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The 'symplectic camel principle' and semiclassical mechanics

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Abstract

We propose a theory of semiclassical mechanics in phase space based on the notion of quantized symplectic area. The definition of symplectic area makes use of a deep topological property of symplectic mappings, known as the 'principle of the symplectic camel' which places stringent conditions on the global geometry of Hamiltonian mechanics. Following this principle, symplectic mappings—and hence Hamiltonian flows—are much more rigid than Liouville's theorem suggests. The dynamical objects of our semiclassical theory are 'waveforms', whose definition requires the notion of square root of de Rham forms. The arguments of these square roots are calculated by using the properties of a generalized Maslov index. The motion of waveforms is determined by Hamiltonian mechanics, and the local expressions of these moving waveforms on configuration space are the usual approximate solutions of WKB-Maslov theory.

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1. Introduction

Non-relativistic physics is governed by two sciences with distinct domains of applicability: classical mechanics (CM) and quantum mechanics (QM). The paradigm of CM is Newton's second law

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = F$$

while that of QM is Schrödinger's equation

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = \widehat{H}\Psi.$$

Both equations describe motions (of particles in the first case, and of waves in the second) in *configuration space* $\mathbb{R}^n_x$. However, CM and QM differ profoundly, both physically and mathematically. They differ *physically*, because QM renounces to the idea of material systems with sharply defined positions and momenta, and incorporates instead complex probability amplitudes in its dynamics. They differ *mathematically*, because while Newton's second law can immediately be interpreted in terms of phase space variables using the Hamiltonian formalism, there is no simple and obvious way to define 'phase space wavefunctions'. On the other hand, one of the most useful manifestations of QM, both in physics and chemistry, is *semiclassical mechanics* (*SM*), which applies when the scale relative to $\hbar$ of certain parameters (e.g. position, time, or mass) in a system is large. Systems to which *SM* applies exhibit a behaviour which is both classical and quantal: while certain quantities (for instance, energy or angular momentum) remain quantized, the *motion* of the system is governed by CM. (*SM* is sometimes described as a way of doing a simplified path-integral formalism with a focus on 'classical paths'.)

The aim of this paper is to present a unifying and mathematically rigorous theory of *semiclassical mechanics in phase space* based on a deep and striking topological property of Hamiltonian flows, the non-squeezing theorem. This theorem, also known as the 'principle of the symplectic camel', says that no Hamiltonian flow will ever be able to squeeze a phase space ball into a phase space cylinder of smaller radius based on a plane of conjugate variables x_j, p_j. We will use the principle of the symplectic camel, together with a simple physical postulate related to the quantization of action, to quantize phase space in such a way that we recover the usual semiclassical energy levels for integrable systems by a *purely topological argument*, without any reference, whatsoever, to the WKB method or to approximate wavefunctions constructed by other methods.

Our paper consists of two parts, which can be read independently:

- In the first part (sections 2 and 3) we begin by reviewing the 'principle of the symplectic camel' (which seems to be little known by physicists). We define the related notion of symplectic area, which we then use to quantize energy shells by an appropriate physical postulate on the *periodic orbits* they carry. This postulate remarkably leads to the correct ground energy levels for the anisotropic harmonic oscillator in arbitrary dimensions (it can also be used to derive a classical form of Heisenberg's inequalities as we have shown in [19]). We show that our postulate leads, by a topological argument, to the usual Keller–Maslov quantization condition
$$\frac{1}{2\pi\hbar}\oint_\gamma p\,\mathrm{d}x - \frac{1}{4}\mathrm{m}(\gamma) \text{ is an integer}$$
in the integrable case (γ a loop on the 'invariant torus'). Our quantization procedure is actually much more general than those found in the literature (it quantizes periodic orbits and energy shells), and could thus be applied with profit to systems exhibiting chaotic behaviour.
- The second part (sections 4–7) begins with the study of a simple example, the one-dimensional harmonic oscillator. It contains in a embryonic form the whole theory which is being further developed in sections 5–7. We then proceed to survey the notion of phase of a Lagrangian submanifold, as defined by Leray [26] and the cohomological theory of the Maslov index which we have developed in [11, 13, 16]. We are thereafter able to define our 'waveforms': they are phase objects whose phase is expressed in terms of the universal covering of the Lagrangian submanifold, and whose amplitude is the square root of an arbitrary 'twisted' (or de Rham) form. Our study of the Maslov index will allow us to assign the proper argument to these square roots. Our constructions apply whether the underlying manifold is oriented or not (in contrast with other quantization theories where orientability is a *sine qua non* requirement, as for instance in [32]). Finally, we

show that the local expressions on configuration space of our waveforms, whose motion is Hamiltonian, are just the usual WKB wavefunctions.

Notations and terminology. The letter z denotes the generic point (x, p) of the phase space $\mathbb{R}^{2n} = \mathbb{R}^n_x \times \mathbb{R}^n_p$. We equip $\mathbb{R}^{2n}$ with the standard symplectic form $\Omega = \mathrm{d}(p\,\mathrm{d}x)$:

$$\Omega = \mathrm{d}p \wedge \mathrm{d}x = \sum_{j=1}^{n} \mathrm{d}p_j \wedge \mathrm{d}x_j.$$

We will denote by $\Lambda(n)$ (resp. $Sp(n)$) the Lagrangian Grassmannian (resp. the symplectic group) of the symplectic space $(\mathbb{R}^{2n}, \Omega)$: $\ell \in \Lambda(n)$ if and only if ℓ is an n-dimensional linear subspace of $\mathbb{R}^{2n}$ having the property that $\Omega(z, z') = 0$ for all z, z'. The symplectic group $Sp(n)$ consists of all automorphisms s of $\mathbb{R}^{2n}$ such that $s^*\Omega = \Omega$, that is $\Omega(sz, sz') = \Omega(z, z')$ for all z, z'. The universal coverings of $\Lambda(n)$ and $Sp(n)$ will be denoted by $\Lambda_\infty(n)$ and $Sp_\infty(n)$.

By definition, a symplectic transformation (or canonical transformation) is a diffeomorphism of phase space whose Jacobian matrix belongs to $Sp(n)$ at every point at which it is defined. Also recall that a Lagrangian submanifold of phase space $\mathbb{R}^n_x \times \mathbb{R}^n_p$ is an n-dimensional submanifold $V \subset \mathbb{R}^n_x \times \mathbb{R}^n_p$ whose tangent spaces are all Lagrangian planes. Equivalently, $\iota_V^*\Omega = 0$, ι_V being the inclusion operator $V \subset \mathbb{R}^n_x \times \mathbb{R}^n_p$.

We will also use in section 6 some elementary notations from singular (co-) chain theory. Let X be a non-empty set, $(G, +)$ an Abelian group and p an integer $\geqslant 0$. A G-valued p-cochain on X is a mapping $c : X^{p+1} \to G$. The coboundary of c is the $(p+1)$-cochain ∂c defined by

$$\partial c(x_0, \ldots, x_{p+1}) = \sum_{j=0}^{p+2} (-1)^j c(x_0, \ldots, \hat{x}_j, \ldots, x_{p+2})$$

where the cap '^' deletes the term it covers. If $\partial c = 0$, c is called a p-cocycle; if $c = \partial b$ for some $(p-1)$-cochain, it is called a coboundary. We have $\partial^2 c = 0$, hence a coboundary is a cocycle.

2. Symplectic camel quantization

Let $B(R)$ be a closed ball in phase space with radius R:

$$B(R) = \{(x, p) : |x - x_0|^2 + |p - p_0|^2 \leqslant R^2\}$$

and $Z_j(r)$ a cylinder with radius r:

$$Z_j(r) = \{(x, p) : (x_j - x_{0,j})^2 + (p_j - p_{0,j})^2 \leqslant r^2\}$$

$(1 \leqslant j \leqslant n)$ based on the x_j, p_j plane (we will call hereafter the $Z_j(r)$ *symplectic cylinders*). Gromov [21] proved in the mid-1980s that there cannot exist a symplectic transformation sending $B(R)$ inside $Z_j(r)$ unless $R \leqslant r$. In particular, a Hamiltonian flow can never squeeze a phase space ball inside a symplectic cylinder with smaller radius. Gromov's theorem is an equivalent statement of the principle of the symplectic camel:

Proposition 1. *Let* $\mathrm{Pr}_j : \mathbb{R}^n_x \times \mathbb{R}^n_p \longrightarrow \mathbb{R}_{x_j} \times \mathbb{R}_{p_j}$ *be the projection operator. For every symplectic transformation* f*, we have*

$$\mathrm{Area}\, \mathrm{Pr}_j\, f(B(R)) \geqslant \pi R^2. \quad (1)$$

(See the proof in [19] where we used (1) to derive a classical form of Heisenberg's uncertainty relations.)

This result is of course striking, because it seems to contradict the common conception of Liouville's theorem, which is that under a Hamiltonian flow a volume in phase space can be made as thin as one likes (cf Gibbs [9] who calls this the 'principle of extension in phase'; also see the discussion of Liouville's theorem in Penrose [31]). However, what is overseen is that the proof of Liouville's theorem only uses the fact that Hamiltonian flows are divergence free. In fact, Hamiltonian flows consist of symplectic transformations, and this is a much stronger property than being just volume preserving as soon as $n > 1$. For instance, the statement

'f is a volume-preserving transformation of phase space'

is equivalent to saying that if $(x, p) = f(x', p')$ then the Jacobian matrix

$$f'(z) = \begin{pmatrix} \dfrac{\partial x}{\partial x'} & \dfrac{\partial x}{\partial p'} \\ \dfrac{\partial p}{\partial x'} & \dfrac{\partial p}{\partial p'} \end{pmatrix}$$

has a determinant equal to one, while the statement

'f is a symplectic transformation of phase space'

means that the entries of $f'(z)$ satisfy the much more stringent conditions

$$\begin{cases} \left(\dfrac{\partial x}{\partial x'}\right)^{\mathrm{T}} \dfrac{\partial p}{\partial x'}, \left(\dfrac{\partial p}{\partial p'}\right)^{\mathrm{T}} \dfrac{\partial x}{\partial p'} \text{ are symmetric} \\ \left(\dfrac{\partial x}{\partial x'}\right)^{\mathrm{T}} \dfrac{\partial p}{\partial p'} - \left(\dfrac{\partial p}{\partial x'}\right)^{\mathrm{T}} \dfrac{\partial x}{\partial p'} = I_{n\times n}. \end{cases}$$

No 'easy' proofs of Gromov's theorem are known. In Gromov's original paper and in Hofer–Zehnder [23] the reader will find proofs making use of the theory of pseudo-holomorphic curves. Viterbo gives in [37] a very interesting alternative proof using the notion of generating function.

2.1. Symplectic area and periodic orbits

Let $\mathcal{D}$ be a subset of $\mathbb{R}^n_x \times \mathbb{R}^n_p$. We will call *symplectic radius* of $\mathcal{D}$ the supremum $R_{\max}$ of all $R \geqslant 0$ such that we can send the phase space ball $B(R)$ inside $\mathcal{D}$ using a symplectic transformation. We will call *symplectic area* of $\mathcal{D}$, and denote by $\mathcal{A}(\mathcal{D})$ the number $\pi R^2_{\max}$:

$$\mathcal{A}(\mathcal{D}) = \sup_{f \text{ symplectic}} \{\pi R^2 : f(B(R)) \subset \mathcal{D}\}.$$

($\mathcal{A}(\mathcal{D})$ is also sometimes called the *symplectic capacity* of $\mathcal{D}$; see, e.g., [23]). It immediately follows from the definition of $\mathcal{A}(\mathcal{D})$ that $A(f(\mathcal{D})) = \mathcal{A}(\mathcal{D})$ for every symplectic transformation f of phase space: symplectic area is thus a *symplectic invariant*.

Remark. The notion of symplectic area was first introduced by Ekeland and Hofer in [7]; there are other non-equivalent definitions of symplectic areas/capacities (see, e.g., [23]).

The principle of the symplectic camel can obviously be restated as

$$B(R) \subset \mathcal{D} \subset Z_j(R) \Longrightarrow \mathcal{A}(\mathcal{D}) = \pi R^2 \tag{2}$$

showing that subsets of phase space with very different shapes and volumes can have the same symplectic area. Let, for instance,

$$\mathcal{E} : \sum_{j=1}^{n} \frac{1}{R_j^2} \left(p_j^2 + x_j^2\right) \leqslant 1$$

be a phase space ellipsoid; we assume that $R_1 \leqslant \cdots \leqslant R_n$. (The equation of every ellipsoid in phase space can be put in the form above by a suitable symplectic change of coordinates.) It follows from property (2) that the symplectic area of this ellipsoid is

$$\mathcal{A}(\mathcal{E}) = \pi R_1^2. \tag{3}$$

The symplectic area of a set has, as the terminology suggests, the dimension of an area. In the case $n = 1$ the symplectic area is, in fact, just the usual area

$$\mathcal{A}(\mathcal{D}) = \left| \int_{\mathcal{D}} \mathrm{d}p \, \mathrm{d}x \right|. \tag{4}$$

Note that the symplectic area of a ball $B(R)$, or of a symplectic cylinder, is independent of the dimension of the ambient phase space, as it is always πR^2. The symplectic area and the volume of a ball $B(R)$ in $\mathbb{R}^n_x \times \mathbb{R}^n_p$ are related by the formula

$$\mathrm{vol}\, B(R) = \frac{1}{n!} [\mathcal{A}(B(R))]^n \tag{5}$$

since $B(R)$ has volume $\pi^n R^{2n}/n!$.

2.2. Symplectic area and periodic orbits

Consider a bounded domain $\mathcal{D}$ with boundary γ in the phase plane $\mathbb{R}^2$. Obviously, formula (4) can be written using Stoke's theorem as

$$\mathcal{A}(\mathcal{D}) = \left| \int_{\gamma} p \, \mathrm{d}x \right|$$

showing that

'symplectic area = action'

in the case $n = 1$. It turns out—and this is an another striking feature of the principle of the symplectic camel—that this relation holds in any dimension. In fact, symplectic area is related to the action of periodic orbits of Hamiltonian systems. Let us begin by some general considerations. Consider an infinitely differentiable function ('Hamiltonian') $H : \mathbb{R}^n_x \times \mathbb{R}^n_p \longrightarrow \mathbb{R}$ and $X_H = (\nabla_p H, -\nabla_x H)$ the associated Hamilton vector field. The *periodic orbits* of X_H are defined as follows: let (f_t) be the flow of X_H and assume that there exists z and $T > 0$ such that $f_t(z) = f_{t+T}(z)$. Then $\gamma(t) = f_t(z), 0 \leqslant t \leqslant T$ is a periodic orbit through z. The action of the periodic orbit γ is then the integral

$$\oint_{\gamma} p \, \mathrm{d}x = \int_0^T p(t) \, \mathrm{d}x(t)$$

where $(x(t), p(t)) = f_t(z)$.

By definition an 'energy shell' Σ of H is a non-empty regular level set of the H:

$$\Sigma = \left\{ (x, p) \in \mathbb{R}^n_x \times \mathbb{R}^n_p : H(x, p) = E \right\}.$$

Any smooth hypersurface of phase space can, of course, be viewed as the energy shell of some Hamiltonian function H: it suffices to choose for H any C^∞ function on $\mathbb{R}^n_x \times \mathbb{R}^n_p$ keeping the constant value E in a tubular neighbourhood of Σ. By definition, a periodic orbit of Σ is then a periodic orbit of the flow determined by H, and lying on the energy shell Σ. Of course, for this definition to make sense, we have to show that these periodic orbits are independent of the choice of the Hamiltonian having Σ for energy shell. This follows from the following well-known result:

Lemma 2. *Let H and K be two Hamiltonians, and suppose that there exist two constants h and k such that*

$$\Sigma = \{z : H(z) = h\} = \{z : K(z) = k\} \tag{6}$$

with $\nabla_z H \neq 0$ and $\nabla_z K \neq 0$ on Σ. Then the Hamiltonian vector fields X_H and X_K have the same periodic orbits on Σ.

Proof. It suffices to show that X_H and X_K have the same integral curves, up to a reparametrization. Since $\nabla_z H(z) \neq 0$ and $\nabla_z K(z) \neq 0$ are both normal to Σ at z, there exists a function $\alpha \neq 0$ on Σ such that $X_K = \alpha X_H$ on Σ. Let now (f_t) and (g_t) be the flows of H and K, respectively, and define a function $t = t(z, s)$, $s \in \mathbb{R}$ as being the solution of the ordinary differential problem

$$\frac{\mathrm{d}t}{\mathrm{d}s} = \alpha(f_t(z)) \qquad t(z, 0) = 0$$

(where z is being viewed as a parameter). We claim that

$$g_s(z) = f_t(z) \qquad \text{for} \quad z \in \Sigma. \tag{7}$$

In fact, by the chain rule

$$\frac{\mathrm{d}}{\mathrm{d}s} f_t(z) = \frac{\mathrm{d}}{\mathrm{d}t} f_t(z) \frac{\mathrm{d}t}{\mathrm{d}s} = X_H(f_t(z))\alpha(f_t(z))$$

that is, since $X_K = \alpha X_H$:

$$\frac{\mathrm{d}}{\mathrm{d}s} f_t(z) = X_K(f_t(z))$$

which shows that the mapping $s \longmapsto f_{t(z,s)}(z)$ is a solution of the differential equation $\dot{z} = X_H(z)$ passing through z at time $s = t(z, 0) = 0$. By the uniqueness theorem on solutions of systems of differential equations, this mapping must be identical to the mapping $s \longmapsto g_s(z)$; hence (7). Both Hamiltonians H and K thus have the same periodic orbits. □

The general problem of the existence of periodic orbits on a given energy shell Σ is a very difficult one, which has not yet been completely solved. We have, however, the following partial result (see [23], and references therein):

Proposition 3. *If the hypersurface Σ is the boundary of a compact star-shaped submanifold of phase space, then it carries at least one periodic orbit.*

(Recall that a submanifold M of an Euclidean space is called star-shaped if there exists a point $z \in M$ such that the line segment joining z to any other point $z' \in M$ lies inside M.) In particular, the boundary of every closed convex submanifold thus carries a periodic orbit.

The essential relation between the action of periodic orbits and symplectic area is given by the following theorem:

Theorem 4. *Let M be a compact star-shaped submanifold in phase space. Then (1) every periodic orbit γ on $\Sigma = \partial M$ is such that*

$$\left| \oint_\gamma p \, \mathrm{d}x \right| \geqslant \mathcal{A}(M) \tag{8}$$

and (2) there exists at least one periodic orbit $\gamma_{\min}$ whose action is the symplectic area of M:

$$\left| \oint_{\gamma_{\min}} p \, \mathrm{d}x \right| = \mathcal{A}(M).$$

(See again Hofer–Zehnder's treatise [23] for a proof.)

Remark. We conjecture that the property of the symplectic camel is the key to a better understanding of not only quantum mechanics, but also classical phenomena. Consider, for example, adiabaticity. While it is rather well understood in one dimension (cf 'Einstein's pendulum'), one must take the usual physical statements and 'proofs' of adiabatic invariance in higher dimensions with more than a critical eye. The existence of the symplectic invariant $\mathcal{A}(M)$ shows that the symplectic geometry is, in a sense, a two-dimensional geometry 'projected' in higher dimensions. Perhaps a general adiabatic principle could be derived from proposition 1 by showing that adiabatic invariance in the phase plane is sufficient for deducing more general results. We also conjecture that the principle of the symplectic camel might play a fundamental role in thermodynamics and statistical physics (e.g., Bose–Einstein and Fermi–Dirac statistics). Viterbo [38] has given other interesting physical interpretations of the principle of the symplectic camel.

3. Phase space quantization

The property of the symplectic camel discussed above can be used to quantize phase space in a very simple way. We will, in particular, recover the correct ground energy level for the n-dimensional anisotropic oscillator.

3.1. A physical postulate

We now make the following postulate of physical nature:

Minimum symplectic area postulate. *The only physically admissible periodic orbits are those which lie on hypersurfaces Σ which are boundaries of convex subsets M of phase space with symplectic area at least $\frac{1}{2}h$. Moreover, if $A(M) = \frac{1}{2}h$ then Σ effectively carries a physically admissible minimal periodic orbit $\gamma_{\min}$.*

Note that in view of theorem 4 such a minimal periodic orbit satisfies

$$\oint_{\gamma_{\min}} p\,\mathrm{d}x = \frac{1}{2}h \tag{9}$$

hence our postulate implies quantization of action. It actually implies much more, as we are going to see: because of the principle of the symplectic camel, it is not a mere restatement of (9). As we noted in the introduction to this paper, our postulate quantizes energy shells and periodic orbits, and thus applies beyond integrable systems.

We begin by giving an immediate striking application, by showing that the minimum symplectic area postulate leads to the correct energy levels of the anisotropic multi-dimensional harmonic oscillator.

Proposition 5. *Consider the n-dimensional harmonic oscillator with Hamiltonian*

$$H = \sum_{j=1}^{n} \frac{1}{2m_j}\left(p_j^2 + m_j\omega_j^2 x_j^2\right). \tag{10}$$

The minimum symplectic area postulate implies that the ground energy level of that Hamiltonian is

$$E_0 = \sum_{j=1}^{n} \frac{1}{2}\hbar\omega_j. \tag{11}$$

Proof. Let L be the diagonal matrix with diagonal entries $(m_j\omega_j)^{-1/2}$. The symplectic change of variables $(x,p)\longmapsto(Lx,L^{-1}p)$ changes H into

$$H'=\sum_{j=1}^{n}\frac{\omega_j}{2}\left(p_j^2+x_j^2\right).$$

This change of variables preserving both action integrals and symplectic areas, it is sufficient to prove the theorem for H'. Each orbit

$$\gamma:\begin{cases}x_1=x_1'\cos\omega_1 t+p_1'\sin\omega_1 t & p_1=x_1'\sin\omega_1 t-p_1'\cos\omega_1 t\\ \cdots\cdots\cdots\cdots\cdots\cdots & \cdots\cdots\cdots\cdots\cdots\\ x_n=x_n'\cos\omega_n t+p_n'\sin\omega_n t & p_n=x_n'\sin\omega_n t-p_n'\cos\omega_n t\end{cases}$$

lies, not only on the ellipsoid which is the energy shell of the Hamiltonian H', but also on each of the symplectic cylinders

$$Z_j(R_j)=\left\{(x,p):x_j^2+p_j^2=R_j^2\right\}$$

with $R_j^2=x_j'^2+p_j'^2$ and $1\leqslant j\leqslant n$. These cylinders carry periodic orbits, and their symplectic areas must thus satisfy the conditions

$$\mathcal{A}(Z_j(R_j))=\pi R_j^2\geqslant\tfrac{1}{2}h$$

in view of our postulate. If $\gamma_{\min}$ is a minimal periodic orbit, it will thus satisfy

$$E(\gamma_{\min})=\sum_{j=1}^{n}\frac{1}{2}\omega_j R_j^2=\sum_{j=1}^{n}\frac{1}{2}\hbar\omega_j$$

which is the result predicted by the standard quantum mechanics. □

3.2. Quantization of integrable systems

Let us next consider a completely integrable system with the Hamiltonian H. There are thus n independent constants of the motion $F_1=H,F_2,\ldots,F_n$ in involution: $\{F_j,F_k\}=0$ for $1\leqslant j,k\leqslant n$. Given an energy shell Σ of H, through every point $z_0=(x_0,p_0)$ of Σ passes a Lagrangian submanifold V carrying the orbits passing through z_0. Moreover, when V is connected (which we assume) there exists a symplectic transformation

$$f:V\longrightarrow(S^1)^k\times\mathbb{R}^{n-k} \tag{12}$$

where $\left(S_j^1\right)^k$ is the product of k unit circles S_j^1, each lying in some coordinate plane x_j,p_j (f can be constructed using 'action-angle variables', see, e.g., [1, 10]). The minimum symplectic area postulate imposes a condition on the energy shells of any Hamiltonian. The condition is that there should be no periodic orbits with action less than $\frac{1}{2}h$, and that there should exist 'minimal periodic orbits' having precisely $\frac{1}{2}h$ as action. In fact, we have the following result which ties the minimum symplectic area/action principle to the Maslov index of loops:

Theorem 6. *Let V be a Lagrangian submanifold associated with a Liouville integrable Hamiltonian H and carrying minimal action periodic orbits. Then we have*

$$\frac{1}{2\pi\hbar}\oint_\gamma p\,\mathrm{d}x-\frac{1}{4}m(\gamma)=0 \tag{13}$$

for every loop on V.

Proof. Since the actions of loops are symplectic invariants, we can use the symplectomorphism (12) to reduce the proof to the case $V = (S^1)^k \times \mathbb{R}^{n-k}$. Since the first homotopy group of V is

$$\pi_1((S^1)^k \times \mathbb{R}^{n-k}) \equiv \pi_1(S^1)^k \equiv (\mathbb{Z}^k, +)$$

it follows that every loop in V is homotopic to a loop of the type

$$\gamma(t) = (\gamma_1(t), \ldots, \gamma_k(t), 0, \ldots, 0) \qquad 0 \leqslant t \leqslant T$$

where γ_j are the loops on S^1: $\gamma_j(0) = \gamma_j(T)$. On the other hand, every loop on S^1 is homotopic to a loop $\varepsilon_j(t) = (\cos\omega_j t, \sin\omega_j t)$, $0 \leqslant t \leqslant T_j$ so that there must exist positive integers μ_j $(1 \leqslant j \leqslant n)$ such that $\mu_1 T_1 = \cdots = \mu_k T_k = T$. We can thus identify γ_j with $\mu_j\varepsilon_j$, the loop ε_j described 'μ_j times':

$$\mu_j\varepsilon_j(t) = (\cos\omega_j t, \sin\omega_j t) \qquad 0 \leqslant t \leqslant T$$

and it follows that any loop in $V = (S^1)^k \times \mathbb{R}^{n-k}$ is homotopic to a loop $\gamma = \mu_1\varepsilon_1 + \cdots + \mu_k\varepsilon_k$. We thus have

$$\oint_\gamma p\,\mathrm{d}x = \sum_{j=1}^{k} \mu_j \oint_{\varepsilon_j} p_j\,\mathrm{d}x_j$$

and using the same argument as that leading to the proof of formula (11) in proposition 5, we must have

$$\oint_{\gamma_j} p_j\,\mathrm{d}x_j = \frac{1}{2}h \qquad (1 \leqslant j \leqslant k)$$

and hence

$$\oint_\gamma p\,\mathrm{d}x = \frac{1}{2}\left(\sum_{j=1}^{k}\mu_j\right)h.$$

Now, the Maslov index of such a loop γ in $(S^1)^k \times \mathbb{R}^{n-k}$ is by definition

$$m(\gamma) = 2\sum_{j=1}^{k}\mu_j$$

(see formula (51) in example 12, section 6), hence the Keller–Maslov condition (13). □

This result motivates the following definition:

Definition 7. *A Lagrangian submanifold V is said to be* quantized *if*

$$\frac{1}{2\pi\hbar}\oint_\gamma p\,\mathrm{d}x - \frac{1}{4}m(\gamma) \textit{ is an integer} \tag{14}$$

for every loop γ in V.

This definition is, of course, nothing else than the usual Maslov–Keller quantization condition [24, 29, 30], originating historically from the WKB theory. We arrived to it by purely topological considerations.

4. Waveforms on the circle

We consider in this section the one-dimensional oscillator with the Hamiltonian function

$$H = \frac{1}{2}(p^2 + x^2).$$

Since the flow determined by Hamilton's equations for H consists of the rotations

$$s_t = \begin{pmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{pmatrix}$$

the phase-space trajectories are the circles $S_r^1 = \{|z| = r\}$. These circles carry a natural length element denoted by, with the usual abuse of notation, $\mathrm{d}s = r\,\mathrm{d}\theta$, where θ is the polar angle.

4.1. Position of the problem

One wants to define on S_r^1 objects whose vocation is to play the role of waveforms in phase space, in the sense that their local expressions are, at best the 'true' wavefunction, at worst their semiclassical approximation (i.e. approximations for 'small $\hbar$'). One looks for an expression of the type

$$\Psi(z) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\varphi(z)} a(z)\sqrt{\mathrm{d}s} \tag{15}$$

where the phase φ and the amplitude a are real functions, and $\sqrt{\mathrm{d}s}$ is supposed to have some well-defined meaning. Unfortunately, one immediately encounters two difficulties when one tries to define φ and $\sqrt{\mathrm{d}s}$. First of all, if one wants the theory to be consistent with the semiclassical mechanics, one must require that the differential of the phase be the action form

$$\mathrm{d}\varphi = p\,\mathrm{d}x = -r^2 \sin^2\theta\,\mathrm{d}\theta. \tag{16}$$

Unfortunately, there exists no such function φ because the 1-form $p\,\mathrm{d}x$ is not exact on S_r^1. We can, however, define a function φ satisfying (16) on the universal covering $\pi : \mathbb{R} \to S_r^1$ of S_r^1. That covering is defined by $\pi(\theta) = r(\cos\theta, \sin\theta)$ and one immediately checks that

$$\varphi(\theta) = \frac{r^2}{2}(\sin\theta\cos\theta - \theta) \tag{17}$$

satisfies (16). We are thus led to consider $\Psi(z)$ as being an expression of the type

$$\Psi(\theta) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\varphi(\theta)} a(\theta)\sqrt{r\,\mathrm{d}\theta}$$

where one allows θ to take any real value, which amounts to defining the candidate for being a phase space wavefunction on the *universal covering* of the circle. However, there is a second, more serious obstruction because one does not see how to define unambiguously the square root $\sqrt{\mathrm{d}s} = \sqrt{r\,\mathrm{d}\theta}$. The simplest way out of this difficulty is to decide that one should only consider the (for instance, positive) square root of the *density* $|\mathrm{d}s|$, that is that we take

$$\Psi(\theta) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\varphi(\theta)} a(\theta)\sqrt{|r\,\mathrm{d}\theta|} \tag{18}$$

which indeed has a well-defined meaning. However, there is a serious rub with that choice because it leads to the wrong energy levels: since we are actually interested in a single-valued function on S_r^1, we have to impose the condition

$$\Psi(\theta + 2\pi) = \Psi(\theta) \tag{19}$$

on the expression (18), which is equivalent to the condition

$$\varphi(\theta + 2\pi) = \varphi(\theta) - 2N\pi\hbar$$

for some integer N. By definition of (17) this is in turn equivalent to $r^2 = 2N\hbar$, which leads to the energy levels $E_N = N\hbar$, instead of the physically correct $E_N = \left(N + \frac{1}{2}\right)\hbar$.

4.2. The need for de Rham forms

The way out of these difficulties, and which leads to the correct quantization conditions, is the inclusion in the theory of de Rham's [5] 'forms of odd kind' (also called 'twisted' or 'pseudo'-forms in the literature) which are to ordinary differential forms what 'pseudo-vectors' are to ordinary vectors. By this we mean that the local expressions of the de Rham forms depend on the orientation of the local charts used to define them (rigorously speaking, the de Rham forms are just ordinary forms, but defined on the oriented double cover of the manifold). In the case of the harmonic oscillator, this leads to the following constructions. Consider the atlas of S_r^1 consisting of the four half-circles

$$S^1_{r,\mathrm{up}} = \{z : |z| = r, \mathrm{Im}\, z > 0\} \qquad S^1_{r,\mathrm{down}} = \{z : |z| = r, \mathrm{Im}\, z < 0\}$$

$$S^1_{r,\mathrm{left}} = \{z : |z| = r, \mathrm{Re}\, z < 0\} \qquad S^1_{r,\mathrm{right}} = \{z : |z| = r, \mathrm{Re}\, z > 0\}$$

together with the projections $f_{\mathrm{up}}, f_{\mathrm{down}} : (x, p) \longrightarrow x$ and $f_{\mathrm{left}}, f_{\mathrm{right}} : (x, p) \longrightarrow p$. The atlas thus defined is *not* oriented; for example, the transition function on $S^1_{r,\mathrm{left}} \cap S^1_{r,\mathrm{down}}$ has negative sign. The local expressions of $\mathrm{d}\theta$ in the charts defined above are, respectively,

$$\begin{aligned} (\mathrm{d}\theta)_{\mathrm{up}} &= \varepsilon(r^2 - x^2)^{-1/2}\,\mathrm{d}x \qquad & (\mathrm{d}\theta)_{\mathrm{down}} &= \varepsilon(r^2 - x^2)^{-1/2}\,\mathrm{d}x \\ (\mathrm{d}\theta)_{\mathrm{left}} &= \varepsilon(r^2 - p^2)^{-1/2}\,\mathrm{d}p \qquad & (\mathrm{d}\theta)_{\mathrm{right}} &= \varepsilon(r^2 - p^2)^{-1/2}\,\mathrm{d}p \end{aligned} \tag{20}$$

where $\varepsilon = \pm 1$ is the orientation induced from the x, p axes on S^1_{up}, etc by the diffeomorphisms f_{up}, etc. Thus, if the axes come equipped with their usual orientations, then $\varepsilon = -1$ for $(\mathrm{d}\theta)_{\mathrm{up}}$ and $(\mathrm{d}\theta)_{\mathrm{left}}$ and +1 for $(\mathrm{d}\theta)_{\mathrm{down}}$ and $(\mathrm{d}\theta)_{\mathrm{right}}$, and a change of orientation has the effect of reversing the sign of ε. The formulae (20), which are characteristics for de Rham forms, suggest that we *define* the 'argument' of $\mathrm{d}\theta$ by

$$\arg \mathrm{d}\theta = \begin{cases} m(\theta)\pi & \text{in} \quad S^1_r \setminus \{\pm r\} \\ (m(\theta) + 1)\pi & \text{in} \quad S^1_r \setminus \{\pm \mathrm{i}r\} \end{cases} \tag{21}$$

where the integer $m(\theta)$ is defined by

$$m(\theta) = [\theta/\pi] + 1 \tag{22}$$

the square brackets meaning 'integer part of'. Note that a change of orientation of the frame x, p amounts to replacing $m(\theta)$ by $m(\theta + \pi) = m(\theta) + 1$. Formulae (21) and (22) allow us to define the square root of $\mathrm{d}s = r\,\mathrm{d}\theta$ in each of the sets $S^1_r \setminus \{\pm r\}$ and $S^1_r \setminus \{\pm \mathrm{i}r\}$. In fact,

$$\begin{cases} \sqrt{\mathrm{d}s} = \mathrm{i}^{m(\theta)}\sqrt{|r\,\mathrm{d}\theta|} & \text{in} \quad S^1_r \setminus \{\pm r\} \\ \sqrt{\mathrm{d}s} = \mathrm{i}^{m(\theta)+1}\sqrt{|r\,\mathrm{d}\theta|} & \text{in} \quad S^1_r \setminus \{\pm \mathrm{i}r\} \end{cases}$$

(Note that both expressions do not coincide on the overlaps). We are thus led to give the following definition of $\Psi(\theta)$: it is the phase space object whose expression on $S^1_r \setminus \{\pm r\}$ is given by

$$\Psi_0(\theta) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\varphi(\theta)} a(\theta)\, \mathrm{i}^{m(\theta)}\sqrt{|r\,\mathrm{d}\theta|} \tag{23}$$

and on $S^1_r \setminus \{\pm \mathrm{i}r\}$ by $\Psi_1(\theta) = \mathrm{i}\Psi(\theta)$:

$$\Psi_1(\theta) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\varphi(\theta)} a(\theta)\, \mathrm{i}^{m(\theta)+1}\sqrt{|r\,\mathrm{d}\theta|}. \tag{24}$$

With that definition the single-valuedness condition (19) becomes

$$\Psi_j(\theta + 2\pi) = \Psi_j(\theta) \qquad j = 1, 2 \tag{25}$$

and is equivalent to $r^2 = (2N + 1)\hbar$, which yields the true energy levels $E_N = \left(N + \frac{1}{2}\right)\hbar$ predicted by quantum mechanics.

We show that this construction of phase space waveforms can be extended to *any* physical system to which a Lagrangian submanifold can be associated. We begin by defining a notion of phase on arbitrary Lagrangian manifolds generalizing (17).

5. The Lagrangian phase

In the rest of this paper the letter V will denote a connected Lagrangian submanifold. Lagrangian submanifolds are associated in a natural way with integrable classical physical systems, and with every quantum system.

Example 8. The integrable systems of classical mechanics: V is then topologically an 'invariant torus', or, more generally a product of k circles and $n-k$ lines.

Example 9. Let $\psi(x) = a(x)\,\mathrm{e}^{\frac{i}{\hbar}\Phi(x)}$ where a and Φ are defined on some connected open subset of configuration space. The graph $V = \{(x, \nabla_x\Phi(x))\}$ is a Lagrangian submanifold.

5.1. Definition of the phase

Consider the universal covering $\pi : \check{V} \longrightarrow V$ of the Lagrangian submanifold V. Since $\check{V}$ is simply connected there exists a differentiable mapping $\varphi : \check{V} \longrightarrow \mathbb{R}$ such that

$$\mathrm{d}\varphi(\check{z}) = p\,\mathrm{d}x \qquad \text{if} \quad \pi(\check{z}) = (x, p). \tag{26}$$

We will call, following Leray [26], such a function φ a *phase* of V. The phase can be explicitly constructed in the following way: choose an 'origin' $z_0 \in V$, and identify $\check{z} \in \check{V}$ with the homotopy classes (with fixed endpoints) of paths in V originating at z_0; the projection $\pi(\check{z})$ is then the endpoint z of an element γ_{z_0z} of the homotopy class $\check{z}$. A phase function is then given by the formula

$$\varphi(\check{z}) = \int_{\gamma_{z_0z}} p\,\mathrm{d}x. \tag{27}$$

Clearly, the integral only depends on the homotopy class $\check{z}$ of γ_{z_0z} in view of Stoke's theorem, because $\Omega = \mathrm{d}(p\,\mathrm{d}x)$ is zero on V. Also,

$$\mathrm{d}\varphi(\check{z}) = p\,\mathrm{d}x \qquad \text{if} \quad \pi(\check{z}) = (x, p). \tag{28}$$

We observe that the action of the first homotopy group $\pi_1(V) = \pi_1(V, z_0)$ on $\check{V}$ is reflected by the formula

$$\varphi(\gamma\check{z}) = \varphi(\check{z}) + \int_{\gamma} p\,\mathrm{d}x \tag{29}$$

for all $\gamma \in \pi_1(V)$. Thus, φ is defined on V if and only if all the periods $\int_\gamma p\,\mathrm{d}x$ of $p\,\mathrm{d}x$ vanish, i.e. if V is contractible. We leave it to the reader to check that formula (27) leads to the function (17) if we require that $\varphi(0) = 0$.

5.2. The action of Hamiltonian flows on the phase

Consider a function $H = H(x, p, t)$ defined on some open subset $D \times \mathbb{R}_t$ of the extended phase space $\mathbb{R}^n_x \times \mathbb{R}^n_p \times \mathbb{R}_t$. We do not assume here that H has any particular form (for instance, 'kinetic energy + potential'), but only that it is a continuously differentiable function; we also make the simplifying, but not essential, assumption that the solutions of the corresponding Hamilton equations

$$\dot{x} = \nabla_p H \qquad \dot{p} = -\nabla_x H$$

exist for all times, and are uniquely determined by their values at a time t'. We denote by $(f_{t,t'})$ the associated time-dependent flow: $f_{t,t'}$ is the symplectic transformation that takes a point

$(x', p') = (x(t'), p(t'))$ to the point $(x, p) = (x(t), p(t))$. When $t' = 0$, we write simply $f_{t,0} = f_t$. The time-dependent flow satisfies the Chapman–Kolmogorov relation

$$f_{t,t'} f_{t',t''} = f_{t,t''} \tag{30}$$

for all times t, t', t''.

Suppose that we are given, at some time t', a Lagrangian submanifold $V_{t'}$, and select a base point $z_{t'}$ on $V_{t'}$. This allows us to define the phase $\varphi(\check{z}, t')$ of $V_{t'}$ by formula (27), with z_0 replaced by $z_{t'}$, $\check{z}$ being an element of the universal covering $\check{V}_{t'}$. The manifold $V_t = f_{t,t'}(V_{t'})$ is also Lagrangian; defining a base point $z_t \in V_t$ by $z_t = f_{t,t'}(z_{t'})$, we identify the universal covering $\check{V}_t$ with $\check{V}_{t'}$, defining the projection $\pi_t : \check{V}_t \to V_{t'}$ by $\pi_t(\check{z}) = z(t)$ if $\pi_{t'}(\check{z}) = z(t')$. Denoting by $\varphi(\check{z}, t)$ the phase of $V_{t'}$, we have

Proposition 10. *The phases $\varphi(\check{z}, t)$ and $\varphi(\check{z}, t')$ are related by the formula*

$$\varphi(\check{z}, t) = \varphi(\check{z}, t') + \int_{z(t')}^{z(t)} p\,\mathrm{d}x - H\,\mathrm{d}t \tag{31}$$

where the integral is calculated along the trajectory $s \to f_{s,t'}(z(t'))$ $(t' \leqslant s \leqslant t)$ leading from $z(t') \in V_{t'}$ to $z(t) \in V_t$.

Proof. We first note that in view of the relative invariance of the Poincaré–Cartan form (see [28]), we have

$$\varphi(\check{z}, t') + \int_{z(t')}^{z(t)} p\,\mathrm{d}x - H\,\mathrm{d}t = \int_{f_{t,t'}(\gamma_{z_0 z})} p\,\mathrm{d}x + \int_{z_{t'}}^{z_t} p\,\mathrm{d}x - H\,\mathrm{d}t \tag{32}$$

where the integral in the left-hand side is calculated along the trajectory $s \to f_{s,t'}(z_{t'})$ $(t' \leqslant s \leqslant t)$, and $f_{t,t'}(\gamma_{z_0 z})$ is the image in V_t by $f_{t,t'}$ of a path in $V_{t'}$ whose homotopy class is $\check{z}$. Denoting by $\chi(\check{z}, t)$ the left-hand side of (32), we thus have, for fixed t:

$$\mathrm{d}\chi(\check{z}, t) = p(t)\,\mathrm{d}x(t)$$

so that $\chi(\check{z}, t)$ and $\varphi(\check{z}, t)$ differ by a function $K(t)$ only depending on t. Since $\chi(\check{z}, t') = \varphi(\check{z}, t')$, we must have $K = 0$. □

5.3. Phase and generating functions

The notion of phase of a Lagrangian submanifold is related (as is the action integral, see [18]) to the notion of generating function.

Recall (see, for instance, Arnold [1] or Goldstein [10]) that a symplectic transformation f is *free* if there exists a function W defined on twice the configuration space and such that if $(x, p) = f(x', p')$ then

$$p\,\mathrm{d}x = p'\,\mathrm{d}x' + \mathrm{d}W(x, x'). \tag{33}$$

The function W is then called a *free generating* function (or generating function of the second kind) for f. When f is free, the relation $(x, p) = f(x', p')$ uniquely determines x' in terms of x. In fact, (33) being equivalent to

$$p = \nabla_x W(x, x') \qquad \text{and} \qquad p' = -\nabla_{x'} W(x, x') \tag{34}$$

we have by the implicit function theorem:

$$\det \frac{\partial(x', x)}{\partial(x', p')} = \det \frac{\partial x}{\partial p'} \neq 0. \tag{35}$$

Suppose now that H is a Hamiltonian function of the type

$$H = \sum_{j=1}^{n} \frac{1}{2m_j}(p_j - A_j(x,t))^2 + U(x,t). \tag{36}$$

It is then easy to prove (see [18]) that there exists $\varepsilon > 0$ such that for

$$0 < |t - t'| < \varepsilon \tag{37}$$

the mappings $f_{t,t'}$ are free ($(f_{t,t'})$ is the time-dependent flow determined by H). Let now $V_{t'}$, V_t be as in proposition 10. Keeping initial position and time x' and t' *fixed*, every point x is thus reached, after time $t - t'$, by a *unique* trajectory Γ emanating from x. Suppose now $z = (x, p) \in V_t$. That point is the image by $f_{t,t'}$ of a unique point $z' = (x', p') \in V_{t'}$. The mapping $x \longmapsto x'$ thus defined is a local diffeomorphism, whose inverse we will denote by $f^X_{t,t'}$. Thus, by definition, $f^X_{t,t'}(x')$ is the unique element of $\mathbb{R}^n_x$ such that

$$f_{t,t'}(x', p') = \left(f^X_{t,t'}(x'), p\right). \tag{38}$$

The action integral is then, by definition, the integral of the Poincaré–Cartan form along that trajectory; we note that the function

$$S(x, x'; t, t') = \int_{x',t'}^{x,t} p\,\mathrm{d}x - H\,\mathrm{d}t \tag{39}$$

satisfies Hamilton–Jacobi's equation with initial condition $t = t'$:

$$\frac{\partial S}{\partial t} + H(x, \nabla_x S, t) = 0 \qquad S_{x't'}(x, x'; t, t) = 0. \tag{40}$$

From these considerations we easily get the following consequence of proposition 10:

Corollary 11. *Under the assumptions above on the $f_{t,t'}$ we have*

$$\varphi(\check{z}, t) = \varphi(\check{z}, t') + S(x, x'; t, t') \tag{41}$$

where $\check{z}$ has projection $\pi_{t'}(\check{z}) = (x', p')$ on $V_{t'}$, and $(x, p) = f_{t,t'}(x', p')$. The local expression

$$\Phi(x, t) = \Phi(x', t') + S(x, x'; t, t') \tag{42}$$

of $\varphi(\check{z}, t)$ satisfies Hamilton–Jacobi's equation.

Formula (41) is an immediate consequence of (31) and (39); formula (42) follows from (40). (See [18] for a detailed study of the relationship between the action integral and free generating functions.)

Remark. When H is a quadratic homogeneous polynomial in the x_i, p_j, Euler's identity for homogeneous functions yields

$$H = \tfrac{1}{2}(x \cdot \nabla_x H + p \cdot \nabla_p H)$$

hence, using Hamilton's equations:

$$\varphi(\check{z}, t) = \varphi(\check{z}, t') + \tfrac{1}{2}(p \cdot x - p' \cdot x') - H(z, t)(t - t'). \tag{43}$$

6. The argument index

The construction of an index generalizing the function $m(\theta) = [\theta/\pi] + 1$ to arbitrary Lagrangian manifolds is rather technical and will be done in several steps. We have exposed elsewhere (see [15–17]) a direct cohomological construction of the argument index based on previous work by Leray [26, 27] and the author [16, 17]. We adopt here a more concrete point of view by making use of Souriau's identification of the Lagrangian Grassmannian with the manifold of all symmetric unitary matrices (see Souriau's original paper [33] and also [16, 18]). This approach has the advantage that it allows straightforward numerical computations and that it does not require any prior knowledge of chain intersection theory.

6.1. Maslov and argument indices for paths

We begin by recalling some results from Lagrangian analysis [16, 18, 26].

The 'Souriau mapping' is the mapping $w : \Lambda(n) \longrightarrow U(n)$ defined by

$$w(\ell) = u\overline{u}^* = u(u^{\mathrm{T}}) \qquad \text{if} \quad \ell = u\left(\mathbb{R}^n_p\right) \tag{44}$$

where $u \in U(n)$. This mapping is indeed well defined, because if $u\left(\mathbb{R}^n_p\right) = u'\left(\mathbb{R}^n_p\right)$ then $u' = uh$ for some $h \in O(n)$ and hence $u'\overline{u'}^* = u\overline{u}^*$. The mapping w is in fact a *diffeomorphism*, and hence identifies the Lagrangian Grassmannian $\Lambda(n)$ with the manifold

$$W(n) = \{w \in U(n), w = w^{\mathrm{T}}\} \tag{45}$$

of all symmetric unitary matrices. The universal covering $\Lambda_\infty(n)$ of $\Lambda(n)$ can then be identified with the subset

$$W_\infty(n, \mathbb{C}) = \{(w, \alpha) : w \in W(n, \mathbb{C}), \det(w) = \mathrm{e}^{\mathrm{i}\alpha}\} \tag{46}$$

of $U(n, \mathbb{C}) \times C$, the covering mapping being the projection $(w, \theta) \longmapsto w$. It follows that $\Lambda(n) = W_\infty(n)/\mathbb{Z}$ and hence $\pi_1(\Lambda(n)) \equiv (\mathbb{Z}, +)$. The action of $\pi_1(\Lambda(n))$ on $\Lambda_\infty(n) \equiv W_\infty(n)$ is given by

$$\lambda^k \cdot \check{z} = (w, \alpha + 2k\pi) \tag{47}$$

where λ is the generator of $\pi_1(\Lambda(n))$ whose image in $\mathbb{Z}$ is +1.

Let us write explicitly these identifications in the case $n = 1$. The manifold $\Lambda(1)$ consists of all straight lines ℓ through the origin in the phase plane $\mathbb{R}^2 = \mathbb{R}_x \times \mathbb{R}_p$. We will denote by $\ell(\theta)$ the line through the origin whose angle with the x-axis is $\theta + \frac{\pi}{2}$ (mod π): $\ell(\theta)$ is thus the direction of the tangent to the unit circle at the point $\mathrm{e}^{\mathrm{i}\theta}$. Since $\ell(\theta) = \mathrm{e}^{\mathrm{i}\theta}(\mathbb{R}_p)$ the Souriau mapping (44) associates to $\ell(\theta)$ the complex number $w(\theta) = \mathrm{e}^{2\mathrm{i}\theta}$. It follows that we have the identifications

$$\ell(\theta) \equiv \mathrm{e}^{2\mathrm{i}\theta} \qquad \text{and} \qquad \ell_\infty(\theta) \equiv (\mathrm{e}^{2\mathrm{i}\theta}, 2\theta + 2k\pi) \quad k \in \mathbb{Z}. \tag{48}$$

In particular $\mathbb{R}_p$ is identified with +1 and $(\mathbb{R}_p)_\infty$ with $(1, 2k\pi)$.

Consider now the tangent plane $\ell(z)$ at a point z of the Lagrangian submanifold V. The mapping

$$\ell(.) : V \longrightarrow \Lambda(n) \qquad z \mapsto \ell(z) \tag{49}$$

is continuous and therefore induces a homomorphism $\ell_\star$ from the first homotopy group of V into that of $\Lambda(n)$. In fact, a base point $z_0 \in V$ being chosen once for all, the mapping

$$\ell_\star : \pi_1(V, z_0) \longrightarrow \pi_1(\Lambda(n), \ell_0)$$

(with $\ell_0 = \ell(z_0)$) associates to every loop $\gamma : [0, 1] \to V$ $(\gamma(0) = \gamma(1) = z_0)$ the loop $\ell_\star(\gamma)$ of Lagrangian planes defined by $\ell_\star(\gamma)(t) = \ell(\gamma(t))$, $0 \leqslant t \leqslant 1$. Using the Souriau identification $\Lambda(n) \equiv W(n)$ we can associate to the loop $\ell_\star(\gamma)$ in $\Lambda(n)$ the loop $w_*\gamma$ in $W(n)$ defined by $w_*\gamma(t) = w(\ell_\star(\gamma)(t))$. Lifting that loop to $\Lambda_\infty(n) \equiv W_\infty(n)$ we get a path

$$t \longmapsto (w_*\gamma(t), \arg\det w_*\gamma(t)) \qquad 0 \leqslant t \leqslant 1$$

where $\arg\det w_*\gamma(t)$ is a choice of continuously varying argument, uniquely determined by a choice of $\arg\det w_*\gamma(0)$. Since $w_*\gamma(0) = w_*\gamma(1)$ the quantity

$$m(\gamma) = \frac{1}{2\pi}(\arg\det w_*\gamma(1) - \arg\det w_*\gamma(0)) \tag{50}$$

must be an integer, depending only on the homotopy class of γ. Formula (50) thus defines a function $m : \pi_1(V, z_0) \to \mathbb{Z}$ called *Maslov index for loops*. The integer $m(\gamma)$ can be intuitively interpreted as follows. Since $\pi_1(\Lambda(n)) \equiv (\mathbb{Z}, +)$, $\Lambda(n)$ has a 'hole'. Now, a loop γ in V induces a loop in $\Lambda(n)$, namely the loop $t \mapsto \ell(\gamma(t)) = T_{\gamma(t)}V$, and $m(\gamma)$ is the number of times $\ell_*\gamma$ turns around the 'hole' in $\Lambda(n)$.

Example 12. *Suppose that V is the circle S^1 in $\mathbb{R}_x \times \mathbb{R}_p$ and $\gamma(t) = \mathrm{e}^{2\pi \mathrm{i}t}$, $0 \leqslant t \leqslant 1$. We have $w_*\gamma(t) = \mathrm{e}^{4\pi \mathrm{i}t}$, $0 \leqslant t \leqslant 1$. The argument of $w_*\gamma(t)$ varies from 0 to 4π when t goes from 0 to 1; it follows from definition (50) that $m(\gamma) = 2$. The same argument shows that if $\gamma = \mu_1\varepsilon_1 + \cdots + \mu_k\varepsilon_k$ is a loop in $(S^1)^k$, where $\varepsilon_j(t) = \mathrm{e}^{2\pi \mathrm{i}t}$ $(0 \leqslant t \leqslant 1)$ is a loop on the jth circle, then*

$$m(\gamma) = 2\sum_{j=1}^{k}\mu_j. \tag{51}$$

The fact that $m(\gamma)$ is an even integer in the example above is not fortuitous. In fact, Souriau [34] has proved that

$$V \text{ oriented} \Longrightarrow m(\gamma) \equiv 0 \mod 2 \quad \text{for all } \gamma \in \pi_1(V, z_0) \tag{52}$$

(see [16] for an algebraic proof of this property, and the generalization to 'q-oriented Lagrangian manifolds'; Dazord [4] gives a related cohomological definition).

Let us next generalize the notion of Maslov index to arbitrary paths in $\Lambda(n)$. Let γ_{z_0z} be a path in V joining z_0 to a point z and $\check{z}$ its homotopy class: $\check{z}$ is an element of the universal covering $\check{V}$ of V. If two paths γ_{z_0z} and γ'_{z_0z} are homotopic, then so are their images $\ell_*(\gamma_{z_0z})$ and $\ell_*(\gamma'_{z_0z})$ in $\Lambda(n)$ by

$$\ell(\cdot) : V \ni z \longmapsto T_zV \in \Lambda(n).$$

This mapping induces a continuous mapping

$$\ell_\infty(\cdot) : \check{V} \longrightarrow \Lambda_\infty(n) \tag{53}$$

which to every $\check{z} \in \check{V}$ with representant γ_{z_0z} associates the homotopy class $\ell_\infty(\check{z})$ of $\ell_*(\gamma_{z_0z})$; obviously, the diagram

$$\begin{array}{ccc} \check{V} & \stackrel{\ell_\infty(.)}{\longrightarrow} & \Lambda_\infty(n) \\ \pi\downarrow & & \downarrow\pi \\ V & \stackrel{\ell(.)}{\longrightarrow} & \Lambda(n) \end{array} \tag{54}$$

is commutative (the vertical arrows being the covering projections). In view of the identification $\Lambda(n) \equiv W(n)$ we can associate to γ_{z_0z} a unique continuous path $t \mapsto w(t)$ $(t \in [0, 1])$ in $W(n)$ such that $\arg\det w(t) = \alpha(t)$, provided that we have specified an 'initial argument' $\alpha(0)$ for $w(0) = \ell(z_0)$.

We now impose the following rather restrictive condition on the endpoints of the path γ_{z_0z}: we assume that z is such that

$$\ell(z_0) \cap \ell(z) = 0 \tag{55}$$

and define an 'argument function' $m_0 : \check{V} \longrightarrow \mathbb{R}$ by the formula

$$m_0(\check{z}) = \frac{1}{2\pi}(\alpha(1) - \alpha(0) + \mathrm{i}\,\mathrm{Tr}\,\mathrm{Log}(-w(1)w(0)^{-1})) + \frac{n}{2} \tag{56}$$

where Tr means 'trace of', and where we define the logarithm by

$$\mathrm{Log}(-w(1)w(0)^{-1}) = \int_{-\infty}^{0} \{[\lambda I + w(1)(w(0))^{-1}]^{-1} - (\lambda - 1)^{-1} I\}\, \mathrm{d}\lambda \tag{57}$$

(I is the $n \times n$ identity matrix). The right-hand side of (57) makes sense in view of the following characterization of transversality of Lagrangian planes (see [16, 18, 26, 33]).

Lemma 13. *Let ℓ and ℓ' be two arbitrary Lagrangian planes, and set $w = w(\ell)$ and $w' = w(\ell')$. The condition $\ell \cap \ell' = 0$ is equivalent to* $\det(w(w')^{-1} - I) \neq 0$*, that is, to the condition that $w(w')^{-1}$ has no > 0 eigenvalues.*

We have:

Proposition 14. *(1) The function m_0 is integer-valued. It is locally constant on its domain of definition $\{z \in V : \ell(z) \cap \mathbb{R}^n_p = 0\}$; (2) m_0 coincides with the function defined in (22) when $V = S^1_r$ and $z_0 = +1$; (3) we have for all $\gamma \in \pi_1(V, z_0)$*

$$m_0(\gamma\check{z}) = m_0(\check{z}) + m(\gamma) \tag{58}$$

where $m(\gamma)$ is the Maslov index for loops defined by (50).

Proof. (1) We have, by definition of w,

$$\begin{aligned}\exp(\mathrm{Tr}\,\mathrm{Log}(-w(1)w(0)^{-1}) &= (-1)^n \det(w(1)w(0)^{-1}) \\ &= (-1)^n\,(\exp(\mathrm{i}\alpha(1)) - \exp(\mathrm{i}\alpha(0)))\end{aligned}$$

and hence $\exp(2\pi\mathrm{i}m_0(\check{z})) = (-1)^n\,\mathrm{e}^{\mathrm{i}n\pi} = 1$ so that $m_0(\check{z}) \in \mathbb{Z}$, as claimed. (2) If $n = 1$, $V = S^1_r$, and $z_0 = 1$ then $\ell(\theta) \equiv w(1) = \mathrm{e}^{2\mathrm{i}\theta}$ and $\ell(0) \equiv w(0) = 1$. On the other hand, the logarithm defined by (57) is given, in the case $n = 1$, by

$$\mathrm{Log}(\mathrm{e}^{\mathrm{i}\alpha}) = \mathrm{i}\left(\alpha - 2\left[\frac{\alpha + \pi}{\pi}\right]\pi\right) \tag{59}$$

for $\alpha \neq \pi \pmod{2\pi}$, hence

$$\mathrm{Log}(-w(1)w(0)^{-1}) = \mathrm{Log}(-\mathrm{e}^{2\mathrm{i}\theta}) = \mathrm{i}\left(2\theta - 2\left[\frac{2\theta + 2\pi}{2\pi}\right]\pi\right)$$

from which it follows that $m_0(\check{z}) = [\theta/\pi] + 1$, as claimed. (3) Let $\check{z}$ be the homotopy class of a path γ_{z_0z} and γ the homotopy class of a loop $\gamma_{z_0z_0}$. Then $\gamma\check{z}$ is the homotopy class of the concatenation $\gamma_{z_0z_0} + \gamma_{z_0z}$. Formula (58) follows by definition (56) of the Maslov index for loops. □

The last step in the construction of the complete argument index needs the properties of the Leray index.

6.2. The Leray index

The key to the definition of the Maslov index for paths with endpoints in general position is the cohomological index defined by Leray [26, 27] in the transversal case, and generalized by the author [13] to the non-transversal case. We begin by giving a general definition of the Leray index. Recall that $\Lambda_\infty(n) \equiv W_\infty(n)$ is the universal covering of the Lagrangian Grassmannian $\Lambda(n)$.

Definition 15. *A Leray index on* $(\Lambda_\infty(n))^2$ *is a mapping*

$$m : (\Lambda_\infty(n))^2 \longrightarrow \mathbb{Z}$$

having the two following properties: (1) the coboundary of m, viewed as a 1-cochain, descends to a $Sp(n)$*-invariant cocycle* f *on* $\Lambda(n)$: $\partial m = \pi^* f$ *(*π *the projection* $\Lambda_\infty(n) \longrightarrow \Lambda(n)$*);* (2) *m is locally constant on each of the subsets*

$$\{(\ell_\infty, \ell'_\infty) : \dim(\ell \cap \ell') = k\} \tag{60}$$

$(0 \leqslant k \leqslant n)$ *of* $(\Lambda_\infty(n))^2$.

Condition $\partial m = \pi^* f$ means that

$$m(\ell_\infty, \ell'_\infty) - m(\ell_\infty, \ell''_\infty) + m(\ell'_\infty, \ell''_\infty) = f(\ell, \ell', \ell'') \tag{61}$$

and the $Sp(n)$-invariance of f means that

$$f(s\ell, s\ell', s\ell'') = f(\ell, \ell', \ell'') \qquad \text{for all } s \in Sp(n).$$

Note that the function f automatically is a $\mathbb{Z}$-valued 2-cocycle on $\Lambda(n)$: $\partial f = 0$, locally constant on each of the sets

$$\{(\ell, \ell', \ell'') : \dim(\ell \cap \ell') = k, \dim(\ell' \cap \ell'') = k', \dim(\ell'' \cap \ell) = k''\} \tag{62}$$

$(0 \leqslant k, k', k'' \leqslant n)$. Given a 2-cocycle f on $\Lambda(n)$, there exists at most one Leray index m satisfying (61) (see [13, 16]).

We will also need the following simple general property:

Lemma 16. *Suppose m is a real function defined on all the pairs* $(\ell_\infty, \ell'_\infty)$ *such that* $\ell \cap \ell' = 0$, *and such that (61) holds for some* 2*-cocycle* f *on* $\Lambda(n)$*. Then, the formula*

$$m(\ell_\infty, \ell'_\infty) = m(\ell_\infty, \ell''_\infty) - m(\ell'_\infty, \ell''_\infty) + f(\ell, \ell', \ell'') \tag{63}$$

where ℓ''_∞ *is chosen such that* $\ell \cap \ell' = \ell \cap \ell''$ *defines unambiguously* $m(\ell_\infty, \ell'_\infty)$ *for all* $(\ell_\infty, \ell'_\infty) \in (\Lambda_\infty(n))^2$.

It is sufficient to verify that $m(\ell_\infty, \ell'_\infty)$ is independent of the choice of ℓ''_∞, but this follows from the cocycle property $\partial f = 0$ of f (see [13, 16, 20]).

To every triple (ℓ, ℓ', ℓ'') of Lagrangian planes we can associate an integer $\sigma(\ell, \ell', \ell'')$, called *signature*, and defined as being the difference $\sigma_+ - \sigma_-$ between the numbers of >0 and <0 eigenvalues of the quadratic form

$$Q(z, z', z'') = \Omega(z, z') + \Omega(z', z'') + \Omega(z'', z)$$

on $\ell \oplus \ell' \oplus \ell''$ (see [16, 18, 28]). The signature is an antisymmetric and $Sp(n)$-invariant cocycle: $\partial\sigma = 0$. Introducing the notation $\dim(\ell, \ell') = \dim \ell \cap \ell'$ we moreover have

$$\sigma(\ell, \ell', \ell'') \equiv n + \partial \dim(\ell, \ell', \ell'') \mod 2. \tag{64}$$

Theorem 17. *(1) The function m defined by*

$$m(\ell_\infty, \ell'_\infty) = \frac{1}{2\pi}(\alpha - \alpha' + \mathrm{i}\,\mathrm{Tr}\,\mathrm{Log}(-w(w')^{-1})) + \frac{n}{2} \tag{65}$$

for $\ell_\infty \equiv (w, \alpha)$, $\ell'_\infty \equiv (w', \alpha')$ *with transversal projections:* $\ell \cap \ell' = 0$ *is the Leray index associated with the cocycle*

$$\mathrm{Inert}(\ell, \ell', \ell'') = \tfrac{1}{2}(\sigma(\ell, \ell', \ell'') + n + \partial\dim(\ell, \ell', \ell'')) \tag{66}$$

(Inert *is called the 'index of inertia' of* (ℓ, ℓ', ℓ'')*). (2) That Leray index m has the following properties:*

$$m(\ell_\infty, \ell'_\infty) + m(\ell'_\infty, \ell_\infty) = n + \dim(\ell, \ell') \qquad m(\ell_\infty, \ell_\infty) = n \tag{67}$$

and the action of $\pi_1(\Lambda(n))$ *on m satisfies*

$$m(\lambda^k \cdot \ell_\infty, \lambda^{k'} \cdot \ell'_\infty) = m(\ell_\infty, \ell'_\infty) + k - k' \tag{68}$$

where λ *is the generator of* $\pi_1(\Lambda(n))$ *whose natural image in* $\mathbb{Z}$ *is* +1 *(cf (47)). (3) For* $n = 1$ *we have, with the notations (48),*

$$m(\theta, \theta') = \left[\frac{\theta - \theta'}{\pi}\right] + 1. \tag{69}$$

Proof. We first note that Inert (ℓ, ℓ', ℓ'') is always an integer in view of (64). We have shown in [11, 13] that the function μ defined on all $\{(\ell_\infty, \ell'_\infty) : \ell \cap \ell' = 0\}$ by $\mu = 2m - n$ (m defined by (65)) satisfies

$$\mu(\ell_\infty, \ell'_\infty) - \mu(\ell_\infty, \ell''_\infty) + \mu(\ell'_\infty, \ell''_\infty) = \sigma(\ell, \ell', \ell'').$$

It follows that

$$m(\ell_\infty, \ell'_\infty) - m(\ell_\infty, \ell''_\infty) + m(\ell'_\infty, \ell''_\infty) = \tfrac{1}{2}(\sigma(\ell, \ell', \ell'') + n)$$

if the planes ℓ, ℓ', ℓ'' are pairwise transverse. Since in this case $\partial\dim(\ell, \ell', \ell'') = 0$, the existence of m follows from lemma 16, because Inert is obviously a $Sp(n)$-invariant cocycle. Formulae (66)–(68) are obvious consequences of (47), (65) when $\ell \cap \ell' = 0$, and of (61) in the general case since ℓ_∞ and $\lambda^k \cdot \ell_\infty$ have same projection ℓ on $Lag(n)$. Let us finally prove property (3). Suppose first that $\theta - \theta' \neq 0 \pmod{\pi}$. Then (69) immediately follows from (65). Suppose next that $\theta - \theta' = k\pi$. Choosing θ'' such that $\ell(\theta) \cap \ell(\theta'') = 0$, we have

$$m(\theta, \theta') = k + \mathrm{Inert}(\ell(\theta), \ell(\theta), \ell(\theta'')) = k + 1$$

in view of (63), concluding the proof. □

Remark. There is a deep and interesting connection between the Leray index m and the Maslov index on the metaplectic group $Mp(n)$ (i.e., the unitary representation of the double cover $Sp_2(n)$ of $Sp(n)$) (see [12, 14]).

6.3. Definition of the argument index

We have now developed the machinery we need to define the complete argument index generalizing (21), (22).

Consider again the mapping $\ell_\infty(.) : \check{V} \longrightarrow \Lambda_\infty(n)$ defined by (54). We denote by $\ell_{\alpha,\infty}$ an element of $\Lambda_\infty(n)$ with projection $\ell_\alpha \in \Lambda(n)$.

Proposition 18. *The function* $m_\alpha : \check{V} \longrightarrow \mathbb{Z}$ *defined by*

$$m_\alpha(\check{z}) = m(\ell_\infty(\check{z}), \ell_{\alpha,\infty}) \tag{70}$$

has the following properties: (1) suppose that $\ell_\alpha = \ell_0$ and $\ell_{\alpha,\infty} = \ell_{0,\infty}$ is the homotopy class of the constant loop with origin ℓ_0. Then $m_\alpha(\check{z})$ is given by (56) if $\ell(z) \cap \ell_0 = 0$; (2) we have

$$m_\alpha(\gamma\check{z}) = m_\alpha(\gamma\check{z}) + m(\gamma) \tag{71}$$

for all $\gamma \in \pi_1(V)$ and $\check{z} \in \check{V}$; (3) we have $m_\alpha(\check{z}) = m(\theta)$ when $V = S^1$, $\ell_\alpha = \mathbb{R}_p$ and $z_0 = +1$.

Property (1) is obvious in view of (56) and (65). Property (2) follows from property (68) of the Leray index. Property (3) follows from part (3) of theorem 17.

The following result makes explicit the effect of a change in base point:

Proposition 19. *Let m_α, m_β be the Maslov indices associated by (56) to arbitrary elements $\ell_{\alpha,\infty}$ and $\ell_{\beta,\infty}$ of $\Lambda_\infty(n)$. We have*

$$m_\alpha(\check{z}) - m_\beta(\check{z}) = m(\ell_{\alpha,\infty}, \ell_{\beta,\infty}) - \mathrm{Inert}(\ell_\alpha, \ell_\beta, \ell(z)) \tag{72}$$

where z is the projection on V of $\check{z} \in \check{V}$.

Formula (72) is, of course, an immediate consequence of property (61) with the choice $f = \mathrm{Inert}$.

We next define the waveforms on Lagrangian manifolds.

7. Waveforms

We set out to generalize the construction of the square root of a de Rham form on the circle, as outlined above, to the general case of an n-dimensional Lagrangian submanifold V (which we again suppose connected, but *not necessarily orientable*). We will use the following standard notation and terminology: the *caustic* of V is the closed set

$$C = \left\{z \in V : \ell(z) \cap \mathbb{R}^n_p \neq 0\right\}.$$

More generally, we will call 'caustic of V relatively to the direction $\ell_\alpha \in \Lambda(n)$' the closed set

$$C_\alpha = \{z \in V : \ell(z) \cap \ell_\alpha \neq 0\}$$

and we denote by V_α its complement $V \setminus C_\alpha$:

$$V_\alpha = \{z \in V : \ell(z) \cap \ell_\alpha = 0\}.$$

7.1. De Rham forms and their square roots

Remark. The introduction of de Rham forms in SM should not be too surprising. It is well known in physics that many phenomena exhibit this dependence on orientation, the most elementary example of this phenomenon being the magnetic field, which is a 'pseudo-vector' (see the lucid discussion in Frankel's book [8]). On the other hand, the necessity of the inclusion of *half*-densities (or *half*-forms) in quantum mechanics has been noted a long time ago (it is of course immediately suggested by Van Vleck's formula [36] (also see [18, 22]). (Historically, the systematic use of these objects goes back to the work of Blattner, Kostant and Sternberg (see [3, 25, 39]).)

An *m-density* $\rho \in |\Omega^m(V)|$ on V ($m \in \mathbb{R}$) is a smooth section of the line-bundle $|\Lambda^m(TV)|$ of 1-densities on TV. Recall that by definition every $\rho(z) \in |\Lambda^m(T_zV)|$ is a mapping

$$\rho(z) : \underbrace{T_zV \times \cdots \times T_zV}_{m \text{ times}} \longrightarrow \mathbb{C}$$

such that

$$\rho(z)(u_1,\ldots,u_n) = |\det A|^m\, \rho(z)(Au_1,\ldots,Au_n)$$

for every $A \in GL(n,\mathbb{C})$ and all vectors $u_1,\ldots,u_n$ in T_zV. Let $(U_\alpha, f_\alpha)_\alpha$ be an atlas of V. The local expression ρ_α of $\rho \in |\Omega^m(V)|$ in each chart (U_α, f_α) is $\rho_\alpha(x)|\mathrm{d}x|^m$, the functions $\rho_\alpha \in C^\infty(f_\alpha(U_\alpha))$ satisfy the matching conditions

$$\rho_\alpha(x) = \left|\det \frac{\partial f_{\alpha\beta}}{\partial x}(x)\right|^m \rho_\beta(x) \qquad x \in f_\beta(U_\alpha \cap U_\beta) \tag{73}$$

where we have set $f_{\alpha\beta} = f_\alpha \circ f_\beta^{-1}$. In particular, if f_α and f'_α are two coordinate systems on U_α, then

$$\rho_\alpha(x)|\mathrm{d}x|^m = \left|\det\frac{\partial x}{\partial x'}\right|^m \rho_\alpha(x')|\mathrm{d}x'|^m$$

if $x = f_\alpha(z)$, $x' = f'_\alpha(z)$.

Suppose now that $m = 1$; we write $|\Omega^1(V)| = |\Omega(V)|$ and call elements of $|\Omega(V)|$ simply *densities*. Obviously, each $\rho(z) \in |\Lambda^1(T_zV)|$ is homogeneous with respect to scalar multiplication, but it is not additive. The definition of de Rham forms reinstates additivity: a *de Rham form* $\tilde{\mu} \in \Omega_\tau(V)$ associated with a density $\rho \in |\Omega(V)|$ is a smooth section of the line bundle $\tilde{\Lambda}(V)$ obtained by assigning to each $\rho(z) \in |\Lambda(T_zV)|$ the mapping

$$\mu(z) : \underbrace{T_zV \times \cdots \times T_zV}_{n\ \text{times}} \longrightarrow \mathbb{C}$$

defined by $\mu(z)(u_1,\ldots,u_n) = 0$ if the vectors $u_1,\ldots,u_n$ are linearly dependent, and by

$$\mu(z)(\mathcal{B}^{\pm}(z)) = \pm\rho(z)(\mathcal{B}(z))$$

if they form a basis $\mathcal{B}(z)$ of $\ell(z) = T_zV$; the notation $\pm$ refers to whether this basis is positively or negatively oriented relative to the orientation at z defined by a local chart (U, f) at z. Due to the inclusion of the factor ± 1 in its definition, $\mu(z)$ is linear and antisymmetric.

Let us now be more specific, and assume again that V is a Lagrangian submanifold. We denote by f_α the orthogonal projection of V_α on ℓ_α; it is a local diffeomorphism onto its image, so that each orientation of ℓ_α determines an orientation at $z \in V_\alpha$. Let now U be an open neighborhood of z in V_α. Choosing U sufficiently small, the pair (U, f_α) is a local chart at z. The open set U is orientable, and each of its orientations is determined by the choice of an orientation of ℓ_α, that is by the datum of an element $\tilde{\ell}_\alpha$ of the double cover $\Lambda_2(n)$ with projection ℓ_α. The restriction $\ell_U(\cdot)$ of the mapping $z \mapsto \ell(z)$ to U can be lifted to two continuous mappings $z \mapsto \tilde{\ell}^{\pm}_U(z) \in \Lambda_2(n)$, corresponding to a continuous positive (resp. negative) choice of orientations of the tangent planes. Let $\rho \in |\Omega|\,(U)$ be a density on U, and $\ell^{\pm}_{U,\infty}(z)$ be two elements of $\Lambda_\infty(n)$ with projections $\tilde{\ell}^{\pm}_U(z) \in \Lambda_2(n)$. Let $\ell_{\alpha,\infty}$ be an element of $\Lambda_\infty(n)$ with projection $\tilde{\ell}_\alpha$ on $\Lambda_2(n)$. We claim that

Lemma 20. *The formula*

$$\mu_U(z)(\mathcal{B}^{\pm}(z)) = (-1)^{m(\ell^{\pm}_{U,\infty}(z),\ell_{\alpha,\infty})}\rho(z)(\mathcal{B}(z)) \tag{74}$$

defines a de Rham form on U.

In fact, if we change $\mathcal{B}^+(z)$ into $\mathcal{B}^-(z)$, then we have to change $\ell^+_{U,\infty}(z)$ into $\ell^-_{U,\infty}(z)$ in formula (74). Since both $\ell^+_{U,\infty}(z)$ and $\ell^-_{U,\infty}(z)$ have same projection $\ell(z) \in \Lambda(n)$, we must have $\ell^+_{U,\infty}(z) = \lambda^k \cdot \ell^-_{U,\infty}(z)$ for some integer k and hence, by (68)

$$m\left(\ell^+_{U,\infty}(z), \ell_{\alpha,\infty}\right) = m(\ell^-_{U,\infty}(z), \ell_{\alpha,\infty}) + k.$$

Now, the integer k must be odd, because if it were even, then $\ell^+_{U,\infty}(z)$ and $\ell^-_{U,\infty}(z)$ would have same projection $\tilde{\ell}^+_U(z)$ on $\Lambda_2(n)$. Thus

$$\mu_U(z)(\mathcal{B}^+(z)) = -\mu_U(z)(\mathcal{B}^-(z).$$

Similarly, if we reverse the orientation at z, that is, if we replace $\tilde{\ell}_\alpha$ by an element of $\Lambda_2(n)$ defining the reverse orientation, then we must replace $\ell_{\alpha,\infty}$ by $\lambda \cdot \ell_{\alpha,\infty}$, which leads to replace $m\big(\ell^\pm_{U,\infty}(z), \ell_{\alpha,\infty}\big)$ by

$$m\left(\ell^\pm_{U,\infty}(z), \lambda \cdot \ell_{\alpha,\infty}\right) = m\left(\ell^\pm_{U,\infty}(z), \ell_{\alpha,\infty}\right) - 1$$

and thus again reverses the sign of $\mu_U(z)(\mathcal{B}^\pm(z))$. The lemma follows, noting that the mappings $z \mapsto \ell^\pm_{U,\infty}(z)$ are locally constant, and hence smooth.

Formula (74) allows us to define locally the argument of a de Rham form by

$$\arg \mu_U(z) = m\left(\ell^+_{U,\infty}(z), \ell^+_{\alpha,\infty}\right)\pi \tag{75}$$

and hence the square root of μ_U by the formula

$$\sqrt{\mu_U}(z)(\mathcal{B}^\pm(z)) = \mathrm{i}^{m(\ell^\pm_{U,\infty}(z),\ell_{\alpha,\infty})}\sqrt{\rho(z)(\mathcal{B}(z))}. \tag{76}$$

It turns out that this formula cannot generally be extended to define a global argument for a de Rham form (cf, for example, the density $r|\mathrm{d}\theta|$ on the circle S^1_r). However, we show that this can always be done outside the caustic C_α relative to ℓ_α, provided that we work on the universal covering of V.

Proposition 21. *Let μ be a de Rham form on V, associated with a density $\rho \in |\Omega|(V)$. For every V_a there exists a choice of $\ell_{\alpha,\infty} \in \Lambda_\infty(n)$ such that the restriction μ_α of μ to V_a is given, for $\check{z} \in \pi^{-1}(V_\alpha)$, by*

$$\mu_\alpha(\check{z})(\mathcal{B}^\pm(z)) = (-1)^{m^\pm_\alpha(\check{z})}\rho(z)(\mathcal{B}(z)) \tag{77}$$

where $m^+_\alpha(\check{z}) = m(\ell_\infty(\check{z}), \ell_{\alpha,\infty})$ and $m^-_\alpha(\check{z}) = m(\ell_\infty(\check{z}), \lambda \cdot \ell_{\alpha,\infty})$. We can thus define the square root of μ of V_a by the formula

$$\sqrt{\mu_\alpha}(\check{z})(\mathcal{B}^\pm(z)) = \mathrm{i}^{-m^\pm_\alpha(\check{z})}\sqrt{\rho(z)(\mathcal{B}(z))}. \tag{78}$$

If $z \in V_\alpha \cap V_\beta$, then

$$\sqrt{\mu_\alpha}(\check{z}) = \mathrm{i}^{-m_{\alpha\beta}(z)}\sqrt{\mu_\beta}(\check{z}) \tag{79}$$

where the function $m_{\alpha\beta} : V_\alpha \cap V_\beta \to \mathbb{Z}$ is given by

$$m_{\alpha\beta}(z) = m(\ell_{\alpha,\infty}, \ell_{\beta,\infty}) - \mathrm{Inert}(\ell_\alpha, \ell_\beta, \ell(z)). \tag{80}$$

Remark. We have introduced similar notions in [15, 17]; however, the choice $\mu_\alpha = \mathrm{i}^{-m_\alpha(\check{z})}\sqrt{\rho}$ for the square root of a half-density was postulated in a rather ad hoc manner.

It is instructive to interpret the constructions above in terms of the oriented double covering $\tilde{V}$ of the manifold V. Recall (see, for instance, [6], X, section 4) that $\tilde{V}$ is constructed, for an arbitrary submanifold V, in the following way: let $(U_\alpha, f_\alpha)_\alpha$ be an atlas, and define, for $U_\alpha \cap U_\beta \neq \varnothing$, locally constant mappings $g_{\alpha\beta} : U_\alpha \cap U_\beta \longrightarrow \{+1, -1\}$ by

$$g_{\alpha\beta}(z) = Df_{\alpha\beta}(f_\beta(z))|Df_{\alpha\beta}(f_\beta(z))|^{-1} \tag{81}$$

where the $f_{\alpha\beta} = f_\alpha f_\beta^{-1}$ are the transition functions. Evidently, $g_{\alpha\beta}g_{\beta\gamma}g_{\gamma\alpha}(z) = z$ for $z \in U_\alpha \cap U_\beta \cap U_\gamma$, hence there exists a twofold covering $\tilde{\pi} : \tilde{V} \longrightarrow V$ with trivializations

$$\tau_\alpha : \tilde{\pi}^{-1}(U_\alpha) \longrightarrow U_\alpha \times \{+1, -1\}.$$

The transition functions

$$\tau_{\alpha\beta} = \tau_\alpha\tau_\beta^{-1} : U_\beta \times \{+1, -1\} \longrightarrow U_\alpha \times \{+1, -1\}$$

are given by $\tau_{\alpha\beta}(z,\varepsilon) = (z, g_{\alpha\beta}(z))$ for $z \in U_\alpha \cap U_\beta$ and $\varepsilon = \pm 1$. This allows one to construct an orientable atlas $(\tilde{U}_{\alpha,\varepsilon}, \tilde{f}_{\alpha,\varepsilon})_{\alpha,\varepsilon}$ of $\tilde{V}$ by setting $\tilde{U}_{\alpha,\varepsilon} = \tau_\alpha^{-1}(U_\alpha \times \{\varepsilon\})$ and defining $\tilde{f}_{\alpha,\varepsilon} : \tilde{V}_{\alpha,\varepsilon} \longrightarrow \mathbb{R}^n$ by the formulae

$$\tilde{f}_{\alpha,\varepsilon}\left(\tau_\alpha^{-1}(z,\varepsilon)\right) = \begin{cases} f_\alpha(z) & \text{for} \quad \varepsilon = +1 \\ \sigma f_\alpha(z) & \text{for} \quad \varepsilon = -1 \end{cases}$$

where σ is $\mathbb{R}^n \longrightarrow \mathbb{R}^n$ changes, for instance, the coordinate x_1 into $-x_1$ and leaves the other coordinates unchanged. One has the following property: *V is orientable if and only if the double covering $\tilde{V}$ is trivial: $\tilde{V} = V \times \{+1, -1\}$, and $\tilde{V}$ is connected if and only if V is not orientable.*

When V is Lagrangian, we have the following interesting result that shows that the oriented double cover can always be identified with the product $V \times \{+1, -1\}$ (but of course not equipped with the product topology when V is non orientable!):

Proposition 22. *Suppose that V is not orientable. Then, each of the mappings*

$$\tilde{\Phi}_\alpha : \tilde{V} \longrightarrow V \times \{+1, -1\}$$

defined by $\tilde{\Phi}_\alpha(\tilde{z}) = (z, (-1)^{m_\alpha(\check{z})})$ where $\check{z} \in \check{V}$ has projection $\tilde{z} \in \tilde{V}$, is a bijection. The restriction Φ_α of $\tilde{\Phi}_\alpha$ to $\tilde{V}_\alpha = \{\tilde{z} : \ell(z) \cap \ell_\alpha\}$ is a homeomorphism, and the transitions $\Phi_{\alpha\beta} = \Phi_\alpha \Phi_\beta^{-1}$ are given by

$$\Phi_{\alpha\beta}(\tilde{z}) = (z, m(\ell_{\alpha,\infty}, \ell_{\beta,\infty}) - \mathrm{Inert}(\ell_\alpha, \ell_\beta, \ell(z))) \tag{82}$$

for $\tilde{z} \in \tilde{V}_\alpha \cap \tilde{V}_\beta$.

Proof. We first note that $\tilde{\Phi}_\alpha$ is well defined: if $\check{z}'$ and $\check{z}$ both have projection $\tilde{z} \in \tilde{V}$, then $\check{z}' = \gamma\check{z}$ for $\gamma \in \pi_1(\tilde{V})$, and hence

$$m_\alpha(\check{z}') = m_\alpha(\gamma\check{z}) = m_\alpha(\check{z}) \mod 2$$

in view of (52) since $\tilde{V}$ is orientable. A similar argument shows that each mapping $\tilde{\Phi}_\alpha$ is injective: if $\tilde{\Phi}_\alpha(\tilde{z}') = \tilde{\Phi}_\alpha(\tilde{z})$, then $z' = z$ and $\check{z}' = \gamma\check{z}$ with $m(\gamma)$ even, so that $\gamma \in \pi_1(\tilde{V})$, and $\tilde{z}' = \tilde{z}$. To prove that $\tilde{\Phi}_\alpha$ is surjective, it suffices to note that if $\tilde{\Phi}_\alpha(\tilde{z}) = (z, \varepsilon)$, then $\tilde{\Phi}_\alpha(\tilde{z}') = (z, -\varepsilon)$ where $\tilde{z}'$ is the projection on $\tilde{V}$ of $\gamma\check{z}$, $\check{z}$ has projection $\tilde{z}$, and $\gamma \in \pi_1(V)$ is such that $m(\gamma) = 1$ (the existence of such a γ follows from (52) since we are assuming V non-orientable). Finally, Φ_α is locally constant on V_α, and hence continuous; formula (82) follows from (72). □

7.2. Definition of waveforms

Let φ be the phase of the Lagrangian submanifold V, and μ a de Rham form associated with a density ρ on V.

Definition 23. *A waveform on $\check{V}$ is the datum, for each $\ell_\alpha \in \Lambda(n)$ of an expression*

$$\Psi_\alpha(\check{z}) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\varphi(\check{z})}\sqrt{\mu_\alpha}(\check{z})$$

where the μ_α are associated with a same density ρ on V. Equivalently,

$$\Psi_\alpha(\check{z}) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\varphi(\check{z})}\mathrm{i}^{-m_\alpha(\check{z})}\sqrt{\rho}(z).$$

Defining the action of $\pi_1(V)$ on Ψ by $\gamma\Psi(\check{z}) = \Psi(\gamma\check{z})$, we say that Ψ is defined on V if $\gamma\Psi = \Psi$ for all $\gamma \in \pi_1(V)$.

The following result relates our constructions to the minimum symplectic area postulate:

Proposition 24. *(1) A waveform is defined on V if and only if V satisfies the Maslov quantization condition*

$$\frac{1}{2\pi\hbar}\int_\gamma p\,\mathrm{d}x - \frac{1}{4}m(\gamma) \text{ is an integer} \tag{83}$$

for every loop γ in V. (2) When V is oriented, condition (83) reduces to the condition

$$\frac{1}{\pi\hbar}\int_\gamma p\,\mathrm{d}x \in \mathbb{Z} \qquad \text{for all } \gamma \in \pi_1(V). \tag{84}$$

Proof. The second statement of the theorem follows from the first in view of (52). By definition of a waveform we have to prove that the condition $\Psi(\check{z}) = \Psi(\gamma\check{z})$ is equivalent to (83). In view of (29) and (71) we have

$$\gamma\Psi(\check{z}) = \exp\left[\mathrm{i}\left(\frac{1}{\hbar}\int_\gamma p\,\mathrm{d}x - \frac{\pi}{2}m(\gamma)\right)\right]\Psi(\check{z})$$

hence $\gamma\Psi = \Psi$ is equivalent to

$$\frac{1}{\hbar}\int_\gamma p\,\mathrm{d}x - \frac{\pi}{2}m(\gamma) = 0 \mod 2\pi$$

which is, of course, the same thing as (83). □

7.3. The Hamiltonian motion of waveforms

The waveforms we have defined are time-independent, they are thus adequate for the study of stationary processes. However, if we want to use them for the dynamical study of quantum systems we have to define how Hamiltonian flows act on them.

Consider an arbitrary function $H = H(x, p, t)$ defined on some open subset $D \times \mathbb{R}_t$ of the extended phase space $\mathbb{R}^n_x \times \mathbb{R}^n_p \times \mathbb{R}_t$; we denote the time-dependent flow of $X_H = (\nabla_p H, -\nabla_x H)$ by $f_{t,t'}$.

We need the following property of the Leray index. Let $Sp_\infty(n)$ be the universal covering of $Sp(n)$; the usual action $Sp(n) \times \Lambda(n) \longrightarrow \Lambda(n)$ induces an action $Sp_\infty(n) \times \Lambda_\infty(n) \longrightarrow \Lambda_\infty(n)$. We claim that the following essential formula holds,

$$m(s_\infty\ell_\infty, s_\infty\ell'_\infty) = m(\ell_\infty, \ell'_\infty) \tag{85}$$

for all $(s_\infty, \ell_\infty) \in Sp_\infty(n) \times \Lambda_\infty(n)$.

Formula (85) follows from the fact that the cocycle f associated with a Leray index is $Sp(n)$-invariant and from the uniqueness of the Leray index associated with a given cocycle (see lemma 16): both mappings $(\ell_\infty, \ell'_\infty) \longmapsto m(\ell_\infty, \ell'_\infty)$ and $(\ell_\infty, \ell'_\infty) \longmapsto m(s_\infty\ell_\infty, s_\infty\ell'_\infty)$ satisfy the conditions in definition 15, and are hence identical.

The Jacobian matrix $s_{t,t'}(z)$ of $f_{t,t'}$ at z being symplectic, we can lift the mapping $t \mapsto s_{t,t'}(z) \in Sp(n)$ to a mapping

$$t \mapsto (s_{t,t'}(z))_\infty \in Sp_\infty(n)$$

such that $(s_{t,t}(z))_\infty$ is the identity of $Sp_\infty(n)$. Setting

$$m_0(\check{z}, t) = m(\ell_{0,\infty}, (s_{t,t'}(z))_\infty\ell(\check{z})) \tag{86}$$

we then define the value of Ψ at time t by the formula

$$\Psi(\check{z}, t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\varphi(\check{z},t)}\mathrm{i}^{-m_0(\check{z},t)}\sqrt{(f_t)_*\rho}(z). \tag{87}$$

Let $\check{f}_{t,t'}$ be the mapping which to $\Psi(\check{z}, t')$ associates $\Psi(\check{z}, t)$. These mappings satisfy the Chapman–Kolmogorov condition

$$\check{f}_{t,t'}\check{f}_{t',t''} = \check{f}_{t,t''} \tag{88}$$

as immediately follows from the fact that

$$(f_{t,t'}f_{t',t''})_*\rho = (f_{t,t'})_*(f_{t',t''})_*\rho.$$

7.4. Shadows and their motion

Suppose that the Lagrangian submanifold V is a simply connected graph $p = \nabla_x\Phi(x)$. V is then automatically quantized, because $m(\gamma) = 0$ for every loop γ in V. We denote by $\mathcal{S}$ the operator which to every waveform Ψ on V associates the coefficient of its local expression in the chart (V_t, π_X) where π_X is the projection $(x, p) \longmapsto x$ on configuration space. Thus, if Ψ has local expression $\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Phi(x)}a(x)|\mathrm{d}x|^{1/2}$ in (V, π_X), then

$$\mathcal{S}(\Psi)(x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Phi(x)}a(x).$$

We will call $\Sigma(\Psi)$ the *shadow* of Ψ. Suppose now that V is an arbitrary Lagrangian submanifold (i.e. we relax the conditions that V be a graph, or simply connected). We moreover assume that the quantization condition (83) holds for V. Then, given a point x there will, in general, be several charts (U_j, π_X) such that $x \in \pi_X(U_j)$. In this case we define the shadow of a waveform Ψ as being the sum

$$\mathcal{S}(\Psi)(x) = \sum_j \mathrm{i}^{m(x_j)}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Phi(x,p_j)}a(x_j)$$

calculated at the point (x, x'_j, t, t'), and m_j is the *Morse index* of the trajectory from x'_j to x: it is the number of conjugate points along that trajectory, that is, the number of points where $\det \mathrm{Hess}_{x,x'}(S)$ is zero, or infinite.

Write now the wavefunction at time t' in the familiar 'oscillatory' form

$$\Psi(x, t') = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Phi(x,p_j)}a(x, t')$$

where Φ and a are smooth functions, $a \geqslant 0$, both defined for $(x, t') \in X \times \mathbb{R}_t$, X some open subset of $\mathbb{R}^n_x$ (we do not assume that X is simply connected). For fixed t' the function $\psi(\cdot, t')$ is the local expression of a Lagrangian waveform $\check{\Psi}(., t')$ on the graph $V_{t'}$ of the gradient of the phase $\Phi(., t')$:

$$V_{t'} = \{(x, p) : p = \nabla_x\Phi(x, t')\}.$$

In fact,

$$\Psi(\check{z}, t') = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\varphi(\check{z},t')} f^*(a(x, t')|\mathrm{d}^n x|^{1/2}) \tag{89}$$

where $f^*(a(x)|\mathrm{d}^n x|^{1/2})$ is the pull-back to $V_{t'}$ of the half-density $a(x)|\mathrm{d}^n x|^{1/2}$ on $\mathbb{R}^n_x$.

Let us finally relate our waveforms to the approximate solutions to Schrödinger's equation studied by Maslov [29] and Maslov and Fedoriuk [30]. Writing the initial wavefunction as $\Psi_0(x) = \exp\left[\frac{\mathrm{i}}{\hbar}S_0(x)\right]$, these authors propose expressions of the type

$$\Psi(x, t) = \sum_j \mathrm{i}^{\mu_j(x,t,t')}\left|\frac{\mathrm{d}x}{\mathrm{d}x'_j}\right|^{-1/2} \exp\left[\frac{\mathrm{i}}{\hbar}S_j(x, t)\right]\Psi_0(x'_j, t') \tag{90}$$

where x'_j, S_j and $\mu_j(x, t, t')$ are defined as follows: let again $(f_{t,t'})$ be the time-dependent flow of H, and denote by V_t the image by $f_{t,t'}$ the image of the Lagrangian submanifold $V_{t'} : p = \nabla_x S(x, t')$. Given a point x of the projection of V_t on $\mathbb{R}^n_x$ there is (under adequate assumptions on U and $\Psi_{t'}$) a finite number of points $(x, p_j) \in V_t$ and $(x'_j, p'_j) \in V_{t'}$ such that $(x, p_j) = f_{t,t'}(x'_j, p'_j)$. The phase $S_j(x, t)$ in (90) is then given by the integral

$$S_j(x,t) = S(x, x'_j; t, t') = \int_{x'_j, t'}^{x,t} p\, \mathrm{d}x - H\, \mathrm{d}s \tag{91}$$

calculated along the trajectory leading from x'_j at time t' to x at time t. The integers $\mu_j(x, t, t')$ in (90) are the *Morse indices* of these trajectories; these indices are obtained by counting the number of *conjugate points* along each trajectory. It turns out that for short time intervals $t - t'$ formula (90) reduces to

$$\Psi(x,t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x,t)}\Psi(x', t') \left|\det \frac{\partial x}{\partial x'}\right|^{-1/2} \tag{92}$$

where S is just the classical action function evaluated from (x', t') to (x, t). In fact, if $t - t'$ is sufficiently small then V_t will be a graph and there will exist exactly *one* point x' such that $(x, p) = f_{t,t'}(x', p')$ for $(x, p) \in V_t$. (Formula (92) was actually already discovered in 1928 by Van Vleck [36].)

8. Conclusion

We have achieved our goal, which was to construct a semiclassical mechanics based on a topological principle without any reference to the usual semiclassical approximations based on the WKB method (from which SM historically originates). Semiclassical mechanics thus appears to be a theory in its own right. We have not examined in which sense our theory approximates CM or QM, nor have we given any applications. As is the case for CM or QM, the domain of validity of SM can be determined by experience. It would certainly be interesting to develop further the consequences of the minimum symplectic area postulate in the following directions:

(1) The quantization of non-integrable systems: it is well known that periodic orbits play a fundamental role in such systems (see, e.g., [2, 22]); the theory of Lagrangian paths as outlined in section 6 and further developed in [20] is certainly useful in this context (this theory gives a mathematically rigorous justification of the recent constructions in Sugita [35].

(2) Statistical mechanics and thermodynamics: the minimum symplectic area postulate could be used to push further phase space 'cell quantization' as we outlined in [19]. Formula (5) relating symplectic area and volume shows that the volume of such cells corresponding to a quantized ball $B(\sqrt{\hbar})$ is $h^n/2^n n!$, which is consistent with Bose–Einstein statistics.

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