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Semi-classical approximation and microcanonical ensemble

by

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ABSTRACT. — For quantum mechanical systems with spherically symmetric potential the improved W.K.B. approximation of Elworthy and Truman corresponds to the classical microcanonical ensemble in the limit where \hbar goes to zero, at least for small time.

RÉSUMÉ. — Pour des systèmes quantiques à potential radial, l'approximation WKB améliorée d'Elworthy et Truman correspond à l'ensemble microcanonique classique dans la limite où \hbar tend vers zéro, au moins pour des temps petits.

§ 1. MOTIVATIONS

Since the very beginnings of quantum theory a lot of interest has been paid to the relationship between classical and quantum mechanics. Many

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results have been proved in this direction more or less rigorously and are part of the folklore. More specifically recently there has been a revival of interest in the semiclassical approximations in quantum mechanics (see e. g. [9] [10] and [4] for a review of the problem and for the references therein). Especially an « improved » W.K.B. approximation has been obtained in [1] [2]. It is an approximate solution of the Schrödinger equation which is localized in some region of space.

Our purpose in this note is to emphasize the classical meaning of this approximation, by showing its relation with the microcanonical ensemble of classical mechanics. More precisely, we prove that in the limit of \hbar going to zero expectation values defined by this state approach, for a suitable set of observables on phase space, the microcanonical expectation value of the corresponding classical observables. This result is explicitly proven for one dimensional systems but it holds as well for all integrable systems in the classical sense (see Appendix B).

This result has to be compared with the known fact (see e. g. (C.4)) that expectation values corresponding to eigenstates of the Harmonic oscillator behave in a similar way.

The paper is organized as follows: In Section 2 we rederive in our case the Elworthy-Truman expression for the approximate solution of the Schrödinger equation and prove some estimates on the way it approaches the solution of the Schrödinger equation. In Section 3 we derive the main result of the paper, viz. for any observable whose support is limited in a given region of space there exists an « improved WKB approximation » for sufficiently high energies such that if one computes the expectation value within this state, it approaches the microcanonical expectation value. Finally, we indicate in Appendices A and B the way to generalize these results to the case of respectively spherically symmetric potentials and completely integrable systems. In Appendix C we derive a result on the eigenstates of harmonic oscillator.

§ 2. APPROXIMATE SOLUTION OF THE SCHRÖDINGER EQUATION

Let us consider a quantum mechanical system of mass m with n degrees of freedom. Let $x \in \mathbb{R}^n \rightarrow V(x)$ be the potential, then the wave function $\psi(x, t)$, $x \in \mathbb{R}^n$, $t \in \mathbb{R}$ satisfies the Schrödinger equation:

$$i\hbar \frac{\partial \psi}{\partial t}(x, t) = -\frac{\hbar^2}{2m} \sum_{i=1}^n \frac{\partial^2 \psi}{\partial x_i^2}(x, t) + V(x)\psi(x, t) \quad (2.1)$$

and some boundary condition

$$\lim_{t \downarrow 0} \psi(x, t) = \psi_0(x) \quad \psi \in L_2(\mathbb{R}^n, dx). \quad (2.2)$$

In the previous formula \hbar is the Planck constant divided by 2π .

As is well known, if we make the ansatz:

$$\psi(x, t) = R(x, t)^{1/2} \exp \left\{ \frac{i}{\hbar} S(x, t) \right\} \quad (2.3)$$

then the functions R and S obey a system of coupled partial differential equations:

$$\frac{\partial R}{\partial t}(x, t) = -\frac{1}{m} \sum_{i=1}^n \frac{\partial}{\partial x_i} \left(R(x, t) \frac{\partial}{\partial x_i} S(x, t) \right) \quad (2.4)$$

$$\begin{aligned} \frac{\partial S}{\partial t}(x, t) = & -\frac{1}{2m} \sum_{i=1}^n \left(\frac{\partial}{\partial x_i} S(x, t) \right)^2 - V(x) \\ & + \frac{\hbar^2}{2m} R(x, t)^{-1/2} \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2} R^{1/2}(x, t). \end{aligned} \quad (2.5)$$

These equations are close to the well-known equations of classical mechanics (see e. g. [3]), and one has the obvious remark that if R^c and S^c are solutions of the set of equations

$$\frac{\partial R^c}{\partial t}(x, t) = -\frac{1}{m} \sum_{i=1}^n \frac{\partial}{\partial x_i} \left(R^c(x, t) \frac{\partial S^c}{\partial x_i}(x, t) \right) \quad (2.6)$$

$$\frac{\partial S^c}{\partial t}(x, t) = -\frac{1}{2m} \sum_{i=1}^n \left(\frac{\partial S^c}{\partial x_i}(x, t) \right)^2 - V(x) \quad (2.7)$$

with appropriate boundary conditions, then ψ^c defined as

$$\psi^c(x, t) = R^c(x, t)^{1/2} \exp \left\{ \frac{i}{\hbar} S^c(x, t) \right\} \quad (2.8)$$

satisfies an approximate Schrödinger equation in the sense that:

$$\begin{aligned} i\hbar \frac{\partial \psi^c}{\partial t}(x, t) + \frac{\hbar^2}{2m} \sum_{i=1}^n \frac{\partial^2 \psi^c}{\partial x_i^2}(x, t) - V(x) \psi^c(x, t) \\ = -\frac{\hbar^2}{2m} \exp \left\{ + \frac{i}{\hbar} S^c(x, t) \right\} \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2} (R^c(x, t))^{1/2}, \end{aligned} \quad (2.9)$$

namely up to order \hbar^2 . This is the starting point of a well-known approximation scheme, see e. g. [4] and references therein.

Given a solution of equations (2.6) and (2.7) then (2.8) defines a good approximation of the solution of the Schrödinger equation. More precisely:

PROPOSITION (2.1). — Let $x \in \mathbb{R}^n \rightarrow V(x)$ be a potential such that the operator H

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2} + V \quad (2.10)$$

is self-adjoint. Let R^c and S^c be solutions of the system of equations (2.6)

and (2.7). Furthermore, assume that $x \rightarrow \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2} R^c(x, t)^{1/2}$ is $L_2(\mathbb{R}^n, dx)$

for each $t \in [0, T]$ then one has the estimate

$$\|\psi^c(\cdot, t) - \psi(\cdot, t)\| \leq \frac{\hbar}{2m} \int_0^t \|\Delta R^{c1/2}(\cdot, \tau)\| d\tau \quad (2.11)$$

where $\|\varphi(\cdot)\|$ denotes the L_2 norm of $x \in \mathbb{R}^n \rightarrow \varphi(x)$ and

$$(x, t) \in \mathbb{R}^n \times \mathbb{R} \rightarrow \psi(x, t)$$

denotes the exact solution of the Schrödinger equation (2.1) with boundary condition

$$\lim_{t \downarrow 0} \psi(x, t) = \psi^c(x, 0). \quad (2.12)$$

Proof. — Let φ be a unit vector in $L_2(\mathbb{R}^n, dx)$ and define

$$\varphi(\cdot, t) = \exp \left\{ -\frac{i}{\hbar} Ht \right\} \varphi(\cdot),$$

namely as the solution of the Schrödinger equation with φ as initial condition. Unitarity of $\exp \left\{ -\frac{i}{\hbar} Ht \right\}$ as well as the fact that both ψ and ψ^c have the same boundary conditions implies that

$$(\varphi(\cdot, t) | \psi^c(\cdot, t) - \psi(\cdot, t)) = \int_0^t d\tau \frac{d}{d\tau} (\varphi(\cdot, \tau) | \psi^c(\cdot, \tau)) \quad (2.13)$$

where $(|)$ denotes the scalar product in $L_2(\mathbb{R}^n, dx)$.

However, ψ^c satisfies an approximate Schrödinger equation (2.9) and H is self-adjoint, hence

$$\frac{d}{d\tau} (\varphi(\cdot, \tau) | \psi^c(\cdot, \tau)) = -\frac{i\hbar}{2m} \left(\varphi(\cdot, \tau) \left| \exp \left\{ \frac{i}{\hbar} S^c(\cdot, \tau) \right\} \Delta \{ R^{c1/2}(\cdot, \tau) \} \right. \right). \quad (2.14)$$

Taking the supremum on φ of both sides of (2.13) the inequality (2.11) follows.

Previous method can be used to give approximate eigenstates of the Hamiltonian H . Indeed, assume that there is a solution R^c and S^c of equations (2.6) and (2.7) of the form

$$S^c(x, t) = S_0(x) - Et \quad (2.15)$$

for some E and at least in the interval $[0, T]$, $T > 0$. Then one has the following estimate:

$$\| (H - E)\psi^c(\cdot, 0) \| \leq \hbar \| R^{c1/2}(\cdot, 0)' \| + \frac{\hbar^2}{2m} \| \Delta R^{c1/2}(\cdot, 0) \| \quad (2.16)$$

where $R^{c1/2}(\cdot, 0)'$ denotes the time derivative at $t = 0$.

Proof. — Let us denote $\psi^c(\cdot, 0)$ by ψ_0 then

$$\| \psi(\cdot, t) - \psi^c(\cdot, t) \| = \left\| \exp \left\{ \frac{-i}{\hbar} (H - E)t \right\} \psi_0 - \frac{R^{c1/2}(\cdot, t)}{R^{c1/2}(\cdot, 0)} \psi_0 \right\|. \quad (2.17)$$

It follows that:

$$\| \psi(\cdot, t) - \psi^c(\cdot, t) \| \geq \left\| \left(\exp \left\{ \frac{-i}{\hbar} (H - E)t \right\} - 1 \right) \psi_0 \right\| - \| R^{c1/2}(\cdot, t) - R^{c1/2}(\cdot, 0) \| \quad (2.18)$$

Combining this result with the one in Proposition (2.1) the estimate (2.16) follows.

In this sense ψ^c is an approximate eigenstate of the Hamiltonian H . This is the intuitive reason for which the corresponding state of quantum mechanics approaches the microcanonical ensemble as we shall see later (see also Appendix C, true eigenfunctions behave in the same way). However, before proving this result we shall show that the previous scheme can be explicitly implemented at least in some cases. In what follows we restrict ourselves to one dimensional systems (or, more generally, to collections of uncoupled one-dimensional systems). Furthermore, we assume that the potential V is:

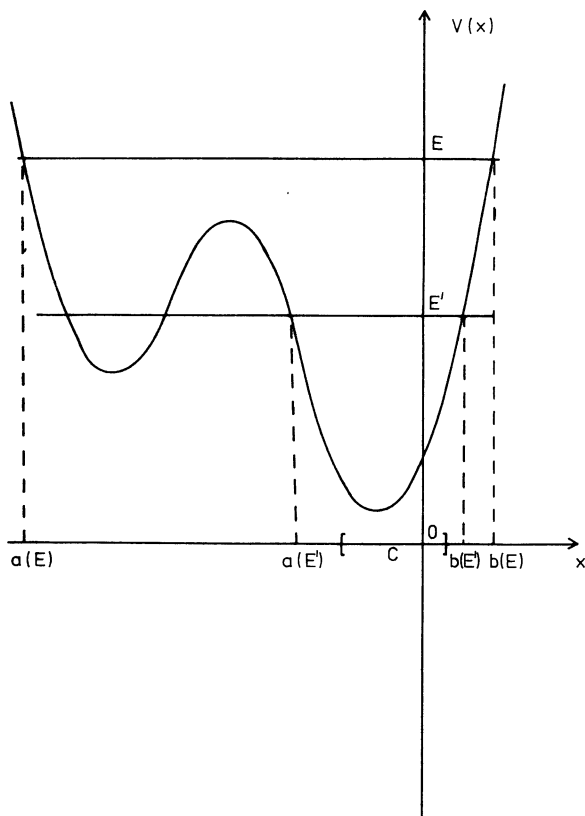
- i)* Continuous and lower bounded (say positive)
- ij)* Increasing at infinity.

For each $E > 0$ we choose an interval $\Delta_E = [a(E), b(E)]$ such that

- j)* $V(a(E)) = V(b(E)) = E$
- ij)* $x \in [a(E), b(E)]$ implies that $V(x) \leq E$.

In what follows we shall choose E sufficiently large in order that *j* and *ij* define Δ_E in a unique way (see figure).

Under our assumption, for sufficiently large E , $[a(E), b(E)]$ is completely



defined by the second condition. Then the Jacobi equation has an obvious solution, viz.

$$S^c(x, t) = S_0(x) - Et = \int_{a(E)}^x dy(2m(E - V(y)))^{1/2} - Et, \quad x \in \Delta_E. \quad (2.19)$$

Now, let us consider the classical problem, viz. let

$$\phi_s(x_0) = x(x_0, (2m(E - V(x_0)))^{1/2}, s) \quad (2.20)$$

be the solution at time s of Newton's equations with initial position x_0 and momentum $(2m(E - V(x_0)))^{1/2}$. ϕ_s is a well defined one to one differentiable map of any interval $C \subset \Delta_E$ for time $s \in [0, T]$, with $T > 0$ depending on C . It allows to define a solution of the continuity equation at least for small t ; more precisely

LEMMA 2.2. — For any $\Theta \in C_0^\infty(C)$ and for those t such that $\phi_s(\text{supp. } \Theta) \subset \Delta_E, s \in [0, t]$. Then

$$\tilde{J}(x, t) = (E - V(x))^{-1/2} \Theta \circ \phi_t^{-1}(x) \quad (2.21)$$

satisfies the continuity equation

$$\frac{\partial \tilde{J}}{\partial t}(x, t) + \frac{1}{m} \frac{\partial}{\partial x} \left(\tilde{J}(x, t) \frac{\partial S^c}{\partial x}(x, t) \right) = 0. \quad (2.22)$$

Proof. — Observe that $(E - V(x))^{-1/2}$ is a solution of the continuity equation (2.22) for x inside Δ_E . Moreover, $\theta(x, t) = \Theta(\phi_t^{-1}(x))$ satisfies

$$\frac{\partial \theta}{\partial t}(x, t) + \frac{1}{m} \frac{\partial \theta}{\partial x}(x, t) \frac{\partial S}{\partial x}(x, t) = 0 \quad (2.23)$$

because of the equations of motion.

According to our previous results $\psi(x, t) = \tilde{J}(x, t)^{1/2} \exp \left\{ \frac{i}{\hbar} S_c(x, t) \right\}$ is an approximate solution (up to order \hbar^2) of the Schrödinger equation at least for small time, which is localized in a finite region.

It is convenient to compare the result we obtained with a more general previous one [1] [2]. For this we make the following observation

LEMMA 2.3. — For small t let $x_0(x, t)$ be $\phi_t^{-1}(x)$, then

$$\frac{\partial x_0}{\partial x}(x, t) = \left(\frac{E - V(x_0)}{E - V(x)} \right)^{1/2}, \quad x \in \Delta_E. \quad (2.24)$$

Proof is obvious using the classical equation of motion:

$$t = \left(\frac{m}{2} \right)^{1/2} \int_{x_0(x, t)}^x \frac{dy}{(E - V(y))^{1/2}}. \quad (2.25)$$

Consequently, one can rewrite the semi-classical solution of the Schrödinger equation according to the

PROPOSITION 2.4. — [1] [2]. Let $\Theta \in C_0^\infty(\mathbb{C})$ then:

$$\psi^c(x, t) = \frac{\Theta(x_0(x, t))}{\left(\frac{2}{m} (E - V(x_0(x, t))) \right)^{1/4}} \left(\frac{\partial x_0(x, t)}{\partial x} \right)^{1/2} \exp \left\{ \frac{i}{\hbar} S_0(x) - \frac{i}{\hbar} Et \right\}$$

for sufficiently small t satisfies the Schrödinger equation up to order \hbar^2 .

As a last observation let us remark that we have chosen the plus sign for the definition of S . We can as well choose the other sign defining another solution with the same properties except for the initial condition.

Finally, for completely integrable systems one can explicitly reproduce the previous results, viz. find a solution S of the Jacobi equation and a solution R for the continuity equation. See Appendix A and B.

§ 3. CLASSICAL LIMIT OF WIGNER FUNCTIONALS

As we have shown in the previous section, for those systems we have considered it is possible to build an approximate solution of the Schrödinger equation which is for small time localized in a finite region. We want to show the physical meaning of these wave functions in the classical limit, viz. when \hbar goes to zero.

However, as it is known, wave functions have a singular behaviour when \hbar goes to zero, especially the ones we have considered since they contain an oscillatory term $\exp \left\{ \frac{i}{\hbar} S^c(x, t) \right\}$. On the other hand, wave functions define expectation values on the quantum observables and one can expect that these expectation values have a much nicer behaviour [5].

More precisely, let ϕ be a normalized wave function then it is associated with a Wigner function W_ϕ (see e. g. [5] and references therein).

$$W_\phi(x, p) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} d\xi \bar{\phi}\left(x + \frac{\hbar}{2}\xi\right) e^{ip\xi} \phi\left(x - \frac{\hbar}{2}\xi\right), \quad (x, p) \in \mathbb{R}^{2n}. \quad (3.1)$$

From which one obtains the quantum expectation value $\langle \phi f \rangle_Q$ in the state ϕ of a quantum observable whose classical functions is f (which for the sake of simplicity we choose in $L_1(\mathbb{R}^n \times \mathbb{R}^n)$), as

$$\langle \phi f \rangle_Q = \int_{\mathbb{R}^{2n}} f(x, p) W_\phi(x, p) dx dp. \quad (3.2)$$

Let us come back to the semi-classical wave function we have considered. Let f be an $L_1(\mathbb{R} \times \mathbb{R})$ function on phase space which is of compact support in x , independently of p , viz.

$$\text{Supp } f(\cdot, p) \subset C \quad \forall p \in \mathbb{R}$$

and decreasing sufficiently fast in p for given x . Then there exists $E > 0$ such that $C \Subset \Delta_E$. Consequently, there exists a function $\Theta \in C_0^\infty(\mathbb{R})$ with support C' such that

$$\begin{aligned} j - C &\Subset C' \Subset \Delta_E \\ ij - \Theta \upharpoonright_C &= 1. \end{aligned} \quad (3.3)$$

For small enough time t let us compute up to normalization the quantum

expectation value $\langle f \rangle_Q$ within the semi-classical state associated with Θ :

$$\langle \phi_+^c f \rangle_Q = \left(\frac{m}{2}\right)^{1/2} (2\pi)^{-1} \int_{\mathbb{R}} d\xi \int_{\mathbb{R}^2} dx dp \exp \left\{ \frac{i}{\hbar} \left(S_0^c \left(x - \frac{\hbar}{2} \xi \right) - S_0^c \left(x + \frac{\hbar}{2} \xi \right) \right) \right\} \quad (3.4)$$

$$\Theta^{1/2} \left(\phi_t^{-1} \left(x - \frac{\hbar}{2} \xi \right) \right) \Theta^{1/2} \left(\phi_t^{-1} \left(x + \frac{\hbar}{2} \xi \right) \right) e^{ip\xi}$$

$$\left(E - V \left(x - \frac{\hbar}{2} \xi \right) \right)^{-1/4} \left(E - V \left(x + \frac{\hbar}{2} \xi \right) \right)^{-1/4} f(x, p).$$

However, for \hbar going to zero and by Lebesgue dominated convergence theorem, using $(\min_{y \in C} (E - V(y)))^{-1/2} \left| \int e^{ip\xi} f(x, p) dp \right|$ as majorant, the previous expression tends to

$$\langle \phi_+^c f \rangle_Q \xrightarrow{\hbar \downarrow 0} (2\pi)^{-1} \int_{\mathbb{R}} d\xi \int_{\mathbb{R}^2} dx dp \exp \left\{ i\xi \left(p - \frac{\partial S_0}{\partial x} \right) \right\} \quad (3.5)$$

$$\left(\frac{2}{m} (E - V(x)) \right)^{-1/4} f(x, p).$$

It can also be written as

$$\langle \phi_+^c f \rangle_Q \xrightarrow{\hbar \downarrow 0} \int_{\mathbb{R}^2} dx dp f(x, p) \frac{1}{\left(\frac{2}{m} (E - V(x)) \right)^{1/2}} \delta(p - (2m(E - V(x)))^{1/2}) \quad (3.6)$$

As we mentioned in Section 2, there exists another solution ϕ_-^c , for which we can repeat a similar calculation and obtain

$$\langle \phi_-^c f \rangle_Q \xrightarrow{\hbar \downarrow 0} \int_{\mathbb{R}^3} dx dp f(x, p) \frac{1}{\left(\frac{2}{m} (E - V(x)) \right)^{1/2}} \delta(p + (2m(E - V(x)))^{1/2}). \quad (3.7)$$

On the other hand, if we consider the matrix elements of the quantum observables corresponding to a function f on the phase space, between ϕ_+^c and ϕ_-^c one is left with the following expression

$$\left(\frac{m}{2}\right)^{1/2} (2\pi)^{-1} \int_{\mathbb{R}} d\xi \Theta^{1/2} \left(x_0 \left(x + \frac{\hbar}{2} \xi, t \right) \right) \Theta^{1/2} \left(x_0 \left(x - \frac{\hbar}{2} \xi, t \right) \right) \quad (3.8)$$

$$\left(E - V \left(x + \frac{\hbar}{2} \xi \right) \right)^{-1/4} \left(E - V \left(x - \frac{\hbar}{2} \xi \right) \right)^{-1/4}$$

$$\exp \left\{ \frac{i}{\hbar} \left(S \left(x - \frac{\hbar}{2} \xi \right) + S \left(x + \frac{\hbar}{2} \xi \right) \right) \right\}$$

which is an oscillatory integral with respect to \hbar and goes to zero pointwise as \hbar goes to zero.

Consequently (reintroducing the normalization), we can state the

THEOREM 3.1. — Let ψ^c be the approximate solution of the Schrödinger equation given by

$$\psi^c(x, t) = \psi_+^c(x, t) + \psi_-^c(x, t) \quad (3.9)$$

for a given energy E . Then for any function f on the classical phase space whose support in configuration space is (strictly) contained in Δ_E (independently of the momentum), for sufficiently small time t , the normalized quantum expectation value satisfies:

$$\lim_{\hbar \rightarrow 0} \langle \psi^c f \rangle_Q = \langle f \rangle_{\text{microcanonical}}. \quad (3.10)$$

$\langle f \rangle_{\text{microcanonical}}$ means the average of f with respect to the microcanonical measure on the phase space

$$\langle f \rangle_{\text{microcanonical}} = \int_{\mathbb{R}^2} f(x, p) \delta(H(x, p) - E) \Big/ \int_{\mathbb{R}^2} \delta(H(x, p) - E) \Theta(\dot{x}).$$

Let us observe that the result does not depend on the relative phase between ψ_+^c and ψ_-^c a result which has something to do with the fact that we are dealing with a short time.

Finally, if we observe that the norm convergence of the wave function implies the pointwise convergence of the Wigner function by the obvious estimate:

$$|W_\varphi(x, p) - W_{\varphi'}(x, p)| \leq 2 \|\varphi - \varphi'\|.$$

We can conclude by the:

THEOREM 3.1. — Let $t \rightarrow \psi(x, t)$ the solution of the Schrödinger equation with initial condition

$$\Theta^{1/2}(x)(E - V(x))^{-1/4} \left(e^{\frac{i}{\hbar}S(x)} + e^{i\alpha - \frac{i}{\hbar}S(x)} \right) \quad (3.11)$$

then for any function f on the phase space whose support in configuration space is (strictly) contained in Δ_E for any value of the momentum, and such that $\Theta \upharpoonright \text{supp } f = 1$, for sufficiently small t , we have:

$$\lim_{\hbar \downarrow 0} (\psi_t f)_Q = \langle f \rangle_{\text{microcanonical}}. \quad (3.12)$$

APPENDIX A

THE CASE OF SPHERICALLY SYMMETRIC POTENTIALS

This case is the prototype of completely integrable systems and it is for this reason that we want to treat it completely. However, for the sake of notational simplicity we restrict ourselves to the two dimensional case, the general case will be treated along quite similar lines (Appendix B).

Let us consider a classical system in two dimensions whose Hamiltonian is

$$\begin{aligned} \mathbf{H}((x, y, p_x, p_y)) &= \frac{1}{2m} (p_x^2 + p_y^2) + \mathbf{V}(r) \\ r &= (x^2 + y^2)^{1/2}. \end{aligned} \quad (\text{A.1})$$

It is convenient in this case to introduce polar coordinates

$$x = r \cos \varphi \quad (\text{A.2})$$

$$y = r \sin \varphi$$

$$p_x = p_r \cos \varphi - \frac{1}{r} p_\varphi \sin \varphi \quad (\text{A.3})$$

$$p_y = p_r \sin \varphi + \frac{1}{r} p_\varphi \cos \varphi.$$

Consequently, the invariant measure on the phase space satisfies

$$dx dy dp_x dp_y = dr d\varphi dp_r dp_\varphi. \quad (\text{A.4})$$

the Hamiltonian function rewrites as

$$\mathbf{H}(r, \varphi, p_r, p_\varphi) = \frac{1}{2m} \left(p_r^2 + \frac{1}{r^2} p_\varphi^2 \right) + \mathbf{V}(r) \quad (\text{A.5})$$

and p_φ is a constant of motion.

Again we assume that \mathbf{V} is a positive potential which increases at infinity. For any $E > 0$ and $n \in \mathbb{Z}$ we define the function

$$\mathbf{S}_\pm(r, \varphi, t) = \mathbf{S}_\pm(r) + n(\varphi - \varphi_0) - Et \quad (\text{A.6})$$

$$\mathbf{S}_\pm(r) = \pm \left[\int_{\rho_0}^r \left[2m(E - \mathbf{V}(\rho)) - \frac{n^2}{\rho^2} \right]^{1/2} d\rho \right]$$

for those r such that $2m(E - \mathbf{V}(r)) - \frac{n^2}{r^2} \geq 0$, $r \neq 0$.

LEMMA A.1. — $\mathbf{S}_\pm(r, \varphi, t)$ satisfies the Jacobi equation, viz.

$$\frac{1}{2m} |\Delta \mathbf{S}_\pm|^2 + \mathbf{V}(r) - E = 0.$$

Furthermore, it is easy to prove that again on the same domain

$$\mathbf{J}(r) = \left(2m(E - \mathbf{V}(r)) - \frac{n^2}{r^2} \right)^{-1/2} \quad (\text{A.7})$$

satisfies the continuity equation:

$$\nabla \cdot (\mathbf{JVS}_{\pm}) = 0. \quad (\text{A. 8})$$

Consequently, if we consider the mapping ϕ , induced by the Newton equation with the given value n of p_{φ}

$$\psi_{\pm}(r, \varphi) = \Theta^{1/2} \left(\phi_{\pm}^{-1}(r, \varphi) \right) \left(2m(E - V(r)) - \frac{n^2}{r^2} \right)^{-1/4} \exp \left\{ \frac{i}{\hbar} (\mathbf{S}_{\pm}(r) + n(\varphi - \varphi_0) - Et) \right\} \quad (\text{A. 9})$$

is an approximate solution of the Schrödinger equation (up to order \hbar^2) and for given small time it approaches the true solution in norm as \hbar goes to zero.

As previously, when \hbar goes to zero the Wigner function $\mathbf{W}(x, y, p_x, p_y)$ built out of this function, up to the factor $\left[2m(E - V(r)) - \frac{n^2}{r^2} \right]^{1/2}$ approaches the Dirac measure on

$$p_x = \frac{\partial \mathbf{S}}{\partial x} \quad (\text{A. 10})$$

$$p_y = \frac{\partial \mathbf{S}}{\partial y}.$$

However, using inverse formulas to (A.3) this amounts to replacing p_r by

$$\left(2m(E - V(r)) - \frac{n^2}{r^2} \right)^{1/2} \quad \text{and} \quad p_{\varphi} \quad \text{by} \quad n.$$

Consequently, as in the one dimensional case with suitable combination of ψ_+ and ψ_- for small time and for functions in the phase space with limited support in r , the corresponding expectation value approaches the one given by the microcanonical ensemble

$$\delta(\mathbf{H}(r, \varphi, p_r, p_l) - E) \delta(p_{\varphi} - n). \quad (\text{A. 11})$$

Finally, let us quote the result for the three dimensional case. The function \mathbf{S} depends on two constants of motion beside the energy E , viz. l^2 and l_z the length of the angular momentum and the value of its third component

$$\mathbf{S}(r, \theta, \varphi, t) = \int_{r_0}^r d\rho \left(2m(E - V(\rho)) - \frac{l^2}{\rho^2} \right)^{1/2} + \int_{\theta_0}^{\theta} d\theta' \left(l^2 - \frac{l_z^2}{\sin^2 \theta'} \right)^{1/2} + l_z(\varphi - \varphi_0) - Et \quad (\text{A. 12})$$

whereas the \mathbf{J} function which in the proper domain satisfies the continuity equation can be written as

$$\mathbf{J}(r, \theta, \varphi) = \frac{m}{2} \left(2m(E - V(r)) - \frac{l^2}{r^2} \right)^{-1/2} \left(l^2 - \frac{l_z^2}{\sin^2 \theta} \right)^{-1/2}, \quad (\text{A. 13})$$

it does not depend on φ .

Again in (A.12) different signs can be taken for the square roots and it is the proper combination, up to phase, which leads to the microcanonical ensemble in the limit where \hbar goes to zero.

APPENDIX B

COMPLETELY SEPARABLE CASE

Now we consider a conservative system, which is completely integrable. In this case, it is known [6, § 48] that there exists a solution of the Hamiltonian Jacobi equation of the form:

$$\mathcal{S} = \sum_k \mathcal{S}_k(q_k, \alpha_1, \dots, \alpha_s) - E(\alpha_1, \dots, \alpha_s)t \tag{B.1}$$

$q_i \ i = 1, \dots, s$ being coordinates of the systems and $\alpha_i \ i = 1, \dots, s$ being the constants of motion. Indeed, in that case one can find functions $\varphi_1, \dots, \varphi_{s-1}$, such that

$$H(q_i, p_i) = \Phi(\varphi_1(q_1, p_1), \varphi_2(q_2, p_2, \varphi_1(p_1 q_1)) \dots \varphi_{s-1}(q_{s-1}, p_{s-1}, \varphi_1 \dots), q_s p_s). \tag{B.2}$$

Consequently, the Hamiltonian Jacobi equation is equivalent to the set of equations:

$$\begin{aligned} \varphi_1 \left(q_1, \frac{\partial \mathcal{S}}{\partial q_1} \right) &= \alpha_1 \\ \varphi_i \left(q_i, \frac{\partial \mathcal{S}}{\partial q_i}, \alpha_1, \dots, \alpha_{i-1} \right) &= \alpha_i \\ &\dots \dots \dots \\ \Phi \left(\alpha_1, \dots, \alpha_{s-1}, q_s, \frac{\partial \mathcal{S}}{\partial q_s} \right) &= E. \end{aligned} \tag{B.3}$$

And the S_i 's are obtained explicitly by: (we assume that H is at most quadratic in the p 's)

$$\frac{\partial S_i}{\partial q_i} = \varepsilon_i f_i(q_i, \alpha_1 \dots \alpha_i), \quad \varepsilon_i = \pm 1$$

and then by a simple quadrature.

It is obvious that the function

$$J = \prod_{i=1}^s f_i(q_i, \alpha_1 \dots \alpha_i)^{-1} \tag{B.5}$$

satisfies the continuity equation outside of its singular points. Consequently, the wave function

$$\psi_{i_0}^{\Theta}(q, t) = (\Theta^{1/2})_t J^{1/2} \exp \left\{ \frac{i}{\hbar} \left(\prod_{i=1}^s \varepsilon_i \int f_i(q_i, \alpha_1 \dots \alpha_i) dq_i - E(\alpha_1 \dots \alpha_s) t \right) \right\} \tag{B.6}$$

where $(\Theta^{1/2})_t$ denotes for small $t(\Theta(q_{i_0}(q_j, t))^{1/2}$, Θ being a smooth function of compact support, and $q_{i_0}(q_i, t)$ the solution of the classical equation of motion corresponding to the constants $\alpha_1 \dots \alpha_s$, is an approximate solution of the Schrödinger equation. Therefore, we can state the

THEOREM. — If Θ is one on a compact region K of the phase space, then the Wigner function associated to the wave function :

$$\psi^\Theta(q, t) = \sum_{\varepsilon_i = \pm} \psi_{|\varepsilon_i|}^\Theta(q, t)$$

for small enough t , and for functions in the phase space whose support is contained in K , approaches the microcanonical measure as \hbar goes to zero.



APPENDIX C

CLASSICAL LIMIT OF THE EXCITED STATES OF THE HARMONIC OSCILLATOR

In this appendix we want to show on an example that true eigenstates of the Hamiltonian operator can behave in the same way as the states we have considered. The example we are considering is the one dimensional harmonic oscillator.

The Fourier transform of the Wigner function corresponding to an eigenvector $|n\rangle$ (in the standard notations) is given by

$$(\mathcal{F} W_n)(u, v) = \exp\left(\frac{i\Theta |^2}{4}\right) L_n\left(\frac{| \Theta |^2}{2} u\right) \tag{C.1}$$

where

$$\Theta = \left(\frac{\hbar}{m\omega}\right)^{1/2} v + i(\hbar m\omega)^{1/2} u \tag{C.2}$$

and L_n is the n 'th Laguerre polynomial.

When \hbar goes to 0 $\mathcal{F} W_n$ goes pointwise to one. However, if one looks for another limit where $\hbar \rightarrow 0$ and n goes to infinity in such a way that

$$n\hbar = \frac{E}{\omega} = C$$

then using the known result [7]

$$\lim_{n \rightarrow \infty} n^{-\nu} L_n^\nu\left(\frac{z}{n}\right) = z^{-\frac{\nu}{2}} J_\nu(2z^{1/2}) \tag{C.3}$$

uniformly for bounded z , and the integral representation of the Bessel functions (see e. g. [8], p. 372) it is easy to prove that

$$\lim_{\substack{n \rightarrow \infty \\ \hbar \rightarrow 0 \\ \hbar n = \frac{E}{\omega}}} (\mathcal{F} W_n)(u, v) = \frac{\omega}{2\pi} \mathcal{F} \left\{ \delta\left(\frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 - E\right) \right\} (u, v) = \mathcal{F} \delta(\dots) \cdot \left[\int \delta(\dots) dp dq \right]^{-1} \tag{C.4}$$

Then

$$\lim_{\substack{n \rightarrow \infty \\ \hbar \rightarrow 0 \\ \hbar n = \frac{E}{\omega}}} \int_{\mathbb{R}^2} dq dp f(q, p) W_n(q, p) = \frac{\omega}{2\pi} \int_{\mathbb{R}^2} dq dp f(q, p) \delta\left(\frac{1}{2m} p^2 + \frac{1}{2} m\omega^2 q^2 - E\right) \tag{C.5}$$

for smooth functions on the phase space as expected.

This result is usually quoted in the literature as the fact that quantum mechanics approaches classical mechanics in the limit of large quantum numbers.

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Note added in proof: As pointed out by Prof. M. Berry we have to remark that, in the case of completely integrable systems, the microcanonical ensemble would correspond to the energy surface not limited to a precise value of constants of motion.

Also we are indebted to him for pointing out the following references dealing with the same problem:

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