Revista Brasileira de Física, Vol. 14, nº 1, 1984

Semiclassical Matrix Elements

A.M. OZORIO DE ALMEIDA

Instituto de Física, Universidade Estadual de Campinas, Caixa Postal 1170, Campinas, 13100, SP, Brasil

Recebido em 27 de junho de 1984

Abstract Semiclassical matrix elements of an observable, with respect to the eigenstates of a classically integrable Hamiltonian, are derived using the Wigner-Weyl representation in ordinary phase space and in action-angle variables. For properties involving the entire matrix, such as the eigenvalues, there is usually little difference between both results, which are simpler to calculate in the actíon-angle formalism. The relative difference for single matrix elements can be important. The theory relies on semiclassical approximations of the Moyal matrix or cross-Wigner function, which generalizes previous work on the pure state Wigner function, together with its interpretation in terms of the geometry of the invariant tori of integrable systems. The semiclassical equivalence between the Weyl transform of an operator and the corresponding classical function is also discussed.

1. INTRODUCTION

The attempt to understand the quantum mechanics of systems whose classical motion is unintegrable, i.e. with fewer constants of the motion than degrees of freedom, has hecessarily increased the interest of alternative approaches to semiclassical (SC) mechanics. Of these one of the most promising uses the Wigner-Weyl formulation of quantum mechanics, since the main mathematical results on unintegrable systems are derived in a phase space rather than a coordinate space formalism. Initial work on the Wigner function of integrable systems[1,2,3,4] uncovered a remarkable geometrical relation between the SC Wigner function and the classical invariant manifold (a torus) to which it collapses in the classical limit where Planck's constant $\hbar \to 0$. Unfortunately the SC Wigner function for unintegrable systems has proved as elusive as other representations of the SC state, but the Wigner-Weyl formulation may be used in other ways.

Work partially supported by FAPESP, CNPq and FINEP (Brazilian Government Agencies).

The object of this paper is to derive the SC form of the matrix elements of any observable with a classical limit, with respect to the eigenstates of an integrable system. In the particular case where the observable is an unintegrable Hamiltonian, its SC matrix will be nearly diagonal if the basis used for the expansion are the eigenstates of a good integrable approximation of the Hamiltonian. The spectrum of an unintegrable system thus becomes accessible by merely diagonalizing the SC Hamiltonian. Of course the matrix elements have other uses, such as calculating transition rates, etc.. .

The form of Weyl transform of an operator $\hat{A}$ (function of $\hat{\vec{q}}$ and $\hat{\vec{p}}$, the fundamental coordinate operators of a Hamiltonian system with N degrees of freedom) which I shall use is

$$A(\vec{q},\vec{p}) = \int d\vec{Q}\, \langle \vec{q}+\vec{Q}/2|\hat{A}|\vec{q}-\vec{Q}/2\rangle\, e^{-i\vec{p}\cdot\vec{Q}/\hbar} \tag{1.1}$$

It is not generally true that $A(\vec{q},\vec{p}) = A_c(\vec{q},\vec{p})$, the classical observable, if $\hat{A}$ doesn't depend explicitly on h[5]. However, it will be shown in section 2 that this equality does hold semiclassically.

The matrix representation of $\hat{A}$ in terms of a complete basis of states $|\vec{m}\rangle$ is then

$$\begin{aligned}
\langle\vec{k}|\hat{A}|\vec{m}\rangle &= \int d\vec{q}_1 d\vec{q}_2 \langle\vec{k}|\vec{q}_1\rangle\langle\vec{q}_1|\hat{A}|\vec{q}_2\rangle\langle\vec{q}_2|\vec{m}\rangle \\
&= \int d\vec{q}\; d\vec{Q}\, \langle\vec{k}|\vec{q}+\vec{Q}/2\rangle\, \langle\vec{q}+\vec{Q}/2|\hat{A}|\vec{q}-\vec{Q}/2\rangle\langle\vec{q}-\vec{Q}/2|\vec{m}\rangle \\
&= \left(\frac{1}{2\pi\hbar}\right)^N \int d\vec{p}\; d\vec{q}\; d\vec{Q}\; A(\vec{q},\vec{p})\langle\vec{q}-\vec{Q}/2|\vec{m}\rangle\langle\vec{k}|\vec{q}+\vec{Q}/2\rangle e^{i\vec{p}\cdot\vec{Q}/\hbar} \\
&= \int d\vec{p}\; d\vec{q}\; A(\vec{q},\vec{p})\; \langle\vec{k}|\vec{m}\rangle\; (\vec{q},\vec{p})
\end{aligned} \tag{1.2}$$

where I define the *Moyal Matrix*[6], or the *cross Wigner function*

$$\langle\vec{k}|\vec{m}\rangle(\vec{q},\vec{p}) = \left(\frac{1}{2\pi\hbar}\right)^N \int d\vec{Q}\, \langle\vec{q}+\vec{Q}/2|\vec{m}\rangle\, \langle\vec{k}|\vec{q}-\vec{Q}/2\rangle e^{i\vec{p}\cdot\vec{Q}/\hbar} \tag{1.3}$$

The Moyal matrix elements are simply the Weyl transform of the operators $(2\pi\hbar)^{-N}\; |\vec{m}\rangle\langle\vec{k}|$. Altogether they form a complete orthogonal basis in the set of ***Wigner functions*** corresponding to pure arbitrary states $|\psi\rangle$:

$$<\psi|\psi>(\vec{q},\vec{p}) = \left(\frac{1}{2\pi\hbar}\right)^N \int d\vec{Q} <\vec{q}+\vec{Q}/2|\psi><\psi|\vec{q}-\vec{Q}/2> e^{-i\vec{p}.\vec{Q}/\hbar} \quad (1.4)$$

The expansion

$$|\psi> = \sum_{\vec{m}} a_{\vec{m}}|\vec{m}> \quad (1.5)$$

in eq.(1.4) leads to

$$<\psi|\psi>(\vec{q},\vec{p}) = \sum_{\vec{m},\vec{k}} a^*_{\vec{k}}a_{\vec{m}} <\vec{k}|\vec{m}>(\vec{q},\vec{p}) \quad (1.6)$$

The matrix elements satisfy the relations[6]

$$\int d\vec{q}\ d\vec{Q} <\vec{k}|\vec{m}>(\vec{q},\vec{p})<\vec{k}'|\vec{m}'>^*(\vec{q},\vec{p}) = \left(\frac{2\pi}{\hbar}\right)^N \delta_{kk'}\ \delta_{mm'} \quad (1.7)$$

and

$$\sum_{\vec{m}\vec{k}} <\vec{m}|\vec{k}>(\vec{q},\vec{p})\ <\vec{m}|\vec{k}>^*\ (\vec{q}',\vec{p}') = \left(\frac{2\pi}{\hbar}\right)^N \delta(\vec{q}-\vec{q}')\delta(\vec{p}-\vec{p}') \quad (1.8)$$

as well as the self-orthogonality relations

$$\int d\vec{q}\ d\vec{p} <\vec{m}|\vec{k}>\ (\vec{q},\vec{p}) = <\vec{m}|\vec{k}> = \delta_{\vec{m}\vec{k}} \quad (1.9)$$

and

$$\sum_{\vec{m}} <\vec{m}|\vec{m}> = \left(\frac{2\pi}{\hbar}\right)^N \quad (1.10)$$

The Moyal Matrix is obviously Hermitian,

$$<\vec{m}|\vec{k}>(\vec{q},\vec{p}) = <\vec{k}|\vec{m}>^*\ (\vec{q},\vec{p}) \quad (1.11)$$

even though the operators $|\vec{m}><\vec{k}|$ are not.

From the form of eq.(1.2) it is evident that the first step in the SC theory of matrix representãtion of observables is the generalization of the SC theory of pure state Wigner functions[1,2,3] to Moyal Matrix elements. This is presented in section 3. Finally in section 4 the theory is reworked in action-angle variables. Thecomparisonof these with the results derived in the untransformed phase space revea'ls that the simplicity of the actíon-angle formalism may in some cases entail a significant loss of accuracy of the matrix elements.

2. THE SEMICLASSICAL WEYL TRANSFORM

In the simple case that $\hat{A}$ depends only on $\hat{q}$, it follows from the definition (1.1) that $A(\vec{q},\vec{p}) = A(\vec{q}) = A_c(\vec{q})$. The alternative formof

(1.1) using the momentum representation,

$$A(\vec{q},\vec{p}) = \int d\vec{p}\ \langle\vec{p}+\vec{P}/2|\hat{A}|\vec{p}-\vec{P}/2\rangle\ e^{-i\vec{q}.\vec{P}/\hbar} \qquad (2.1)$$

leads to a similar identity between the Weyl transform and the classical limit of any function of $\hat{\vec{p}}$. The linearity of the Weyl transform thus implies that Hamiltonians with the standard form $\hat{\vec{p}}^2 + V(\hat{\vec{q}})$ have as Weyl transforms $\vec{p}^2 + V(\vec{q})$.

In general, however, the Weyl correspondence may not always hold. Indeed, the best way to quantize a complicated function of $\vec{p}$ and $\vec{q}$ is not always clear[5]. I shall now shaw that these problems are semiclassically negligible by expanding $A(\vec{q},\vec{p})$ as a superposition of Wigner functions. In this way I satisfy a secondary objective of introducing the simplest instance of the Moyal matrix elements to be discussed in the next section. Only a single degree of freedom will be considered.

The expansion of the observable $\hat{A}$ in the basis of its own eigenfunctions

$$\hat{A} = \sum_m |m\rangle A_m \langle m| \qquad (2.2)$$

has the Weyl transform

$$A(q,p) = (2\pi\hbar) \sum_m A_m \langle m|m\rangle(q,p) \qquad (2.3)$$

Semiclassically the state m corresponds to the level curve

$$A_c(q,p) = A_m \qquad (2.4)$$

whose area is $2\pi\ I_m$, where I_m is the classical action selected by the quantization condition

$$I_m = \hbar(m + \alpha/4) \qquad (2.5)$$

Here α is the *Maslov index*, which for the eigenstates of non-linear oscillators equals 2. In the case of more than one degree of freedom, the eigenstate of a complete set of commuting observables corresponds to a phase space N-torus. The quantization condition (2.4) then applies to each one of its N irreducible circuits, defining the set of basis tori.

It was proved by Berry[1] that in the classical limit the Wigner function collapses onto the torus or, in our case, the level curve:

$$<m|m>(q,p) \xrightarrow[\hbar\to 0]{} \frac{\delta(I(q,p) - I_m)}{2\pi} \tag{2.6}$$

In this limit the spacing of the eigen-actions (2.5) tends to zero, so that we may approximate the sum by an integral. Thus, interpolating the A_m using eq. (2.4), we obtain

$$A(q,p) \xrightarrow[\hbar\to 0]{} 2\pi\hbar \int \frac{dI}{\hbar} A_c(q,p) \frac{\delta(I-I(q,p))}{2\pi} = A_c(q,p) \tag{2.7}$$

The classical limit (2.6) of the Wigner function does not hold asymptotically for small non-zero $\hbar$. The uniform SC approximation, valid inside and outside the torus, derived by Berry[1] is

$$<m|m>(q,p) = \frac{\sqrt{2}\left[\frac{3}{2}\,\sigma(q,p)\right]^{1/6} Ai\left(-\left[\frac{3\sigma(q,p)}{2\hbar}\right]^{2/3}\right)}{\pi\hbar^{2/3}\,|\{I_1,I_2\}|^{1/2}} \tag{2.8}$$

where Ai is the Airy function[7]. If the point (q,p) is inside the torus, the area bounded on one side by the torus and on the other by the torus chord, which has (q,p) as its mid-point, is $\sigma(q,p)$. A useful way to construct this Berry chord[2] is to reflect the torus through the point (q,p). The area sandwitched between the torus and the reflected 'anti-torus' is $2\sigma(q,p)$. This is shown in Fig. 1. The chord tips have coordinates (q_j,p_j) and the functions I_j are defined by

$$I_j(q',p') = I(q'-q_j,p'-p_j) \tag{2.9}$$

In the denominator of eq.(2.8) there appears the Poisson Bracket

$$\{I_1,I_2\} = \frac{\partial I_1}{\partial q}\frac{\partial I_2}{\partial p} - \frac{\partial I_1}{\partial p}\frac{\partial I_2}{\partial q} \tag{2.10}$$

with the derivatives evaluated at the origin.

For points (q,p) outside the torus, the chords and the areas $\sigma(q,p)$ are complex, so that the Airy function is exponentially decaying. Inside, where the argument of Ai is much greater than one, we can use the ãsymptotic form[7] of Ai to obtain

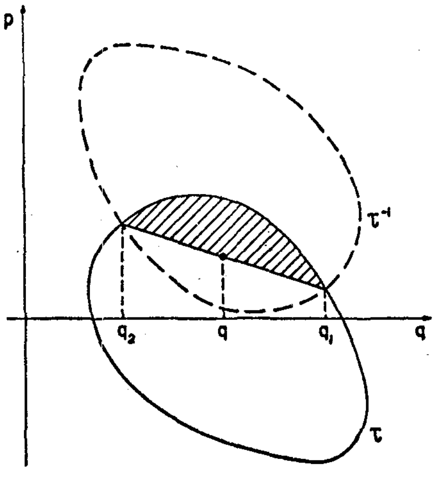

Fig.1 - The antitorus τ^{-1} is obtained by reflecting the torus τ through the evaluation point (q,p). The intersection of τ and τ^{-1} determines the tips of the Berry chord. The area $\sigma(q,p)$ has been shaded in.

$$\langle m|m\rangle(q,p) = \frac{2\cos\left[\sigma(q,p)/\hbar - \frac{\pi}{4}\right]}{|2\pi^3\hbar\{I_1,I_2\}|^{1/2}} \tag{2.11}$$

Thus, as discussed in ref.2, the classical limit eq.(2.6) is not a result of the amplitude inside the torus going to zero, but of the oscillations of the Wigner function becoming infinitely fast. As (q,p) approaches the torus $\{I_1,I_2\} \to 0$ and $a \to 0$. The indeterminacy in eq. (2.8) is resolved in the transitional approximation of the Wigner function

$$\langle m|m\rangle(q,p) = \frac{1}{\pi}(2\hbar^2\delta^2 I)^{-1/3}\, Ai\left[\frac{2(I_m - I(q,p))}{(2\hbar^2\delta^2 I)^{1/3}}\right] \tag{2.12}$$

where

$$\delta^2 I = I_q^2 I_{pp} + I_p^2 I_{qq} - 2I_{pq}I_p I_q \tag{2.13}$$

measures a kind of 'curvature' of the torus, as discussed in ref.3. In the limit $\hbar \to 0$ eq. (2.12) reduces to the δ-function (2.5).

The question is now whether the oscillations of the SC Wigner function break the equality between the Weyl transform and the classical observable. To answer this question we must improve on the crude procedure, of approximating a discrete sum by an integral, through the use of the exact Poisson summation formula[8]

$$\sum_{m=-\infty}^{m} f_m = \sum_{j=-\infty}^{\infty} \int_{-\infty}^{\infty} dm\, f(m)\, \exp(2\pi i j m) \quad (2.14)$$

The terms with $j \neq 0$ supply oscillatory corrections to the standard approximation. Applied to eq.(2.3) the Weyl representation of $\hat{A}$ becomes

$$A(q,p) = \sum_{j=0}^{\infty} e^{ij\alpha\pi} \int_0^{\infty} \frac{dI}{\hbar} A_c(I) \langle I|I\rangle(q,p)\, e^{\frac{2\pi i j I}{\hbar}} \quad (2.15)$$

where $\langle I|I\rangle(q,p)$ stands for the Wigner function corresponding to the (not necessarily quantized) torus with action ■ . Using the approximation (2.11) inside the torus for each integral, we obtain any oscillatory SC contribution to $A(q,p)$ by evaluating the integrals through the method of stationary phase. Since $A_c(I)$ is non-oscillatory, the phase of the j'th integral is just

$$\frac{2\pi j}{\hbar} \pm \left(\frac{\sigma_I(q,p)}{\hbar} - \frac{\pi}{4}\right) \quad (2.16)$$

Note that now it is the centre of the chord (q,p) which is held fixed, whereas the torus I is variabie. The stationary phase condition is

$$\frac{\partial\, \sigma_I(q,p)}{dI} = \pm\, 2\pi j = \pm\, j\, \frac{d(2\pi\, I)}{dI} \quad (2.17)$$

But, since $(2\pi\, I)$ is the area of the whole torus, the chord area can grow with I only as a fraction, not as a multiple of 2π ■ . The only stationary point is thus for

$$j = 0 \quad , \quad \frac{\partial\, \sigma_I(q,p)}{dI} = 0 \quad (2.18)$$

So the approximation of the sum in eq.(2.3) by an integral is justified afterall. Moreover the dorninant stationary action is that of the torus passing exactly through (q,p) - the one with $\sigma_I(q,p) = 0$. Thus, instead of eq.(2.11), we must use the transitional approximation (2.12) in (2.15). Replacing the Airy function by its integral representation

$$Ai(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt\, e^{i(t^3/3 + xt)} \quad (2.19)$$

we get

$$A(q,p) = \frac{1}{\pi} (2\hbar^2\delta^2 I)^{-1/3} \int_{-\infty}^{\infty} dt \int_0^{\infty} dI\, A_c(I)\, \exp\left\{i\left[\frac{t^3}{3} + 2t\, \frac{I-I(q,p)}{(2\hbar^2\delta^2 I)^{1/3}}\right]\right\} \tag{2.20}$$

The only stationary point is at

$$t = 0 \quad , \quad I = I(q,p) \tag{2.21}$$

and the Hessian matrix of the phase at this point has zero signature and determinant $(2(2\hbar^2\delta^2 I)^{1/3})^2$, so that the method of stationary phase gives again

$$A(q,p) = A_c(q,p) \tag{2.22}$$

The SC oscillations of the Wigner function do not affect the Weyl correspondence for systems with one degree of freedom. For two degrees of freedom the transitional approximation of torus Wigner functions reduces to a product of one dimensional Wigner functions, for the simple class of tori discussed in ref.3. This permits the generalization of the foregoing deduction with the same simple result.

3. THE SEMICLASSICAL MOYAL MATRIX

To derive the SC limit of the Moyal matrix elements, one uses the SC form of the wavefunction

$$\langle\vec{q}|\vec{m}\rangle = \frac{1}{\sqrt{2\pi}} \sum_j \left|\det \frac{\partial^2 S_j}{\partial\vec{q}\partial\vec{I}} (\vec{q},\vec{I}_{\vec{m}})\right|^{1/2} \exp\left[\frac{i}{\hbar} S_j(\vec{q},\vec{I}_{\vec{m}}) + i\frac{\pi}{4}\alpha_j\right] \tag{3.1}$$

where

$$S_j(\vec{q},\vec{I}_{\vec{m}}) = \int_{\vec{q}_0}^{\vec{q}} \vec{p}_j(\vec{q}\,',\vec{I}_{\vec{m}}).d\vec{q}\,' \tag{3.2}$$

is the *classical action* along the j'th sheet of the classical torus, labeled by the independent action variables $\vec{I}$, each of them quantized according to eq. (2.5). The index α_j changes by two in passing from sheet to sheet. For a full irreducible circuit on the torus $\Sigma\, \alpha_j = \alpha$, the

Maslov index. (A more detailed exposition of the SC wave function is given in ref.2.) Inserting eq.(3.1) into eq.(1.3) we get the integral representation of the SC Moyal matrix:

$$<\vec{k}|\vec{m}>(\vec{q},\vec{p}) = \left(\frac{1}{(2\pi)^2\hbar}\right)^N \sum_{j,j'} \int d\vec{Q} \left| \det \frac{\partial^2 S_j}{\partial\vec{q}\partial I_{\vec{m}}} \det \frac{\partial^2 S_{j'}}{\partial\vec{q}\partial I_{\vec{k}}} \right|^{1/2}$$

$$\exp\left\{\frac{i}{\hbar}\left[S_j(\vec{q}+\frac{\vec{Q}}{2}, I_{\vec{m}}) - S_j(\vec{q}-\frac{\vec{Q}}{2}, I_{\vec{k}})\right] + \frac{i\pi}{4}(\alpha_j - \alpha_{j'})\right\} \tag{3.3}$$

This integral will be dominated by its stationary points even if these are too close together for the simple stationary phase method to be applied directly. A linear canonical (metaplectic) transformation among the phase space coordinates will usually bring all thestationary points onto a single pair of sheets j,j', so that henceforth, since the metaplectic invariance of the Wigner function proved inref.2 can beextended to the Moyal matrix, these indices and the sum shall be omrnitted.

The modulus of the Moyal matrix elements is uniquely determined, but, unlike the Wigner function, the phase is partly arbitrary. This arbitrariness does not affect integrals over phase space, so we separate it out by defining

$$S\left(\vec{q} \pm \frac{\vec{Q}}{2}\right) = S_0(\vec{q}) + S_{\vec{q}}(\pm \vec{Q}/2) \tag{3.4}$$

The Moyal matrix then takes the form

$$<\vec{k}|\vec{m}>(\vec{q},\vec{p}) = \frac{e^{\frac{i}{\hbar}[S_0(\vec{q},I_{\vec{m}}) - S_0(\vec{q},I_{\vec{k}})]}}{((2\pi)^2\hbar)^N} \int_{-\infty}^{\infty} d\vec{Q} \left| \det \frac{\partial I_{\vec{m}}(\vec{q}+\vec{Q}/2)}{\partial\vec{p}} \right.$$

$$\left. \times \det \frac{\partial I_{\vec{m}}(\vec{q}-\vec{Q}/2)}{\partial\vec{p}} \right|^{-1/2} \exp\left\{\frac{i}{\hbar}[S_{\vec{q}}(\vec{Q}/2, I_{\vec{m}}) - S_q(-\frac{Q}{2}, I_{\vec{k}}) - \vec{p}.\vec{Q}]\right\}$$

(3.5)

where I have used the equality

(3.6)

The two phases in eq.(3.5) have geometrical interpretations. Outside the integral appears the action sandwitched by the $\vec{m}$'th and the $\vec{k}$'th tori between the points with coordinates $\vec{q}_0$ and $\vec{q}$. For one degree of freedom this is just the shaded area between the two level curves shown in Fig. 2. To understand the phase inside the integral it is best to use the 'anti-torus' construction introduced in the previous section. This consists in interpreting

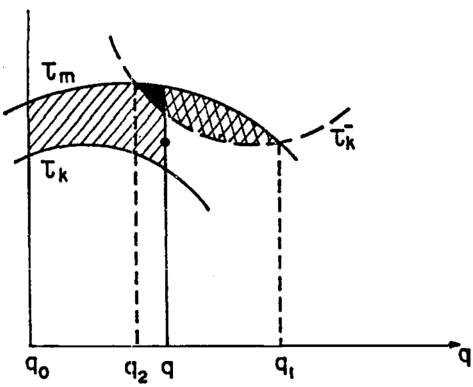

Fig.2 - The figure shows portions of two tori τ_k and τ_m, characterized by actions I_k and I_m and the antitorus τ_k^- obtained by reflecting τ_k through the evaluation point. The sum of rhe cross-hatched and the black areas is proportional to the phase of the integrand in eq. (3.5), whereas the sum of the simply hatched and the black areas is proportional to the phase outside the integral

$$S_{\vec{q}}(-\frac{\vec{Q}}{2}, \vec{I}_k) + \vec{p}.Q \qquad (3.7)$$

as the action from the point with coordinate $\vec{q}$ along the torus $\vec{I} = \vec{I}_{\vec{k}}^-$, obtained by reflecting the torus $\vec{I} = \vec{I}_{\vec{k}}$ through the point $(\vec{q},\vec{p})$, i.e. we take

$$\vec{I}_{\vec{k}}^-(\vec{q}\,',\vec{p}\,') = \vec{I}_{\vec{k}}(-\vec{q}\,'+2\vec{q}, -\vec{p}\,'+2\vec{p}) \qquad (3.8)$$

The phase of the integrand is thus the action between the torus $\tau_{\vec{m}}$, the antitorus $\tau_{\vec{k}}^-$ and the points with coordinate $\vec{q}$ and $\vec{q} + \vec{Q}/2$. as shown for one degree of freedom in Fig.2. In this case there are two stationary points, where the tori intersect, as with the Wigner function, but the stationary points q_1 and q_2 arise for different moduli of Q and the stationary phases also have in general different moduli. The difference between the stationary phases $\phi_{\vec{3}}$ of the Moyal matrix is invariant under metaplectic transformations as long as the initial points on the two tori, from which the actions are evaluated, are kept fixed. This is exemplified for a system with one degree of freedom in Fig. 3.

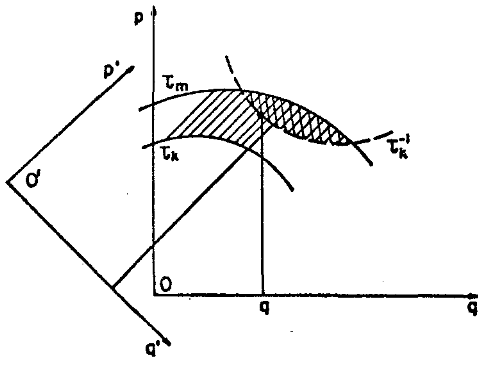

Fig.3 - The two terms of the Moyal matrix element $<k|m>(q,p)$ have phases' which differ by the cross hatched area in both the (p,q) and the (p',q') frames.

For points $(\vec{q},\vec{p})$ such that the antitorus $\tau_{\vec{k}}$ intersects the torus $\tau_{\vec{m}}$, the stationary phase evaluation of eq. (3.5) follows that of the Wigner function in ref.2 with the result

$$<\vec{k}|\vec{m}>(\vec{q},\vec{p}) = \frac{1}{(2\pi^3\hbar)^{1/2}} \sum_j \frac{\exp\{i[\phi_j(\vec{q},\vec{p}) - \hbar\ \pi/4]\}}{|\det\{\vec{I}_{\vec{m}},\vec{I}_{\vec{k}}\}|^{1/2}} \qquad (3.9)$$

where the matrix of Poisson Brackets

$$\{\vec{I}_{\vec{m}},\vec{I}_{\vec{k}}\} = \sum_{n=1}^{N} \left(\frac{\partial \vec{I}_m}{\partial q_n}\frac{\partial \vec{I}_{\vec{k}}}{\partial p_n} - \frac{\partial \vec{I}_m}{\partial p_n}\frac{\partial I_{\vec{k}}}{\partial q_n}\right) \qquad (3.10)$$

are evaluated at the stationary $(\vec{q}_j;\vec{p}'(\vec{q}_j,\vec{I}_{\vec{m}}))$. For one degree of freedom and $\vec{k} = \vec{m}$ eq.(3.9) reduces to the SC Wigner function (2.11).

As the *evaluation point* (q,p) is taken out of the inner torus (I_k in Fig.2), for a single degree of freedom, the stationary phases of the integrand in eq.(3.5) become smaller and, in the limit where the torus and antitorus meet non-transversely, the single Poisson bracket in eq. (3.10) goes to zero. It is easy to see that the locus of these 'catastrophes', where stationary points coalesce, is a closed curve interpolated between the two tori. If m = k this *Wigner caustic*, discussed in refs.1,2 coincides with the torus itself. There is another Wigner caustic corresponding to the locus of evaluation points for which the antitorus of τ_k touches τ_m from the inside instead of the outside, referred to as the L curve in ref.1, where it is shown that it contains cusps (Fig. 4). The situation for two degrees of freedom analysed in ref.2 is much more complicated, since the Wigner caustic is then a connected three-dimensional surface which envelops the two-dimensional torus where it becomes singular.

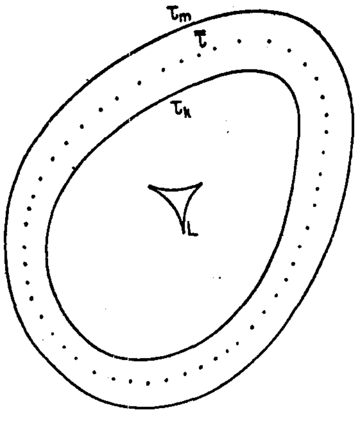

Fig.4 - For the case of one degree of freedom the Moyal matrix element $<k|m>(q,p)$ has two Wigner caustics: The reflection of the torus τ_k with respect to any point of the interpolated torus $\bar{\tau}$ (the dotted line) will be tangent to τ_m from the outside, whereas reflection of τ_k with respect to a point on L leads to tangency from the inside of τ_m.

The uniform approximation of the non-diagonal Moyal matrix elements, valid through the caustic, is more complicated than eq. (2.8), because of the lower symmetry in their geometrical constructions. For our purpose, which involves integration over phase space, it is sufficient to derive the classical delta-function type of approximation like eq. (2.6). To do this for the case of one degree of freedom we must expand the action functions $S(q',I_m)$ and $S(q',I_k)$ near the points $q \pm Q/2$, for which

$$\frac{\partial p}{\partial q'}\left(q + \frac{Q_0}{2}, I_m\right) = \frac{\partial p}{\partial q'}\left(q - \frac{Q_0}{2}, I_k\right) \qquad (3.11)$$

This condition, that a pair of points on the two tori have parallel tangents, locates their midpoint on the Wigner caustic as can be seen in Fig. 5. Setting $Q = Q_0$ in the amplitude of the integrand of eq. (3.5), expanding the exponent to first order in $Q-Q_0$ (or second order, using eq. (3.11) and using

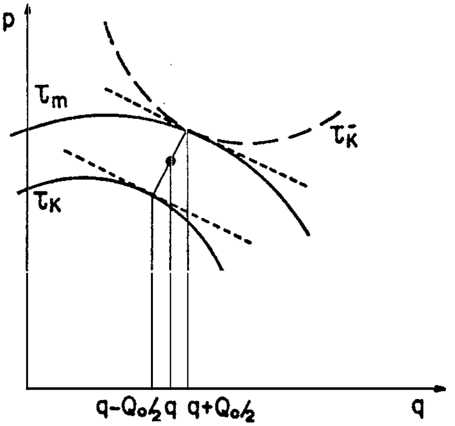

Fig.5 - The Wigner caustic is the locus of midpoints of segments of joining points on τ_k and τ_m with parallel tangents.

$$p(q',I) = \frac{\partial S}{\partial q'}(q',I) \tag{3.12}$$

the Moyal matrix becomes

$$<k|m>(p,q) = \frac{e^{\frac{i}{\hbar}[S_0(q,I_m)-S_0(q,I_k)]}}{(2\pi)^2\hbar}\left|\frac{\partial p}{\partial I_m}\left(q+\frac{Q_0}{2},I_m\right)\frac{\partial p}{\partial I_k}\left(q-\frac{Q_0}{2},I_k\right)\right|^{1/2}$$

$$\int dQ \exp\left\{\frac{i}{\hbar}(Q-Q_0)\left[\frac{p\left(q+\frac{Q_0}{2},I_m\right)+p\left(q-\frac{Q_0}{2},I_k\right)}{2}-p\right]\right\}$$

$$= \frac{1}{2\pi}e^{\frac{i}{\hbar}[S_0(q,I_m)-S_0(q,I_k)]}\left|\frac{\partial p}{\partial I_m}\left(q+\frac{Q_0}{2},I_m\right)\frac{\partial p}{\partial I_k}\left(q-\frac{Q_0}{2},I_k\right)\right|^{1/2}$$

$$\delta\left(p-\frac{p\left(q+\frac{Q_0}{2},I_m\right)+p\left(q-\frac{Q_0}{2},I_k\right)}{2}\right) \tag{3.13}$$

For the Wigner function ($m=k$, $Q_0=0$) this simplifies to eq.(2.6). In the limit $I_k \to I_m$ Q, becomes small, so to second order in (I_m-I_k) and in Q_0 we get

$$<k|m>(q,p) \xrightarrow[I_k\to I_m]{} \frac{1}{2\pi}e^{\frac{i}{\hbar}[S_0(q,I_m)-S_0(q,I_k)]}\,\delta\left(I-\frac{I_k+I_m}{2}\right) \tag{3.14}$$

for the off diagonal elements. Generally, however, the Wigner caustic on which the δ-function of eq. (3.13) is defined, depends exclusively on the geometry of the tori $I_{\vec{k}}$ and $I_{\vec{m}}$ and in no way on any intervening torus of the family.

The derivation of eq. (3.13) has been phrased in terms of the Wigner caustic which coincides with the torus when $I_{\vec{k}} \to I_{\vec{m}}$, but it is equally valid for the inner Wigner caustic shown in Fig. 4. The only difference is that in this case the oscillations in the "amplitude" of the δ-function are much faster and do not disappear in the Wigner function limit.

The picture is more complicated when another degree of freedom is added. The Wigner caustic is then defined by the condition

$$\det \frac{\partial^2}{\partial \vec{Q}^2} \left[S_q(\vec{Q}_0/2, I_{\vec{m}}) - S_q(-\vec{Q}_0/2, I_{\vec{k}})\right] = 0 \tag{3.15}$$

which defines a three-dimensional surface in phase space. Inother words, one of fhe eigenvalues of the above matrix is zero, indicating that the tangrnt planes to the tori at $\vec{p}(\vec{q}+\vec{Q}_0/2, I_{\vec{m}})$ and $\vec{p}(\vec{q}-\vec{Q}_0/2, I_{\vec{k}})$ have a direction in common. The condition that the other eigenvalue is also zero - the case of strong tangency, occurs on a two dimensional surface. In the case of the Wigner function, thoroughly analysed in ref.2, this is the torus itself which is an umbilic (hyperbolic or elliptic) singularity of the Wigner caustic. For $I_{\vec{k}}$ close to $I_{\vec{m}}$ this must also have the global topology of a torus:

$$\frac{\partial \vec{p}}{\partial \vec{q}\,'}\left(\vec{q} + \frac{\vec{Q}_0}{2}, I_{\vec{m}}\right) = \frac{\partial \vec{p}}{\partial \vec{q}\,'}\left(\vec{q} - \frac{\vec{Q}_0}{2}, I_{\vec{k}}\right) \tag{3.16}$$

defines an umbilic interpolating torus.

There is no second order term in the expansion of the phase of the integrand of the Moyal matrix in eq.(3.5) around the points defined by eq.(3.16), so that, in the limit $\hbar \to 0$, repeating the argument that led to eq.(3.14), we obtain

$$<\vec{k}|\vec{m}>(\vec{q},\vec{p}) =$$

$$= \left(\frac{1}{2\pi}\right)^N \exp\left\{\frac{i}{\hbar}\left[S_0(\vec{q}, I_{\vec{m}}) - S_0(\vec{q}, I_{\vec{k}})\right]\right\} \left|\det\frac{\partial \vec{p}}{\partial I_{\vec{m}}}(\vec{q}+\vec{Q}_0/2, I_{\vec{m}}) \det\frac{\partial \vec{p}}{\partial I_{\vec{k}}}(\vec{q}-\vec{Q}_0/2, I_{\vec{k}})\right|^{1/2}$$

$$\delta\left(\vec{p} - \vec{p}\;\frac{(\vec{q}+\vec{Q}_0/2, I_{\vec{m}}) + \vec{p}(\vec{q}-\vec{Q}_0/2, I_{\vec{k}})}{2}\right) \tag{3.17}$$

For simple tori, uniform and transitional approximations for the Moyal Matrix can be derived which generalize the results for the Wigner function[3]. As in the one dimensional case, these are basically fringes, peaked on the Wigner caustic and especially cn the interpolating torus eq.(3.16) and decaying outside the caustic. Projection integrals of the Wigner function, supplying the wave intensity, are correctly given by the 6-function approximation of the Wigner function, as shown in ref.3. This is because the integral averages ove the oscillations (where they are not stationary), inspite of the considerable amplitude inside and especially on the Wigner caustic but outside the interpolating torus. The integral (1.2) for matrix elements of observables, is of twice the dimension of a projection integral and there are no stationary points. The δ-function approximation over all the points which satisfy eq. (3.16) should therefore give correct semiclassical matrix elements. Not only is the 6-function approximation (3.17) much simpler to work with than morei refined approximations, but the derivation of the former can be easily generalized to any number of degrees of freedom, whereas the latter depend on a thorough understanding of the geometry of Lagrõngean manifolds[9] of more than two dimensions.

I have not made a clear distinction between the interpolating torus, which reduces to the quantized torus in the case of the Wigner function, and other curves or surfaces which satisfy eq. (3.16), 'such as the L curve in Fig. 4. The reason is that for neighbouring tori the exponential term in eq.(3.16) oscillates slowly on the interpolating torus and very quickly elsewhere. The phase is nowhere stationary, so that the observable matrix elements will be semiclassically negligible unless all components of $\vec{I}_m - \vec{I}_r$ are of order H for the interpolating torus. The contribution of other surfaces is always negligible.

4. ACTION-ANGLE REPRESENTATION

Is is well known that action-angla variables cannot be quantized directly[10]. However the simplicity of the classical motion in these variables is reflected in the semiclassical wave functions, so that an approximate quantization is extremely useful. The operator $\hat{\vec{I}}$ have the discrete set of semiclasslcal eigenvalues given by the Bohr-

-Sommerfeld quantization rule (2.5) for each component. The stipulation thiit the corresponding eigenfunctions

$$<\vec{\theta}|\vec{m}> = (2\pi)^{-N/2} e^{i\vec{m}.\vec{\theta}} \tag{4.1}$$

are periodic in each conponent of $\vec{\theta}$ implies that in the angle representation

$$\vec{I} = -i\hbar\,\partial/\partial\vec{\theta} + \vec{\alpha}\hbar/4 \tag{4.2}$$

where $\vec{\alpha}$ are the Maslov indices. It is sometimes preferable to use a simpler definition of $\hat{\vec{I}}$ where the $\vec{a}$ are ommitted, at the cost of using Bloch (Foucault) wave functions[11]. The two alternative representation? are related by a gauge transformatiori. Thus the fundamental operators $\vec{I}$, $\hat{\vec{\theta}}$ satisfy the required romnutation relation

$$[\hat{I}_j,\hat{\theta}_j] = -i\hbar\,\delta_{ij} \tag{4.3}$$

The difficulty in working with action-angle variables is that arbitrary periodic functions of $\vec{\theta}$ can be Fourier analysed into superpositions of eigenfunctions of $\hat{\vec{I}}$ with positive and negative components of $\vec{m}$. The freedom of choice of representation prevents us from excluding these unphysical tori, though in the semiclassical limit the expansion coefficients of the terms with negative components of $\vec{m}$, must tend to zero.

The Weyl transform of an operator is defined by

$$A(\vec{I}_{\vec{M}},\vec{\theta}) = \int_{-\pi}^{\pi} d\vec{\Theta}\; e^{-i\vec{M}\vec{\Theta}} <\vec{\theta} + \frac{\vec{\Theta}}{2}|\hat{A}|\theta - \frac{\vec{\Theta}}{2}> \tag{4.4}$$

It is essential that the Weyl representation contain as much information about the operator $\hat{A}$ as the angle representation. This would certainly be the case of the Fourier coefficients of $<\vec{\theta} + \vec{\Theta}|\hat{A}|\vec{\theta}-\vec{\Theta}>$ taken as a periodic function of O. But in the case of N = 1 we can write the m'th Fourier coefficient as

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} d\Theta\; e^{-im\Theta} <\theta+\Theta|\hat{A}|\theta-\Theta> = \frac{1}{2\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\Theta\; e^{-im\Theta} <\theta+\Theta|\hat{A}|\theta-\Theta>$$

$$+\frac{1}{2\pi}\int_{\frac{\pi}{2}}^{\pi} d\Theta\, e^{-im\Theta} \langle\theta+\Theta|\hat{A}|\theta-\Theta\rangle + \frac{1}{2\pi}\int_{-\pi}^{-\pi/2} d\Theta\, e^{-im\Theta} \langle\theta+\Theta|\hat{A}|\theta-\Theta\rangle$$

$$= \frac{1}{4\pi}\int_{-\pi}^{\pi} d\Theta\, e^{-im\Theta/2} \langle\theta+\frac{\Theta}{2}|\hat{A}|\theta-\frac{\Theta}{2}\rangle + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\Theta\, e^{-im(\frac{\Theta}{2}+\pi)} \langle\theta+\pi-\frac{\Theta}{2}|\hat{A}|\theta+\pi-\frac{\Theta}{2}\rangle$$

$$= \frac{1}{4\pi}\left[A(I_{m/2},\theta) + (-1)^m A(I_{m/2},\theta+\pi)\right] \tag{4.5}$$

It follows that the Weyl representation is complete if we allow discrete actions corresponding to half integers $M = m/2$. The curious partnership of the Weyl transform at (I_M,θ) and $(I_M,\theta+\pi)$ had already appeared in the treatment of the pure state condition for the Wigner function[4], though no reference was made in that instance to half integer quantization. It is interesting that in the quantization of linear maps on the torus, Hannay and Berry[12] do use half integer actions without any explanation. For N degrees of freedom the Fourier coefficients take the form

$$\left(\frac{1}{2\pi}\right)^N \int_{-\pi}^{\pi} d\vec{\Theta}\, e^{-i\vec{m}.\vec{\Theta}} \langle\vec{\theta}+\vec{\Theta}|\hat{A}|\vec{\theta}+\vec{\Theta}\rangle = \left(\frac{1}{4\pi}\right)^N \sum_{\gamma} (-1)^{\vec{\varepsilon}_\gamma.\vec{m}} A(I_{\vec{m}/2},\vec{\theta}+\vec{\varepsilon}_\gamma\pi) \tag{4.6}$$

where the vectors $\vec{\varepsilon}$ have N components equal to either zero or one and γ labels each of the 2^N possibilities.

The Moyal matrix elements are particularly simple in the action-angle representation

$$\langle\vec{m}|\vec{k}\rangle(I_{\vec{L}},\vec{\theta}) = \left(\frac{1}{2\pi\hbar}\right)^N \int_{-\pi}^{\pi} d\vec{\Theta}\, e^{-i\vec{L}.\vec{\theta}} \langle\vec{\theta}+\vec{\Theta}|m\rangle\langle k|\vec{\theta}+\vec{\Theta}\rangle$$

$$= \frac{e^{i(\vec{m}-\vec{k}).\vec{\theta}}}{(2\pi\hbar)^N}\, \delta_{(\vec{m}+\vec{k})/2,\vec{L}} \tag{4.7}$$

The need for half integer action labels L is once again manifest. It is important to compare this result with the Moyal Matrix in $(\vec{q},\vec{p})$ space. There we found that for purposes of integration the matrix elements could be *approximated* by a Dirac δ-function on an interpolated torus constructed from the two tori with actions $\vec{I}_{\vec{m}}$ and $\vec{I}_{\vec{k}}$. Here each element is exactly a Kronecker δ-function on the member of the N-parameter family of tori with actions

$$\vec{I} = \hbar \left(\frac{\vec{m}+\vec{k}}{2} + \frac{\vec{\alpha}}{4}\right) \quad (4.8)$$

The tnterpolated torus and the one given by eq. (4.8) only coincide in the case of the Wigner function, for which $\vec{m} = \vec{k}$.

The Wigner function for a state corresponding to a member of another family of tori with action function defined by

$$S(\vec{\theta}) = \int_0^{\vec{\theta}} d\vec{\theta}.I(\vec{\theta},I) \quad (4.9)$$

is obtained from the Weyl transform of $|\psi\rangle\langle\psi|/\hbar$ where

$$\langle\vec{\theta}|\psi\rangle = \left(\frac{1}{2\pi}\right)^{N/2} \left|\frac{\partial^2 S}{\partial\vec{\theta}\partial\vec{I}}\right|^{1/2} e^{iS_I(\vec{\theta})/\hbar} \quad (4.10)$$

If the tori with actions variables $\vec{I}(\vec{q},\vec{p})$ = constant are close to. the tori $\vec{I}(\vec{q},\vec{p})$ = constant the $\vec{I}(\vec{\theta},\vec{I})$ surfaces will be open surfaces periodic in $\vec{\theta}$, as shown in Fig. 6, for one degree of freedom. The result is again given by the antitorus or Berry chord construction, whith the restriction of evaluation points to those with action variables given by eq.(4.8). Such general Wigner functions will therefore be decorated by fringes rising approximately to a Dirac δ-function on the torus, as already noted by Berry[1] and decaying exponentially beyond agiven $I > I_{max}$ and $I < (I_{min} > 0)$.

The wave intensity is given by eq. (4.6) as the sum

$$|\langle\vec{\theta}|\vec{I}\rangle|^2 = 2^{-N} \sum_{\vec{M}} \sum (-1)^{2\vec{\varepsilon}_\gamma.\vec{M}} \langle\vec{I}|\vec{I}\rangle(\vec{I}_{\vec{M}}\vec{\theta}+\vec{\varepsilon}_\gamma\pi) \quad (4.11)$$

I could also present the Moyal Matrix elements corresponding to such other families of tori, but as can be seen from the Wigner function, the advantage of working in the action-angle representation is only felt when dealing with variables specific to the particular family of tori.

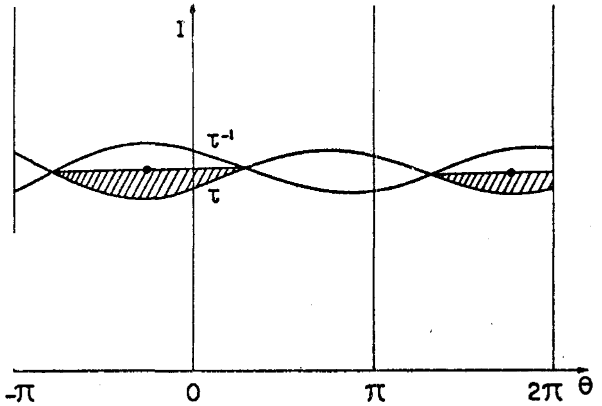

Fig.6 - The only difference between the Berry chord construction in action-angle variables, with respect to the original phase, is that the tori may be open periodic curves.

Assuming the semiclassical equivalence of the Weyl transform of an observable $A(\vec{I}_{\vec{M}},\vec{\theta})$ with the corresponding classical function $A_c(\vec{I}_{\vec{M}},\vec{\theta})$, following the arguments of section 2, we are now in a position to derive a simple expression for the matrix elements. As in the case of eq. (1.2) we can write

$$<\vec{k}|\hat{A}|\vec{m}> = \int_{-\pi}^{\pi} d\vec{\theta}_1 d\vec{\theta}_2 <\vec{k}|\vec{\theta}_1><\vec{\theta}_1|\hat{A}|\vec{\theta}_2><\vec{\theta}_2|\vec{m}>$$

$$= \int_{-\pi}^{\pi} d\vec{\theta}\, d\vec{\Theta} <\vec{k}|\vec{\theta}+\vec{\Theta}/2> <\vec{\theta}+\frac{\vec{\Theta}}{2}|\hat{A}|\vec{\theta}-\frac{\vec{\Theta}}{2}> <\vec{\theta}-\frac{\vec{\Theta}}{2}|\vec{m}> \quad (4.12)$$

where the integration is over one unit cell in the periodic $(\vec{\theta}_1,\vec{\theta}_2)$ space as show in Fig. 7 for one degree of freedom. So, from the Fourier series with coefficients given by eq. (4.6),

$$<\vec{\theta}+\vec{\Theta}/2|\hat{A}|\vec{\theta}-\vec{\Theta}/2> = \left(\frac{1}{4\pi}\right)^N \sum_{\vec{m}} e^{i2\vec{L}.\vec{\Theta}} \sum_{\gamma} (-1)^{2\vec{\varepsilon}_\gamma.\vec{L}} \vec{A}(\vec{I}_{\vec{L}},\ \vec{\theta}+\vec{\varepsilon}_\gamma\pi\ ) \quad (4.13)$$

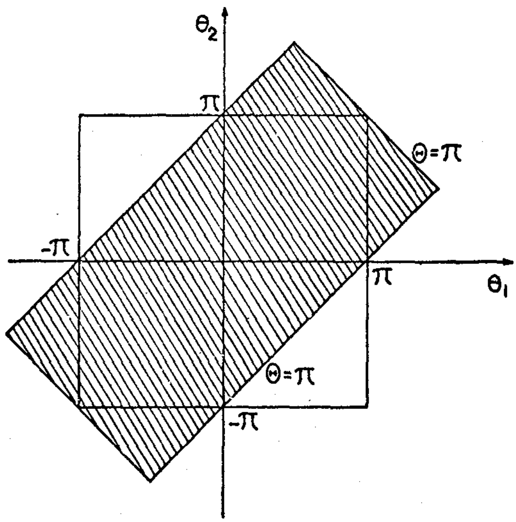

Fig.7 - In the change of variable in eq. (4.12) the domain of integration becomes the shaded rectangle unit cell instead of the square.

we obtain

$$\langle\vec k|\hat A|\vec m\rangle =$$

$$=\left(\frac{1}{4\pi}\right)^N \sum_{\vec L}\sum_{\gamma}(-1)^{2\vec\varepsilon_\gamma\cdot\vec L}\int_{-\pi}^{\pi} d\vec\theta\; A(\vec I_{\vec L},\vec\theta+\vec\varepsilon_\gamma\pi)\int_{-\pi}^{\pi} d\Theta\; e^{i2\vec L\cdot\vec\theta}\,\langle\vec\theta-\frac{\vec\Theta}{2}|\vec m\rangle\langle\vec k|\vec\theta+\frac{\vec\Theta}{2}\rangle$$

$$=\left(\frac{\hbar}{4}\right)^N \sum_{\vec L}\sum_{\gamma}(-1)^{2\vec\varepsilon_\gamma\cdot\vec L}\sum_{\gamma'}(-1)^{2\vec\varepsilon_{\gamma'}\cdot\vec L}\int_{-\pi}^{\pi} d\vec\theta\; A(\vec I_{\vec L},\vec\theta+\vec\varepsilon_\gamma\pi)\;\langle\vec k|\vec m\rangle(\vec I_{\vec L},\vec\theta+\vec\varepsilon_\gamma\pi) \tag{4.14}$$

The greater intricacy of this formula compared with eq.(1.2) now disappears when we use the explicit action-angle Moyal Matrix elements (4.7)

$$\langle\vec{k}|\hat{A}|\vec{m}\rangle = \left(\frac{1}{8\pi}\right)^N \sum_{\gamma\gamma'} (-1)^{(\vec{\varepsilon}_\gamma+\vec{\varepsilon}_{\gamma'})\cdot(\vec{k}+\vec{m})} \int_{-\pi}^{\pi} d\vec{\theta}\, A(I_{\frac{\vec{m}+\vec{k}}{2}}, \vec{\theta}+\vec{\varepsilon}_\gamma \pi)\, e^{i(\vec{m}-\vec{k})\cdot(\vec{\theta}+\vec{\varepsilon}_{\gamma'})\pi}$$

$$= \left(\frac{1}{2\pi}\right)^N \int d\vec{\theta}\; A(\vec{I}_{\frac{\vec{m}+\vec{k}}{2}}, \vec{\theta})\; e^{i(\vec{m}-\vec{k})\cdot\vec{\theta}} \left(\sum_{\gamma\gamma'} (-1)^{(\vec{\varepsilon}+\vec{\varepsilon}_{\gamma'})\cdot 2\vec{m}} / 4^N\right)$$

$$= \left(\frac{1}{2\pi}\right)^N \int d\vec{\theta}\; A(\vec{I}_{\frac{\vec{m}+\vec{k}}{2}}, \vec{\theta})\; e^{i(\vec{m}-\vec{k})\cdot\vec{\theta}} \qquad (4.15)$$

This formula has been presented before by Percival and Richards[13] as a generalization of their work on the Heisenberg correspondence principle for systems with one-degree of freedom. The present derivation relies exclusively on the semiclassical validity of working directly with ãction angle variables in quantum mechanics.

5. CONCLUSION

I have deduced two different expressions for the SC matrix elements of an observable with respect to the eigenstate of a classically integrable Hamiltonian. Working in the original $(\vec{q},\vec{p})$ phase space the approximate matrix elements $\langle\vec{k}|\hat{A}|\vec{m}\rangle$ are given by eq. (3.17) together with eq. (1.2), which reduces to an integral of $A(\vec{q},\vec{p})$ over the torus interpolated between that with actions $\vec{I}_{\vec{m}}$ and the one with actions $\vec{I}_{\vec{k}}$. The other, a simple Fourier integral (4.15), is obtained by working directly in action-angle variabler - it is exact within the assumption of SC validity of this representation.

It is easy to see that as $\vec{I}_{\vec{k}} \to \vec{I}_{\vec{m}}$ the two approximations coincide. Moreover, if $\vec{k}-\vec{m}$ has any large component the Fourier integral will be negligible, as $A(\vec{I}_{\vec{m}+\vec{k}/2},\vec{\theta})$ is arsumed to be a smooth function of $\vec{\theta}$. Since semiclassicaly the quantization condition (2.5) guarantees that the absolute value of each component

$$\left|\vec{I}_{\vec{k}} - \vec{I}_{\vec{m}}\right|_j \ll \left|\vec{m}-\vec{k}\right|_j \qquad (5.1)$$

the dominant matrix elements are not affected by the choice of approximation. The best way to calculate any property which depends on the matrix as a whole, such as the eigenvalues, is thus to use eq. (4.15).

The above statement is valid in the strict limit $\hbar \to 0$. When dealing with a loosely definable 'small semiclassical pãrameter' other factors may have to be taken into account. The most obvious is the geometry of the basis tori. In the simplest case where these are the invariant surfaces of a classical harmonic oscillator of N degrees of freedom, the interpolated torus always coincides with one of the basis tori.

The differences $\vec{m}-\vec{k}$ are therefore not the only relevant parameters, but also the less readily quantifiable nonlinearity or convolutedness of the tori. For one degree of freedom the less variable the curvature of the basis of closed curves, the closer will the closed curve of average action approximate the interpolated closed curve over which the integral should be carried out. Arbitrary canonical transformations, such as those producing 'whorls and tendrills' in closed curves[14,15] will severely distort the interpolated torus, as shown in Fig. 8, so that the direct action-angle theory will no longer be valid.

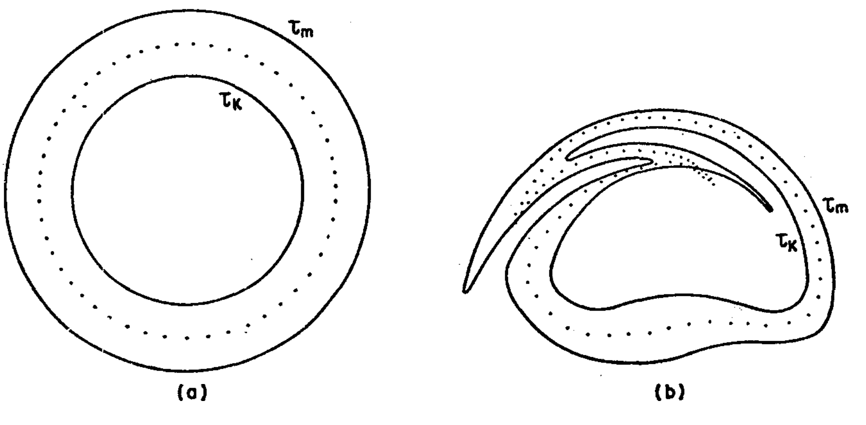

Fig.8 - A very non-linear canonical transformatlon mey misplace considerably the interpolated torus from the torus with the average action. a) For the harmonic oscillator they have the same shape. b) For a family of "convoluted' nested curves the interpolated torus may even intersect one of the basis tori.

Even in the absence of gross distortions, we must be much more careful about features which depend on a single matrix element, such as transition rates[13]. A transition rate between two states may be individually measurable, even if it is negligible with respect to that between other states. In such instances it is the relative difference between the results in sections 3 and 4 which may require the use of the former more complicated formulae. In extreme cases when SC theory is extended to areas of doubful validity, it may become necessary to include in eq. (3.17) all the surfaces defined by eq. (3.16). Beyond that all δ-function approximations break down and full uniform approximations to the Moyal Matrix must be used in the fundamental formula (1.2).

The transformation to action-angle variables has long been known to simplify SC approximations to quantum mechanics, in analogy to its effect in classical mechanics. In the present case the parallel development of an untransformed theory has vitiated this practice, as a rule, while supclying the necessary conditions of validity.

I thank Dr. T.B. Smith for originally drawing my attbntion to the problems discussed in this work.

REFERENCES

1. M.V.Berry, Phil. Trans. Roy. Soc. 287, 237 (1977).
2. A.M. Ozorio de Almeida and J.H.Hannay, Ann.Phys.N.Y. 138, 115(1982).
3. A.M. Ozorio de Almeida, Ann.Phys.N.Y. 745, 100 (1983).
4. A.M. Ozorio de Almeida, Physica *110*A, 501 (1983).
5. J.R. Shewell, Am. J. Phys. 27, 16 (1959).
6. J.E. Moyal, Proc. Camb Phil. Soc. Math. Phys. Sci. 45, 99 (1949).
7. M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions*, U.S. National Bureau of Standards - Washington (1364).
8. M.J. Lighthill, *Introduction to Fourier Analysis and Generalized Functions*, 67 (CUP - London).
9. V.I. Arnold, *Methodes Mathematiques de la Mécanique Classique*, Mir--Moscow (1976).
10. B. Leaf, J.Math. Phys. 9, 65, 769 (1968).
11. A.M. Ozorio de Almeida, J.Chem.Phys. (1984). (In the press).
12. J.H. Hannay and M.V. Berry, Physica D*1*, 267 (1980).

13. I.C. Percival and D. Richards, J.Phys. B3, 1035 (1970).
14. M.V. Berry and N.L. Balazs, J.Phys.A *12*, 625 (1979).
15. M.V. Berry, N.L. Balazs, M. Tabor and A. Voros, Ann. Phys. N.Y. *122*, 26 (1979).

Resumo

Os elementos de matriz de um operador observável, com respeito a uma base de autoestados de uma Hamiltoniana classicamente integrável, são deduzidos na aproximação semiclássica, usando a representação de Wigner-Weyl no espaço de fases comum e em variáveis de ângulo e ação. Os resultados diferem pouco para propriedades que dependem da matriz como um todo, tal como os autovalores, embora sejam mais simples de calcular com as variáveis de ângulo e ação. A diferença relativa para elementos de matriz isolados pode ser importante. A teoria recai em aproximações semiclássicas da matriz de Moyal ou função de Wigner cruzada, que generaliza trabalho anterior sobre a função de Wigner para estados puros, assim como a sua interpretação em termos da geometria dos toros invariantes de sistemas integráveis. Discute-se também a equivalência semiclássica entre a transformada de Weyl de um operador e a função clássica correspondente.