis $\{\Gamma_1, \ldots, \Gamma_l\}$ is the most appropriate to measure the « twist » of any cycle on Λ_α. The Maslov index of Γ_1 is 0.

b) A more dynamical (and always possible) choice $\tilde{\Gamma}_1$ is built with a physical path $x(t)$ $(0 \leq t \leq T_E)$ on Λ_α: since rotations by $(-v_{j'})$ on $\Gamma_{j'}^0$ bring $x(T)$ back onto $x(0)$, the path $x(t)$ can be closed to a cycle $\tilde{\Gamma}_1$ by adding to it arcs $\gamma_{j'}^{-v_{j'}} \subset \Gamma_{j'}^0$, of angles $(-v_{j'})$ (fig. 6). In spite of some arbitrariness, the homotopy class of $\tilde{\Gamma}_1$ is unique; we shall denote the (even) number $n(\tilde{\Gamma}_1)$ which, by continuity is independent of α, the *rotation index* $n(\gamma)$ of the path.

If Γ_1 exists as in *a*) we can express the class of $\tilde{\Gamma}_1$ in the basis, $\{\Gamma_1, \ldots, \Gamma_l\}$:

$\tilde{\Gamma}_1 \sim \Gamma_1 + \sum_2^l \omega^{j'}(\tilde{\Gamma}_1).\Gamma_{j'}$: the coefficient $\omega^{j'}(\tilde{\Gamma}_1)$, linear in $\tilde{\Gamma}_1$, gives the number of turns along $\Gamma_{j'}$. This suggests defining the *absolute* angles of rotation $w_{j'} \in \mathbb{R}$ as:

$$w_{j'} = v_{j'} + 2\pi\omega^{j'}(\tilde{\Gamma}_1) .$$

Since $n(\Gamma_{j'}) = +2$ as for the harmonic oscillator (eq. (70)) we also have:

$$n(\gamma) = n(\tilde{\Gamma}_1) = 2\sum_{2}^{l} \omega^{j'}(\Gamma_{j'}) = \frac{1}{\pi}\sum_{2}^{l}(w_{j'} - v_{j'}) . \quad (^{13})$$

Other remarks about $n(\gamma)$ are given in § 12.

We can now quantize Λ. The Bohr rules are:

$$\oint_{\tilde{\Gamma}_{j'}} pdq = \oint_{\Gamma_{j'}} z_{j'}dy^{j'} = 2\pi\delta E_j = 2\pi\left(n_{j'} + \frac{1}{2}\right)\hbar \qquad (n_{j'} \in \mathbb{N}) \tag{76}$$

$$\oint_{\Gamma_1} pdq = 2\pi\left(N + \frac{n(\gamma)}{4}\right)\hbar \qquad (N \in \mathbb{Z}) .$$

We can write any $x \in \tilde{\Gamma}_1$ as $(\gamma(t) + \delta x')$ with $\delta x'$ transversal, for some t, and we introduce the 2-dimensional surface

$$S = \{ \gamma(t) + \tau\delta x' \mid 0 \leq t < T, 0 \leq \tau \leq 1, \gamma(t) + \delta x' \in \tilde{\Gamma}_1 \} .$$

By the Stokes theorem:

$$\oint_{\tilde{\Gamma}_1} pdq - \oint_{\gamma} pdq = \int_S dp \wedge dq = \int_S \omega . \tag{77}$$

Dynamical ingredients enter now: on the part of S corresponding to $t \neq 0$, ω vanishes (because any plane tangent to S for $t \neq 0$ is spanned by δt and some transversal vector). The part of S where $t = 0$ is a union of circular sectors $S_j^{-v_{j'}} \subset \Gamma_j^0$ spanning the arcs $\gamma_{j'}^{-v_{j'}}$, and:

$$\int_{S_j^{-v_j}} dp \wedge dq = \text{area}\left(S_j^{-v_{j'}}\right) = -v_{j'}.dE_{j'} . \tag{78}$$

The transversal energies $\delta E_{j'}$ are not observed, so the only effect of their quantization should appear in the total energy. Putting together eqs. (76) to (78), we obtain the Bohr rule for $\gamma(t)$:

$$S(E) = \oint_{\gamma} pdq = \left[2\pi N + \sum_{2}^{l} n_{j'}v_{j'} + \frac{1}{2}\left(\sum_{2}^{l} v_{j'} + \pi n(\gamma)\right)\right]\hbar . \tag{79}$$

If Γ_1 exists the RHS can also be written (cf. [*18*]):

$$\left[2\pi N + \sum_{2}^{l}\left(n_{j'}v_{j'} + \frac{w_{j'}}{2}\right)\right]\hbar = \left[2\pi N' + \sum_{2}^{l}\left(n_{j'} + \frac{1}{2}\right)w_{j'}\right]\hbar .$$

(13) After completing this work we have become acquainted with ref. [*52*], where this formula (divided by 2) introduces the rotation index as an invariant for deformations of a parametrically stable system.

Of course the angles $v_{j'}$ are functions of E. The formula is meaningful for $|N| \gg 1$ and $0 < n_{j'} \ll |N|$. In that region the spacing of levels is generated (in the approximation where T(E), $v_{j'}(E)$ are constant) by the numbers $\hbar\omega_1$ where $\omega_1 = \frac{2\pi}{T}$, $\omega_{j'} = \frac{v_{j'}}{T}$. If there is a rational dependence relation of the type $\sum_1 v_j\omega_j = 0$ ($v_j \in \mathbb{Z}$, $|v_{j'}| \ll N$), some levels in eq. (79) will be accidentally quasi-degenerate. If the ω_j are rationally independent but if we put no limit on the size of $n_{j'}$, the levels of eq. (79) become more and more dense everywhere, so quasi-degeneracy occurs again. So we restrict the range of the $n'_{j'}s$ to a set $\{ |n_{j'}| \ll N \}$ small enough so that no two levels in eq. (79) are (quasi) degenerate. Another source of (quasi) degeneracy is when there exist several independent closed paths of energy E which are good candidates for γ; we also exclude this case (the negative effects of discrete degeneracy have been discussed in section 5, § 10). Then to any quantized energy E there correspond a unique path γ, unique values $\{ n_j \}$ and a unique manifold Λ_α. Applying the machinery of section 5 we can construct *unambiguously* a semi-classical wave function of energy E. The limiting Hilbert space $\bigoplus_\alpha L^2(\Lambda_\alpha, \eta_\alpha)$ is a (part of a) Fock space built over the transversal fluctuations. Any description of a state vector using Hermite functions depends on a choice of Γ_1 and is not unique. For this we believe that the best choice is given by the minimally twisted Γ_1 (cf. § 5*a*), if it exists.

6) Error estimates

The linear approximation is totally unappropriate for the classical system since it exhibits a non-generic behaviour for the paths whenever these have rationally dependent angles of rotation; but we hope that in the quantum theory such accidents are smoothed out. Heuristically, the linearized treatment drops all terms of H of order $0(\delta x^3)$ which have a size $0((n'\hbar)^{3/2})$ around the tori Λ_α for small $n' = \sup n_{j'}$; so formally eq. (79) is true with a remainder $0((n'\hbar)^{3/2})$, but this is doubtful for quasi-degenerate levels.

THEOREM 6. — On the phase space $\overset{\circ}{M} = R^{2l}/T\mathbb{Z}$ (with q^1 = coordinate on a circle of period T) let $\overset{\circ}{H}_{cl}(x) = \frac{1}{2}\sum_2^l (p_j^2 + \omega_j^2 q_j^2) + p_1 + 0(x^3)$. Suppose the Weyl-quantized operator $\overset{\circ}{H}$ essentially self-adjoint on the domain of $H_0 = \frac{1}{2}\sum_2^l \left(- \hbar^2 \frac{\partial^2}{\partial q_j^2} + \omega_j^2 q_j^2 \right) - i\hbar \frac{\partial}{\partial q^1}$. Then (79) holds (with

$S(E) = ET$, $w_{j'} = T\omega_{j'}$) up to corrections $0(\hbar^{3/2})$ for stable, simple eigenvalues. Sketch of proof: (79) gives the spectrum of H_0 and the correction results from Kato's perturbation theorem [45] for eigenvalues.

The relevance of this to our problem is that there exists a canonical map S from an annular neighborhood of γ in M to a cylindrical neighborhood of the line $\{ q_2 = \dots = q_l = 0 ; p_2 = \dots = p_l = 0 ; p_1 = E \}$ in $\overset{\circ}{M}$, sending t on q^1 and H_{cl} to a function $\overset{\circ}{H}_{cl}(x) = H_{cl}(S^{-1}x)$. Relating the *quantized* operators H and $\overset{\circ}{H}$ is more difficult; we must assume that S extends to a global one-to-one canonical map. Then $\overset{\circ}{H}$ can be thought of as the « Weyl » quantization of H_{cl} in the curvilinear coordinates induced on M by S. The expansion of $\overset{\circ}{H}_w$ must have the same first two terms as H_w (these are canonically determined by H_{cl}) so the difference is $0(\hbar^2)$. It is reasonable to apply perturbation theory and conclude that the spectra of H and $\overset{\circ}{H}$ differ by $0(\hbar^2)$, but because of the global nature of the problem we see no way to prove this in general.

7) Concrete examples

We check the validity of the method on the separable 3-dimensional central potential, for which we know the exact WKB formulæ (Appendix 2; we use the same notations). For every value of $J_3 = M$ we take for γ the circular equatorial trajectory running at the minimum $W(M^2)$ of the

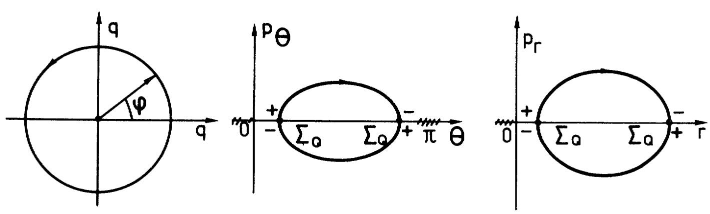

FIG. 7. — Structure of Λ for the $l = 3$ central potential.

effective potential $\left(V(r) + \dfrac{M^2}{2mr^2} \right)$, i. e. γ is the degenerate Lagrangian manifold of equations $\{ H = W(M^2) ; J^2 = M^2 ; J_3 = M \}$, or the path of period $T = \dfrac{2\pi m r_0^2}{M}$ of equations:

$$\begin{cases} r(t) = r_0 & \theta(t) = \dfrac{\pi}{2} & \varphi(t) = \dfrac{Mt}{mr_0^2} \\ p_r(t) = 0 & p_\theta(t) = 0 & p_\varphi(t) = M\,. \end{cases}$$

It is appropriate to remark that $W(M^2)$ is a Legendre transform:

$$W(v) = \left[V\left(\frac{1}{\sqrt{2mu}}\right) + vu \right]_{\frac{dV}{dv} = -v} \qquad \text{where} \qquad u = \frac{1}{2mr^2}$$

so that:

$$\frac{d^2V}{du^2} = -\frac{1}{W''(v)} \qquad \text{for} \qquad v = -\frac{dV}{du} \qquad (\Leftrightarrow u = W'(v)).$$

In particular the radius r_0 of γ satisfies:

$$u_0 = \frac{1}{2mr_0^2} = W'(M^2).$$

The equations of motion of the fluctuations around γ (i. e. $v = M^2$) read:

$$\left(\frac{d}{dt} - A\right)\begin{pmatrix} \delta r \\ \delta\theta \\ \delta\varphi \\ \delta p_r \\ \delta p_\theta \\ \delta p_\varphi \end{pmatrix} = 0 \quad \text{where} \quad A = \begin{pmatrix} 0 & 0 & 0 & m^{-1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 2u_0 & 0 \\ -\lambda & 0 & 0 & 0 & 0 & 2u_0 \\ -m\omega_0^2 & 0 & 0 & 0 & 0 & \lambda \\ 0 & -2M^2u_0^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

and

$$\begin{cases} \lambda = 2^{5/2}M\sqrt{mu_0^3} \\ \omega_0 = (-8W'^3W''^{-1})^{1/2}. \end{cases}$$

Since $\frac{dA}{dt} = 0$, the Poincaré map is just (exp TA). The angles of rotation are (mod 2π) the eigenvalues of $\frac{TA}{i}$: $w_r = T\omega_0$, $w_\theta = 2\pi$, $w_\varphi = 0$. We check that these are the absolute angles of rotation (with the proper signs) when we take the most natural choice for the longitudinal cycle Γ_1 : $\{\delta r = \text{const}, \delta\theta = \text{const}\}$. Quantization of Γ_1 gives $M = m\hbar$; the longitudinal energy being $W(M^2)$, we get the total energy by adding the transversal energies:

$$E_{ml'n'} = W((m\hbar)^2) + \left(l' + \frac{1}{2}\right)\hbar\omega + \left(n' + \frac{1}{2}\right)\hbar\omega_0 \qquad \left(\omega = \frac{2\pi}{T}\right)$$

This is the analog of eq. (79), it holds for large m and small l' and n'. Actually it would have been better to linearize the problem in the $(\delta r, \delta p_r)$ plane only since we know the exact solution in the angular coordinates: then the formula for the levels shows the usual SO(3) degeneracy:

$$E_{ml'n'} = W(v) + \left(n' + \frac{1}{2}\right)\hbar\sqrt{\frac{8W'^3(v)}{-W''(v)}} \qquad v = \left[\left(m + l' + \frac{1}{2}\right)\hbar\right]^2 = \left(l + \frac{1}{2}\right)^2\hbar^2$$

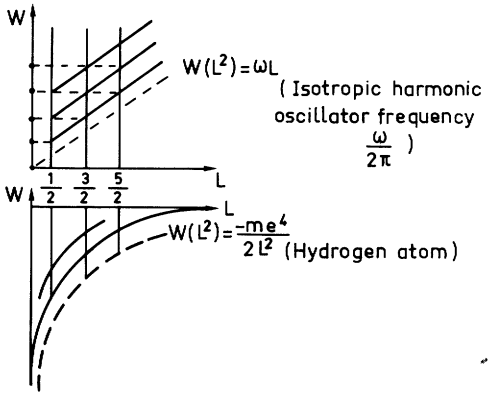

FIG. 8. — Two examples of Regge trajectories.

For fixed n' this formula gives a relation between energy and angular momentum which is nothing else but a *Regge trajectory* (fig. 8).

8) Singular paths

It is possible to relax some of the conditions on the path γ. For instance, the projection $\Pi_Q(\gamma)$ might have multiple or turning points. The latter case creates no difficulty: eq. (79) was derived in phase space and still holds. We can also treat reflections on a hypersurface of $\mathcal{Q}$ as usual by adding a phase shift of π at each reflection point with a Dirichlet boundary condition [16].

9) An interpretation of eq. (79)

In our method, sharp energy levels are generated by a combination of the Balian-Bloch and Gutzwiller mechanisms. We must recall that each Λ_α is generated by (linearized) classical paths, which are generally dense on Λ_α or exceptionally closed. It is the *family* of all such paths wound around the « simple » path γ, and (whenever they are closed) repeated an infinite number of times, that conspires to create the *family* of levels (79). A path can close after p turns only if the angles of rotation are rationally dependent; then the *exact* classical system also admits paths which close after p turns; since $p \geq 2$ except if every $v_{j'} = 0$, those closed paths are not « simple », and under our hypotheses for γ there is no possible double counting (fig. 9).

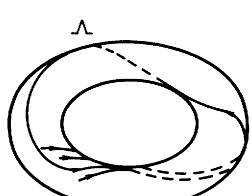

FIG. 9.

The classical perturbation theory around closed paths [39] goes beyond the linear approximation since the angles v_j are allowed to vary continuously with α (they take their linear values for $\alpha = 0$). Consequently the structure of closed paths around a given simple path is extremely complicated [13], and it is satisfying to see that only the central path is relevant to quantization; the other paths (which may have quite different shapes) only contribute through the angles of rotation. We believe that by introducing this classical dependence of the v_j into eq. (79) we should make the formula more accurate ([14]):

$$S(E) = \left[2\pi N + \sum_{2}^{l}\left(n_{j'} + \frac{1}{2}\right)v_j'(E, n_{j'})\right]\hbar .$$

Finally we remark that although the existence proof for the invariant tori relies on classical « perturbation » theory, all the results of this section are non-perturbative in the coupling constants g, i. e. if the classical objects and v_j are known exactly, the semi-classical levels and waves are *functions* of g, not power series (however they are power series of $\hbar$ and we have seen that nothing is known for higher orders in $\hbar$).

10) Partial degeneracy

This section was devoted to systems with closed paths; section 5 treated systems with closed Lagrangian manifolds of dimension l. We give a short treatment of intermediate cases (without proof; details in ref. [53]). Assume that $F_1 = H_{cl}, \ldots, F_p$ are p observables in involution $(1 \leqslant p \leqslant l)$; eq. (18) implies that $[\# dF_j, \# dF_k] = 0$; by the Frobenius theorem, the system has (invariant) p-dimensional integral manifolds, each of which lies in a fixed $(2l - p)$-dimensional manifold $\Sigma_\alpha = \{ F_1 = \alpha_1, \ldots, F_p = \alpha_p \}$ and carries a p-parameter abelian semi-group of canonical mappings $U_t = U^1_{t_1} \ldots U^p_{t_p}$ (where $U^k_{t_k}$ is the flow of F_k). We suppose there exists a (continuous, unique) family $\{ V_\alpha \}$ of *compact* integral manifolds $(V_\alpha \subset \Sigma_\alpha)$; necessarily V_α is a p-dimensional torus. The linearized Poincaré map along a cycle ([15]) $\gamma(t) \subset V_\alpha$ only depends on the homotopy class of the cycle; p such commuting maps $P^1, \ldots, P^p$ correspond to a homotopy basis $\{ \gamma_1, \ldots, \gamma_p \}$ of V_α. Each P^k has the angles of rotation 0 (with multipli-

([14]) With an error $0(\hbar^2)$ only. We are very grateful to Prof. S. Sternberg (Harvard University) for discussions about classical perturbation theory [39].

([15]) The linearized flow around $\gamma(t)$ satisfies the equation $\delta x(t) = \sum_1^p c_i(t) . \nabla_\omega(\delta F_i)$ if the c_i are defined by: $\dot{\gamma}(t) = \sum_1^p c_i(t) . \nabla_\omega F_i(\gamma(t))$; cf. eq. (72).

city p), $v_{p+1}^k, \ldots, v_l^k$ (and we assume parametric stability: $0 < |v_j^k| < \pi$; $v_j^k \neq v_{j'}^k$ for $j \neq j'$). The semi-classical joint spectrum of $F_1, \ldots, F_p$ is then given by the quantization rules for $k = 1, \ldots, p$:

$$S_k(\alpha_1, \ldots, \alpha_p) = \oint_{\gamma_k} pdq = \left[2\pi N_k + \sum_{j=p+1}^{l} n_j^k v_j^k + \frac{1}{2}\left(\sum_{j=p+1}^{l} v_j^k + \pi n(\gamma_k) \right) \right] \hbar \quad (80)$$

where the rotation index $n(\gamma_k)$ is defined in analogy with the case $p = 1$, in which the formula reduces to eq. (79); for $p = l$, $n(\gamma_k)$ is the Maslov index and the rules coincide with eqs. (64).

11) The rotation index

In § 5 we have defined $n(\gamma)$ for a closed, stable physical path γ. If γ belongs to an invariant Lagrangian manifold of a polarization (§ 11 with $p=l$)$n(\gamma)$ is the *Maslov index*. Also, if the classical dynamical flow is locally equivalent to the geodesic flow of a *riemannian* manifold, and if γ is a closed stable geodesic, $n(\gamma)$ is the *Morse index* of γ. Proof: in the $t = 0$ section Λ^0 consider straight lines $L_{j'} \subset \mathbb{R}^2_{j'}$ through 0 such that $L_{j'} \cap \gamma_{j'}^{-v_{j'}} \neq \emptyset$ (they exist since $|v_{j'}| < \pi$). By a symplectic map we put Λ in such a position that the Lagrangian plane generated by the $L_{j'}$ and the velocity $\gamma(0)$ becomes parallel to $\mathcal{Q}$ (we keep the old notations for the rotated objects). The Maslov index of $\tilde{\Gamma}_1$ is just the Maslov index of $x(t)$ $(0 < t < T)$ since the arcs $\gamma_{j'}^{-v_{j'}}$ do not intersect Σ_Q. But for a geodesic problem the (locally) *minimal* action principle is satisfied in *any* canonical coordinates, so the Maslov index of the physical path $x(t)$ is its Morse index ([16]) (cf. 5, § 7). By continuity this is also the Morse index of γ (making $\alpha_{j'} \to 0$). We think that the alternate method given by Gutzwiller for $l = 2$, which keeps track of an absolute angle of rotation all along the path in order to count the focal points, works only for some special (although frequent) problems of the geodesic type.

In conclusion: for a restricted class of paths (physical, closed, stable) we have defined a rotation index which requires neither an invariant Lagrangian manifold $\Lambda \supset \gamma$ (as for the Maslov index) nor the geodesic character of the flow (as for the Morse index): the rotation index takes the place of the Maslov (or Morse) index in the quantization rules (79) or (80).

12) The Laplacian spectrum

The Laplace operator on a compact riemannian manifold is an elliptic PDO of order 2 whose bicharacteristics are precisely the geodesics [*44*]. Therefore we conclude that the semi-classical spectrum of the Laplace operator is given by eqs. (79) of (80) if the hypotheses of § 5 or § 11

([16]) Without the « concavity » term (Dr R. Cushman, private remark).

are satisfied; for isolated paths ($p = 1$) $n(\gamma)$ is the Morse index. The quantization rules give information on the local structure of the spectrum for a high energy quantum number [*50*].

13) Experimental tests

The Poincaré theory we have used in this section finds its most natural application in celestial mechanics. But the literature about the quantum theory of the solar system is far from abundant [*46*] and suggests few experimental ideas. Instead, we might test eqs. (79) or (80) on molecular, atomic or nuclear spectra: in a region of the spectrum around the energy E, not too large but containing a sizable number of eigenvalues, the spacing should be generated by *at most l numbers* if the system has l degrees of freedom [*50*] (provided the family of classical paths $\{ \gamma_E \}$ is *unique* in that region). This structure could vary slowly over broader regions of the spectrum as the $v_{j'}$ vary, and rapidly at energies where the family $\{ \gamma_E \}$ has « accidents ». In theory, agreement should be good only for high energies but, as is often the case, the extrapolation to lower energies might work quite well.

8. CONCLUSIONS

We can sum up the relations between the degree of continuous degeneracy of the system and the possibilities of a semi-classical treatment: $F_1 = H, \ldots, F_p$ are a complete set of commuting admissible observables.

a) $p > l$	WKB-Maslov method (section 5)
b) $p < l$, invariant closed p-manifolds	Approximate WKB method (section 7)
c) $p < l$, no invariant closed p-manifolds	Wigner method (section 4)

In cases *a*) and *c*), the smallest invariant manifolds will in general be the $\Sigma_\alpha^{2l-p} : \{ F_1 = \alpha_1, \ldots, F_p = \alpha_p \}$. The criterion to the possibility of a Hilbert space semi-classical treatment is then that *the invariant stable closed manifolds of the system must be of dimension* $\leq l$ (cases *a*) and *b*)).

Our conclusions are idealized, in assuming that we can localize the analysis to a limited region of interest in phase space. On the other hand they hold for the non-euclidean systems of section 6 as well.

ACKNOWLEDGMENTS

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APPENDIX 1

THE STATIONARY PHASE EXPANSION

Let $\alpha \sim \sum \frac{\alpha_n(q)}{(i\lambda)^n}$ be an asymptotic series for $\lambda \to +\infty$ with $\alpha_n \in \mathcal{S}(\mathbb{R}^l)$ semi-normed uniformly in n, and $\varphi \in C^\infty(\mathbb{R}^l)$ slowly increasing at infinity, with a single critical point $q=0$ ($\nabla_q\varphi(0) = 0$), non-degenerate, i. e. $(Q_{jk}) = \left(\frac{\partial^2\varphi(0)}{\partial q^j \partial q^k}\right)$ has: $\det Q \neq 0$. Let

$$\Phi(q) = \varphi(q) - \varphi(0) - \frac{qQq}{2}.$$

Then

$$I(\lambda) = \int_{\mathbb{R}^l} \alpha(q) e^{i\lambda\varphi(q)} dq = \frac{e^{i\lambda\varphi(0)}}{\lambda^{l/2}} \int_{\mathbb{R}^l} \left[\alpha\left(\frac{q'}{\lambda^{1/2}}\right) \exp\left(i\lambda\Phi\left(\frac{q'}{\lambda^{1/2}}\right)\right)\right] \times \exp\left(i\frac{q'Qq'}{2}\right) dq'$$

has an asymptotic series obtained by integrating term by term the Taylor series at $q' = 0$ of the brackets with the gaussian weight $\exp\left(\frac{iq'}{2}(Q + i\varepsilon)q'\right)$, where ε ($\to 0$) is any *positive definite* quadratic form (the Feynman convergence factor). Integration term by term is legitimate if the contributions to $I(\lambda)$ from $q \to \infty$ are zero (e. g. $\alpha(q) = 0$ *or* $|\nabla_q\varphi| \geq c > 0$ outside a finite region), and the limit $\varepsilon \to 0$ is uniquely determined [*47*]. This gives the contribution of the critical point. By a partition of unity we can isolate the contribution of any region avoiding $q = 0$: φ can be taken as an independent variable, which appears in subintegrals $\int \alpha_1(\varphi) e^{i\lambda\varphi} d\varphi$ ($\alpha_1 \in \mathcal{S}$), but [*28*]:

$$\int \alpha_1 e^{i\lambda\varphi} = \ldots = \int \frac{\partial^N \alpha_1}{\partial\varphi^N} \cdot \frac{e^{i\lambda\varphi}}{(-i\lambda)^N} d\varphi = o\left(\frac{1}{\lambda^N}\right)$$

($\forall$N): this is ~ 0. So, the resulting series for $I(\lambda)$ is local at $q = 0$, it reads:

$$I(\lambda) \sim \frac{(2\pi)^{l/2} e^{i\lambda\varphi(0)}}{(-i\lambda)^{l/2} (\det Q)^{1/2}} \sum_{n,q=0}^{\infty} \sum_{\substack{m \geq 0 \\ |m| = 2q}} \sum_{0 \leq k \leq m} \frac{\alpha_n^{(m-k)}(0)}{(m-k)!}$$

$$\times \sum_{\{s_r\}}' \left(\prod_{|r|=3}^{|k|} \frac{1}{s_r!} \left[\frac{\Phi^{(r)}(0)}{r!}\right]^{s_r} \frac{1}{(i\lambda)^{n+q-\sum_r s_r}} \right) \left(\sum_{\sqcap} (Q^{-1})_{i_1 j_1} \cdots (Q^{-1})_{i_q j_q} \right) \tag{81}$$

where $(-i\lambda)^{l/2} = e^{-il\pi/4} |\lambda|^{l/2}$; $(\det Q)^{1/2} = i^{I(Q)} |\det Q|^{1/2}$, $I(Q)$ being the inertia (number of negative eigenvalues) of Q; m, k, r are l-indices $\left(k \leq m \Leftrightarrow k_i \leq m_i \ (\forall i); \ |r| = \sum_1^l r_j;\right.$ $\left. r! = \prod_1^l r_j!\right)$; $s_r \in \mathbb{N}$ and $\sum'_{\{s_r\}}$ is the sum over those $\{s_r\}$ satisfying $\sum_r s_r . r = k$; finally $\sum_{\sqcap}$ means the sum over all pairs $(i_p, j_p)_{p=1,\ldots,q}$ exhausting the set $\{\underbrace{1, \ldots, 1}_{m_1 \text{ times}}, \ldots, \underbrace{l, \ldots, l}_{m_l \text{ times}}\}$

(Wick's theorem ([16])). Formula (81) is extremely complicated. It shows however that (omitting the overall factor) the coefficient of $1/(i\lambda)^p$ contains a maximum power of $1/(\det Q)^{3p}$ (originating from the contractions $1/(\det Q)^q$, but $\sum s_r . |r| = |k| \leq 2q$ and $|r| \geq 3$ imply $\sum s_r \leqslant \frac{2q}{3}$ and $p \geq q - \sum s_r \geq \frac{q}{3}\Big)$ and is linear in $\alpha_n^{(p')}$ $\left(\text{for } n + \frac{p'}{2} \leq p\right)$.
Assuming $\varphi \in C^\infty$ on Supp α but only $\alpha_0 \in C^2$, $\alpha_1 \in C^0$ we may truncate the expansion and obtain the estimate:

$$\left| \frac{I(\lambda)(-i\lambda)^{l/2} (\det Q)^{1/2}}{(2\pi)^{l/2} e^{i\lambda\varphi(0)}} - \alpha_0(0) \right| \leq \frac{1}{\lambda} (C_1 \sup_{|m| \leq 2} |\alpha_0^{(m)}(0)| + C_2 |\alpha_1(0)|).$$

For the asymptotic Fourier transformation we can derive Hilbert space estimates: the hypothesis $\alpha_0 \in C^2$ must be replaced by the chart-independent condition that $\psi_Q = ae^{i\lambda S_Q}$ belongs to the domain of the operator $(-h^2\Delta_q + q^2)$ (and $S_Q \in C^\infty$).

If $\varphi(q)$ has several *isolated* critical points, each contributes as in eq. (81), and the resulting value for $I(\lambda)$ is simply the sum of the individual terms; there are no interference terms between two critical points. This follows from a partition of unity applied to the amplitude $\alpha(q)$ [*12*] [*21*].

([16]) Eq. (81) expresses the Feynman rules for a « field » theory with l degrees of freedom $\left(\text{free Lagrangian } \frac{1}{2} qQq\text{; interaction } \Phi(q)\right)$; the lowest order corresponds to the sum of tree graphs (ref. [*48*]).

APPENDIX 2

THE CENTRAL POTENTIAL IN 3 DIMENSIONS

Let $H = \frac{p^2}{2m} + V(|q|)$. To separate variables, it is convenient to work in polar coordinates:

$$q = \begin{pmatrix} r \sin\theta \cos\varphi \\ r \sin\theta \sin\varphi \\ r\cos\theta \end{pmatrix} \qquad r \in [0, \infty); \qquad \theta \in [0, \pi]; \qquad \varphi \in [0, 2\pi)$$

At every q there is a euclidean frame in $\mathscr{P}$ of vectors parallel to dr, $d\theta$, $d\varphi$ (except when $\sin\theta = 0$) in which the coordinates of p are:

$$(p_r p_\theta p_\varphi) = (p_1 p_2 p_3)\mathscr{M}; \qquad \mathscr{M} = \begin{pmatrix} \sin\theta\cos\varphi & \cos\theta\cos\varphi & -\sin\varphi \\ \sin\theta\sin\varphi & \cos\theta\sin\varphi & \cos\varphi \\ \cos\theta & -\sin\theta & 0 \end{pmatrix}$$

The fundamental 1-form of M is:

$$\theta_Q = \sum_1^3 p_i dq^i = p_r dr + r p_\theta d\theta + r \sin\theta p_\varphi d\varphi .$$

It is well known that the obrervables H, J^2, J_3 (where $\vec{J} = \vec{q} \times \vec{p}$) are in involution. In our coordinates the Lagrangian foliation is given by:

$$\begin{cases} H = \frac{1}{2m}(p_r^2 + p_\theta^2 + p_\varphi^2) + V(r) = E \\ J^2 = r^2(p_\theta^2 + p_\varphi^2) \qquad = L^2 \\ J_3 = r p_\varphi \sin\theta \qquad = M . \end{cases}$$

In the Q-chart, the equations of a Lagrangian manifold are ($\varepsilon = \pm 1$):

$$p_r = \varepsilon_r \sqrt{2m(E - V(r)) - \frac{L^2}{r^2}}, \qquad p_\theta = \frac{\varepsilon_\theta}{r}\sqrt{L^2 - \frac{M^2}{\sin^2\theta}}, \qquad p_\varphi = \frac{M}{r\sin\theta}$$

(fig. 7) and the invariant density is:

$$\eta = C \frac{D(p_r p_\theta p_\varphi)}{D(E, L^2, M)} d^3 q = \frac{Cm d^3 q}{2r^3 p_r p_\theta \sin\theta} = C' \frac{dr \wedge d\theta \wedge d\varphi}{r p_r p_\theta} . \tag{82}$$

The singular cycle Σ_Q is $\{ p_r = 0 \} \cup \{ p_\theta = 0 \}$ (assume for the moment $M \neq 0$ so that the singularities of the polar coordinate system $r = 0$ and $\sin\theta = 0$ are not encountered). Formula (67) becomes, using (82):

$$\psi_Q(q) = $$

$$= C \frac{\sum_{\varepsilon_r, \varepsilon_\theta} e^{-\frac{i\pi}{4}(\varepsilon_r + \varepsilon_\theta)} \exp \frac{i}{\hbar}\left[\varepsilon_r \int_{r_{\min}}^{r} \left(2m(E-V) - \frac{L^2}{r^2}\right)^{1/2} dr + \varepsilon_\theta \int_{\theta_{\min}}^{\theta}\left(L^2 - \frac{M^2}{\sin^2\theta}\right)^{1/2} d\theta + M\varphi\right]}{r\left[\left(2m(E-V) - \frac{L^2}{r^2}\right)\left(L^2 - \frac{M^2}{\sin^2\theta}\right)\right]^{1/4}}$$

where $r_{\min}$ and $\theta_{\min} = \text{Arc}\sin\frac{M}{L}$ are the lowest turning points. The Bohr rules are

$$\int_0^{2\pi} M d\varphi = 2\pi m\hbar \qquad M = m\hbar \qquad (m \in \mathbb{Z})$$

$$2\int_{\theta_{\min}}^{\pi-\theta_{\min}} \left(L^2 - \frac{M^2}{\sin^2\theta}\right)^{1/2} d\theta = 2\pi\left(l' + \frac{1}{2}\right)\hbar \qquad L = \left(l' + |m| + \frac{1}{2}\right)\hbar \qquad (l' \in \mathbb{N})$$

$$2\int_{r_{\min}}^{r_{\max}} \left(2m(E - V) - \frac{L^2}{r^2}\right)^{1/2} dr = 2\pi\left(n' + \frac{1}{2}\right)\hbar \qquad (n' \in \mathbb{N})$$

We remark that the radial quantization only uses the well-known effective potential $(V + L^2/2mr^2)$ for which we assume a unique minimum $W(L^2)$ for each $L^2 > 0$. Also, the spectrum of L^2 differs from the exact spectrum $J^2 = l(l+1)\hbar^2$ by the constant $\hbar^2/4$; $L^2 = \left(l + \frac{1}{2}\right)^2 \hbar^2$ where $l = l' + |m|$ (this is known as the Langer modification [22]); the eigenvalue $L = \left(l + \frac{1}{2}\right)\hbar$ is $(2l+1)$-degenerate since $m = -l, \ldots, +l$. In our opinion, since the spacing of levels when m varies is correct, the reason for the Langer modification can be found at $m = 0$. Then the cycle $p_\theta = \frac{\varepsilon_\theta}{r}\left(L^2 - \frac{M^2}{\sin^2\theta}\right)^{1/2}$ becomes $p_\theta = \frac{\varepsilon_\theta}{r} L$ and has indeed 2 reflections at $\theta = 0$ and π, giving rise to the shift $l' \to l' + \frac{1}{2}$; but these reflections are due to the singularities of the polar coordinates and are *not* genuine turning points (any meridian circle on the sphere $r = \text{const.}$ is a good representant of the cycle in Q-space). However we cannot discard their effects altogether since the effective potential to be used in the radial Bohr rule is indeed [22] $V(r) + \left(l + \frac{1}{2}\right)\hbar^2/2mr^2$.

Solvable cases:

a) *Spherical harmonics* are obtained by dropping the radial degree of freedom. The normalized semi-classical expression is:

$$Y_m^l(\theta, \varphi) \sim \frac{\sqrt{l + \frac{1}{2}}}{\pi} \cos\left[\left(l + \frac{1}{2}\right) \text{Arccos}\left(\frac{\cos\theta}{\cos\theta_0}\right) - m \,\text{Arctg}\, \frac{\sqrt{\frac{\cos^2\theta_0}{\cos^2\theta} - 1}}{\sin\theta_0} - \frac{\pi}{4}\right] e^{im\varphi}$$

asymptotic for large l and $\cos\theta \ll \cos\theta_0 = \dfrac{\sqrt{\left(l + \frac{1}{2}\right)^2 - m^2}}{l + \frac{1}{2}}$.

b) *The Kepler problem:* the radial quantization rule for bound states is

$$2\int_{r_{\min}}^{r_{\max}} \left(2m\left(E + \frac{Ze^2}{r}\right) - \frac{\left(l + \frac{1}{2}\right)^2 \hbar^2}{r^2}\right)^{1/2} dr = 2\pi\left[\sqrt{\frac{mZ^2e^4}{-2E}} - \left(l + \frac{1}{2}\right)\hbar\right] = 2\pi\left(n' + \frac{1}{2}\right)\hbar$$

so we find the exact levels $\dfrac{-mZ^2e^4}{2(n' + l + 1)\hbar^2}$ with their degeneracy.

It is known that the (radial) relativistic equation with the 4-momentum $p = (p_0, \vec{p})$ is obtained from the non-relativistic one by the substitutions of constants:

$$2mE \to \frac{p_0^2}{c^2} - m^2c^2, \qquad Ze^2 \to \frac{Ze^2p^2}{mc}, \qquad l(l+1) \to \lambda(\lambda+1) = l(l+1) - \frac{Z^2e^4}{c^2}.$$

Since the Langer shift commutes with these substitutions $\left(\lambda + \frac{1}{2}\right)^2 = \left(l + \frac{1}{2}\right)^2 - \frac{Z^2e^4}{c^2}$ the WKB spectrum and the exact spectrum coincide:

$$(p_0)_{n',l} = mc\left[1 + \left(\frac{Ze^2}{\hbar c}\right)^2 \frac{1}{(n' + \lambda + 1)^2}\right]^{1/2}.$$

The WKB method can also be applied to the Dirac equation in a Coulomb field with some approximation (J. Leray, private communication).

c) *The spherical cavity* [*16*] (of radius 1, with Dirichlet boundary conditions) for a momentum $k = \sqrt{2mE}$, the radial Bohr rule is:

$$2\int_{r_{\min}}^{1} \sqrt{k^2 - \frac{L^2}{r^2}}\, dr = 2\sqrt{k^2 - L^2} - 2L \text{ Arccos } \frac{L}{k} = 2\pi\left(n' + \frac{3}{4}\right)\hbar \tag{83}$$

(in the RHS the shift $\frac{3}{4}$ is made from $\frac{1}{4}$ at the turning point $r_{\min} = \frac{L}{k}$ and $\frac{1}{2}$ at the reflection point $r = 1$). This is not very interesting since the level $k_{ln'}$ is better known as the n'-th zero of the spherical Bessel function j_l and it is easy to check that the exact expansion [*49*] for $n' \to \infty$:

$$k_{ln'} \sim \beta\hbar - \frac{l(l+1)\hbar}{2\beta} + 0\left(\frac{1}{\beta^2}\right) \qquad \left(\beta = \left(n' + \frac{l}{2} + 1\right)\pi\right)$$

differs from that resulting from (83):

$$k_{ln'} \sim \beta\hbar - \frac{\left(l + \frac{1}{2}\right)^2 \hbar}{2\beta} + 0\left(\frac{1}{\beta^2}\right).$$

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