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# Semiclassical mechanics of periodic motion: I. General scheme

P Kasperkovitz<sup>†</sup> and M Peev<sup>‡</sup>

<sup>†</sup> Institut für Theoretische Physik, Technische Universität Wien, Wiedner Hauptstr. 8–10, A-1040 Wien, Austria

<sup>‡</sup> Austrian Research Centre Seibersdorf, A-2444 Seibersdorf, Austria

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**Abstract.** A unified treatment of quantum mechanical oscillatory motion in one dimension is presented in a phase space formalism which is especially adapted to the semiclassical energy domain and closely related to a ‘naive’ quantization of action and angle variables. Characteristics of this scheme are non-classical symmetry properties of the phase space functions representing density operators and observables and the inclusion of half-Bohr orbits besides the familiar Bohr orbits. Over long time intervals the quantum evolution can be well approximated by a Hamiltonian flow along these distinguished classical orbits. The interplay of this reduced classical evolution and the symmetry properties of the phase space functions results in a consistent quantitative description of quantum interference effects which are most clearly seen in the revivals of wavepackets.

## 1. Introduction

The last years have seen a steady interest in and development of semiclassical calculation schemes, most of them related to studies of quantum chaos [1]. However, the most natural application of semiclassical ideas are integrable systems whose evolution is characterized by a high degree of regularity (conserved quantities, symmetries, etc). In the following, only the simplest motion of this kind is considered: oscillations of a particle in a one-dimensional potential. Results obtained for these systems are easily generalized to periodic motion in  $D > 1$  dimensions if the considered system is integrable and separable in the classical sense, i.e. if  $D$  pairs of action and angle variables can be explicitly constructed for the classical system.

The discussion presented in this paper aims at the following goals:

(i) to combine a number of known results on action and angle variables in quantum mechanics, phase space representations of operators, semiclassical matrix elements, expectation values and their evolution in time into a single unified and consistent semiclassical phase space formalism ( $S$ -formalism for semiclassical operators);

(ii) to show that for a high energies scheme (i) is essentially equivalent to first reformulating the classical problem in terms of action and angle variables and then quantizing it in a naive way where the action is treated like an angular momentum conjugate to the angle and anti-clockwise rotations are excluded as unphysical;

(iii) to illustrate the fact that there exists no universal quantization scheme, such that the sequence ‘dequantization–canonical transformation–quantization’ could be replaced by a unitary transformation (or at least an isometric one);

(iv) to point out that both (i) and (ii) naturally lead to a doubling of classical orbits which are relevant for semiclassical calculations (half-Bohr orbits besides the familiar Bohr orbits) and to non-classical symmetry properties of the phase space functions representing observables and density operators.

The paper is organized as follows: in section 2 we review the definition of various phase space functions related to operators and fix our notation. In section 3 we first present a list of exact formulae for the quantum mechanical expectation value of a given observable for a given state of the system. In these formulae the input which characterizes both the state and the observable ranges from matrix elements to phase space functions. Among the latter are the well known Wigner–Weyl representatives (*W*-functions) [2, 3], which are considered here as the classical equivalent of the operators. Usually these quantities are given as functions of momentum and position, whereas the variables used in the following discussion are the classical action and angle variables. It is shown that there exists another set of functions of the same variables, which are in one-to-one correspondence with the operators (*S*-formalism), and that expectation values can be calculated by means of these *S*-functions in exactly the same way as it is done in the Wigner–Weyl formalism. After having shown the equivalence of the different formulae for the expectation value we discuss in section 4 how the physical interpretation of the *S*-functions is related to the validity of an approximation used to calculate a matrix representation of the related operators. This approximation, sometimes called the Heisenberg correspondence principle [4], relates the matrix elements of an operator in energy representation to its Weyl representative. It is pointed out that this relation is not valid in general, but makes sense only for a certain class of operators which depends on the dynamics of the system (‘semiclassical’ operators). Seen from a more fundamental point of view, this formula defines a mapping of classical phase space functions onto operators which differs from standard quantization if, and only if, the classical function is not invariant under a certain smoothing procedure (a phase space function which is not ‘semiclassical’). In section 5 we show that a quantum theory, which differs from the restriction of standard quantum mechanics to semiclassical operators only by minor technical details, is obtained along the following route. (i) Consider only a restricted set of phase space functions. (ii) Quantize them by treating the action like an angular momentum and by mapping exponentials in the angle onto unitary operators. (iii) Fix an ordering scheme for products of these basic operators. (iv) Exclude all operators related to anti-clockwise rotations.

In section 6 we turn to the time evolution of quantum mechanical expectation values for the case where both the density operator and the observable are, at least to a good approximation, semiclassical operators. Here we introduce an approximation of the frequencies associated with the matrix elements of the operators in energy representation and distinguish three different levels of accuracy; they give rise to three different time intervals, for which the quantum evolution may be replaced by a dynamics derived from classical mechanics. (i) For short times the quantum evolution is indistinguishable from the classical evolution. (ii) For a much longer time interval the evolution can still be described by a Hamiltonian flow, however not on the whole phase space but only on a selected set of classical orbits; within this period typical quantum (interference) effects do occur and can be well described, both qualitatively and quantitatively, by means of this modified classical dynamics. (iii) For still longer time intervals one has essentially to go back to the quantum evolution; but if the Hamilton operator is also a semiclassical operator one can, instead of solving its eigenvalue problem, use the Maslov (EBK, torus, . . .) quantization condition to obtain the eigenvalues. Our conclusions are summarized in section 7 where our work is also compared to related approaches.

As is clear from the discussion in sections 4 and 5 the usefulness of the present and similar semiclassical schemes for calculating semiclassical expectation values depends crucially on the explicit knowledge of the energy representation of the operators of interest or on the validity of the semiclassical approximation for these matrix elements. A list of conditions an operator has to satisfy, such that the Heisenberg correspondence holds true (within a given error bound), is presented in this paper, as well as equivalent conditions for the related phase space functions. All these conditions depend both on the classical and the quantum mechanical dynamics of the system at hand. While they are useful to discuss structural relations they cannot be applied in a special case without explicit knowledge of the classical action and angle variables and a complete set of eigenfunctions of the Hamilton operator. What would be needed from a practical point of view, especially to estimate the quality of expectation values calculated according to our scheme, are *sufficient* conditions which hold for whole classes of Hamiltonians and operators. For anharmonic oscillators a partial answer to this open question is given in the subsequent paper where certain operators related to coherent states of high energy are shown to have the desired properties.

## 2. Basic concepts and notation

In the following we consider systems with Hamiltonians of the form

$$H(P, X) = \frac{1}{2}P^2 + V(X) \quad (1)$$

where  $V(X) \geq V(0) = 0$  and the potential is assumed to increase indefinitely for  $|X| \rightarrow \infty$ . We further assume that  $V$  is an even function, i.e.  $V(X) = V(-X)$ ; this simplifies the calculations but should have no impact on the qualitative features of our discussion. We consider only energy ranges where the equation  $H(P, X) = E$  describes a single closed curve in the two-dimensional phase plane  $\mathbf{R}^2$ . Under the classical evolution of the system the points of phase space are shifted clockwise along these curves as time proceeds. The description best adapted to this kind of motion uses action and angle variables [5] instead of momentum and position. The new variables  $\mathbf{I}$  and  $\Theta$  vary over a semi-infinite cylinder

$$\mathcal{C}_+ : \quad 0 \leq \mathbf{I} < \infty \quad -\pi \leq \Theta \leq \pi \quad (2)$$

(note that  $\mathbf{I}, \Theta$  and  $\mathbf{I}, \Theta + 2\pi$  represent the same physical state). In terms of these variables the evolution is simply a translation along the lines  $\mathbf{I} = \text{constant}$

$$(\mathbf{I}, \Theta) \rightarrow (\mathbf{I}, \Theta + \omega(\mathbf{I})t) \quad (3)$$

where

$$\omega(\mathbf{I}) = \frac{d}{d\mathbf{I}} \mathbf{H}(\mathbf{I}) \geq 0 \quad (4)$$

$$\mathbf{H}(\mathbf{I}) = \mathbf{H}(\mathbf{I}, \Theta) = H(P, X). \quad (5)$$

Here, and in the following, we consider equations of the form  $\mathbf{F}(\mathbf{I}, \Theta) = F(P, X)$  as identities: if, for instance,  $F(P, X)$  and the functional dependence of  $P$  and  $X$  on  $\mathbf{I}$  and  $\Theta$  are known, then  $\mathbf{F}(\mathbf{I}, \Theta) = F(\mathbf{P}[\mathbf{I}, \Theta], \mathbf{X}[\mathbf{I}, \Theta])$  is the defining equation of the function  $\mathbf{F}$ . The transition  $P, X \rightarrow \mathbf{I}, \Theta$  is a canonical transformation with functional determinant equal to one; hence

$$\int dP dX F(P, X) = \int d\mathbf{I} d\Theta \mathbf{F}(\mathbf{I}, \Theta) \quad (6)$$

where it is understood that the integrations are performed over the plane  $\mathbf{R}^2$  and the cylinder  $\mathcal{C}_+$ , respectively. In the following we will work almost exclusively with the variables  $\mathbf{I}, \Theta$

which, from a practical point of view, requires the explicit knowledge of the canonical transformation  $P, X \rightarrow \mathbf{l}, \Theta$  and its inverse. Instead of a function  $\mathbf{F}(\mathbf{l}, \Theta)$  we will frequently consider the functions  $\mathbf{F}_M(\mathbf{l})$ ,  $M = 0, \pm 1, \pm 2, \dots$  which appear in the decomposition

$$\mathbf{F}(\mathbf{l}, \Theta) = \sum_M \mathbf{F}_M(\mathbf{l}) e^{iM\Theta}. \quad (7)$$

If  $\mathbf{A}$  is the observable of interest and  $(1/h)\mathbf{Z}$  the distribution function which describes the state of the system,

$$\mathbf{Z} = \mathbf{Z}^* \quad \mathbf{Z} \geq 0 \quad \frac{1}{h} \int d\mathbf{l} d\Theta \mathbf{Z}(\mathbf{l}, \Theta) = 1 \quad (8)$$

the classical expectation value is given by

$$\langle A \rangle_{\mathbf{Z}}^C = \frac{1}{h} \int d\mathbf{l} d\Theta \mathbf{A}(\mathbf{l}, \Theta) \mathbf{Z}(\mathbf{l}, \Theta). \quad (9)$$

In general, the distribution function  $(1/h)\mathbf{Z}$  will not be stationary but evolve according to

$$\mathbf{Z}_t(\mathbf{l}, \Theta) = \mathbf{Z}_{t=0}(\mathbf{l}, \Theta - \omega(\mathbf{l})t) \quad (10)$$

(cf equation (3)) and the expectation value (9) will change accordingly.

When the system is quantized its evolution in time is determined by the Hamilton operator  $\hat{H} = H(\hat{P}, \hat{X})$ .

$$\hat{H}|n\rangle = E(n)|n\rangle. \quad (11)$$

The index  $n = 0, 1, 2, \dots$  not only labels the eigenvalues in increasing order,  $E(0) < E(1) < E(2) < \dots$ , but also gives the number of nodes of the eigenfunctions  $\langle x|n\rangle = \psi_n(x)$  (because of time reversal symmetry these functions can always be chosen to be real). Besides the orthonormalized eigenstates  $|n\rangle$  we also need the (normalized) coherent states  $|P, X\rangle$  whose wavefunctions in  $x$ -representation read

$$\langle x|P, X\rangle = (\pi\hbar)^{-1/4} e^{-iPX/2\hbar + iPx/\hbar - (x-X)^2/2\hbar}. \quad (12)$$

The coherent state  $|\mathbf{P}(\mathbf{l}, \Theta), \mathbf{X}(\mathbf{l}, \Theta)\rangle$  is abbreviated as  $|\mathbf{l}, \Theta\rangle$ . Properties of the coherent states used in the following are the scalar product

$$\begin{aligned} \langle P, X|P', X'\rangle &= \exp\left\{-\frac{(P-P')^2 + (X-X')^2}{4\hbar}\right\} \\ &\times \exp\left\{i\frac{(PX - P'X') - (P-P')(X+X')}{2\hbar}\right\} \end{aligned} \quad (13)$$

and the completeness relation

$$\begin{aligned} \hat{1} &= \frac{1}{h} \int dP dX |P, X\rangle \langle P, X| \\ &= \frac{1}{h} \int d\mathbf{l} d\Theta |\mathbf{l}, \Theta\rangle \langle \mathbf{l}, \Theta|. \end{aligned} \quad (14)$$

Besides the Hamiltonian  $\hat{H}$  we consider two sets of operators, namely observables, denoted by the symbol  $\hat{A}$ , and density operators, denoted by  $\hat{Z}$ ; when general properties of these operators are discussed we use the symbol  $\hat{F}$ . We assume that each of these operators is explicitly given in one of the following forms: (i) the energy representation (matrix elements  $\langle n'|\hat{F}|n''\rangle$ ); (ii) the  $x$ -representation (kernel  $\langle x'|\hat{F}|x''\rangle = F(x', x'')$ ), related to (i) by

$$F(x', x'') = \sum_{n', n''} \psi_{n'}(x') \langle n'|\hat{F}|n''\rangle \psi_{n''}(x'')^* \quad (15)$$

or (iii) the Weyl representative (W-function)  $F$ , related to (ii) by [3]

$$F(P, X) = \int_{-\infty}^{\infty} dx e^{-iPx/\hbar} F\left(X + \frac{x}{2}, X - \frac{x}{2}\right) \quad (16)$$

$$F(x', x'') = \frac{1}{h} \int_{-\infty}^{\infty} dP e^{iP(x'-x'')/\hbar} F\left(P, \frac{x'+x''}{2}\right). \quad (17)$$

We identify the  $W$ -function with the classical counterpart of the operator  $\hat{F}$  by assigning the same name to both of them. For example, the term ‘state’ is used for all Weyl representatives of density operators (‘Wigner functions’) although most of them assume negative values in certain regions of phase space. We refrain from giving a physical meaning to every operator or phase space function, even if the name suggest one, but restrict physical interpretation to classical and quantum mechanical expectation values.

The mapping of operators onto phase space functions and *vice versa* depends on the existence and meaning of the integrals (16) and (17). In the following we focus on operators  $\hat{F}$  which belong to the Hilbert–Schmidt class. This set consists of all operators for which

$$\|\hat{F}\|^2 = \langle\langle \hat{F}, \hat{F} \rangle\rangle < \infty \quad (18)$$

where the scalar product of two operators is defined by

$$\begin{aligned} \langle\langle \hat{F}, \hat{G} \rangle\rangle &= \text{Tr } \hat{F}^\dagger \hat{G} \\ &= \frac{1}{h} \int dP dX F(P, X)^* G(P, X) \\ &= \frac{1}{h} \int d\mathbf{l} d\Theta \mathbf{F}(\mathbf{l}, \Theta)^* \mathbf{G}(\mathbf{l}, \Theta). \end{aligned} \quad (19)$$

It is seen from  $\text{Tr } \hat{Z}^\dagger \hat{Z} = \text{Tr } \hat{Z}^2 \leq 1$  and equation (19) that all density operators  $\hat{Z}$  are Hilbert–Schmidt, and that the quantum mechanical expectation value has the form of a scalar product if the observable  $\hat{A}$  is also a Hilbert–Schmidt operator. This formal restriction of the observables under consideration has no physical consequences because the action of these operators is only of interest in a finite-dimensional subspace of the Hilbert space, which is related to a certain energy range and fixed by the density operator. When the elements of an infinite matrix are set equal to zero, except for a finite-dimensional submatrix, the original observable is transformed into a Hilbert–Schmidt operator which has the same physical meaning for the states under consideration. Mathematically the restriction to Hilbert–Schmidt operators has the advantage that this set, endowed with the scalar product (19) and the norm (18), is isomorphic to the Hilbert space of square integrable functions defined on the phase spaces  $\mathbf{R}^2$  or  $\mathcal{C}_+$ , respectively

$$h \langle\langle \hat{F}, \hat{G} \rangle\rangle = \langle \mathbf{F}, \mathbf{G} \rangle_2 \quad h \|\hat{F}\|^2 = \|\mathbf{F}\|_2^2. \quad (20)$$

The norm  $\|\hat{F}_1 - \hat{F}_2\| = \|\mathbf{F}_1 - \mathbf{F}_2\|_2$  provides a natural measure for the difference between two operators or the related phase space functions. This is especially of interest if the density operator or/and the observable are replaced by ‘similar’ ones in an expectation value. Since the expectation value has the form of a scalar product (19) the Schwarz inequality can be used to estimate the error induced by this substitution in terms of the norms  $\|\hat{F}_1 - \hat{F}_2\|$ .

The Weyl representatives are not the only set of phase space functions which contain the same information as the operators. An alternative set is provided by the  $Q$ -functions [6],

$$F^Q(P, X) = \langle P, X | \hat{F} | P, X \rangle \quad (21)$$

which may be obtained from the  $W$ -functions by smoothing

$$F^Q(P, X) = \int dP dX \mathbf{K}(P, X|P', X') F(P', X') \quad (22)$$

$$\mathbf{K}(P, X|P', X') = \frac{2}{h} \exp \left\{ -\frac{(P - P')^2 + (X - X')^2}{\hbar} \right\}. \quad (23)$$

The smoothing kernel (23) appears also in the implicit definition of the  $P$ -functions [6], which constitute a third set of phase space representatives

$$F(P, X) = \int dP dX \mathbf{K}(P, X|P', X') F^P(P', X'). \quad (24)$$

Formally equation (24) can be solved for  $F^P$ ,

$$F^P(P, X) = \exp \left\{ -\frac{\hbar}{4} \left( -\frac{\partial^2}{\partial P^2} + \frac{\partial^2}{\partial X^2} \right) \right\} F(P, X) \quad (25)$$

but the resulting series need not converge. The meaning of a divergent series follows from the combination of a  $P$ - with a  $Q$ -function in the scalar product (19)

$$\langle\langle \hat{F}, \hat{G} \rangle\rangle = \frac{1}{h} \int dP dX F^P(P, X) * G^Q(P, X) = \frac{1}{h} \int d\mathbf{l} d\Theta \mathbf{F}^P(\mathbf{l}, \Theta) * \mathbf{G}^Q(\mathbf{l}, \Theta) \quad (26)$$

where  $G^Q$  is a rapidly decreasing function and  $F^P$  a tempered distribution. Equation (26) follows from (19) and (22)–(24), or from (21) and the 'diagonal representation' [6]

$$\begin{aligned} \hat{F} &= \frac{1}{h} \int dP dX |P, X\rangle F^P(P, X) \langle P, X| \\ &= \frac{1}{h} \int d\mathbf{l} d\Theta |\mathbf{l}, \Theta\rangle \mathbf{F}^P(\mathbf{l}, \Theta) \langle \mathbf{l}, \Theta|. \end{aligned} \quad (27)$$

### 3. The $S$ -formalism

The expectation value of an observable  $\hat{A}$  in a state given by the density operator  $\hat{Z}$  can be calculated in various ways. For a discussion of approximations to the exact quantum mechanical expectation value the following equivalent expressions are of interest.

$$\begin{aligned} \langle\langle \hat{A} \rangle\rangle_{\hat{Z}} &= \langle\langle \hat{A}, \hat{Z} \rangle\rangle \\ &= \sum_{n', n''} \langle n' | \hat{A} | n'' \rangle * \langle n' | \hat{Z} | n'' \rangle \end{aligned} \quad (28)$$

$$= \frac{1}{2\pi} \sum_{\bar{n}} \int d\Theta \mathbf{a}^S(\bar{n}\hbar, \Theta) * \mathbf{z}^S(\bar{n}\hbar, \Theta) \quad (29)$$

$$= \frac{1}{h} \int d\mathbf{l} d\Theta \mathbf{A}^S(\mathbf{l}, \Theta) * \mathbf{Z}^S(\mathbf{l}, \Theta) \quad (30)$$

$$= \frac{1}{h} \int d\mathbf{l} d\Theta \mathbf{A}(\mathbf{l}, \Theta) * \mathbf{Z}(\mathbf{l}, \Theta). \quad (31)$$

Whereas (28) and (31) are familiar formulae the  $S$ -functions  $\mathbf{f}^S(\bar{n}\hbar, \Theta)$ ,  $\mathbf{f} = \mathbf{a}$  or  $\mathbf{z}$ , and  $\mathbf{F}^S(\mathbf{l}, \Theta)$ ,  $\mathbf{F} = \mathbf{A}$  or  $\mathbf{Z}$ , occurring in (29) and (30) call for explanation. Both these functions derive from the matrix elements in the energy representation. The first step in passing from (28) to (29) consists in a special choice of performing the double summation in (28). Instead of the double indices  $n', n''$  one uses the double indices

$$\bar{n} = \frac{1}{2}(n' + n'') \quad \delta n = n' - n'' \quad (32)$$

which range over

$$\bar{n} = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots \quad \delta n = \text{integer.} \quad (33)$$

However, care must be taken in which order the two summations are performed and which pairs of indices correspond to non-negative integer values of both  $n'$  and  $n''$ . If the summation over  $\delta n$  is performed first, then

$$\sum_{n'=0}^{\infty} \sum_{n''=0}^{\infty} \Psi(n', n'') = \sum_{\bar{n}=0}^{\infty} \sum_{\delta n}^{(\bar{n})} \Psi(\bar{n} + \frac{1}{2}\delta n, \bar{n} - \frac{1}{2}\delta n) \quad (34)$$

where

$$\sum_M^{(\bar{n})} \Phi(M) = \sum_{M=-2\bar{n}}^{2\bar{n}} \gamma(2\bar{n} + M) \Phi(M) \quad (35)$$

$$\gamma(m) = \frac{1}{2}[1 + (-1)^m]. \quad (36)$$

The functions  $\mathbf{f}_M^S(\bar{n}\hbar)$ , the Fourier coefficients of the function

$$\mathbf{f}^S(\bar{n}\hbar, \Theta) = \sum_{M=-\infty}^{\infty} \mathbf{f}_M^S(\bar{n}\hbar) e^{iM\Theta} \quad (37)$$

are then defined by

$$\mathbf{f}_M^S(\bar{n}\hbar) = \gamma(2\bar{n} + M) \langle \bar{n} + \frac{1}{2}M | \hat{F} | \bar{n} - \frac{1}{2}M \rangle \quad \text{for } |M| \leq 2\bar{n} \quad (38)$$

and

$$\mathbf{f}_M^S(\bar{n}\hbar) = 0 \quad \text{for } |M| > 2\bar{n}. \quad (39)$$

These definitions and the orthogonality relations of the exponentials  $\exp\{iM\Theta\}$  ensure that (29) and (28) yield the same result. Note that the factor  $\gamma(2\bar{n} + M)$  in (38) entails that for integer  $\bar{n}$  only exponentials with even  $M$  occur in the sum (37) while for half-integer  $\bar{n}$  the function  $\mathbf{f}^S(\bar{n}\hbar, \Theta)$  has only Fourier coefficients with odd index  $M$ . Accordingly

$$\int d\Theta \mathbf{f}^S(\bar{n}\hbar, \Theta) \mathbf{g}^S(\bar{m}\hbar, \Theta) = 0 \quad \text{if } \bar{n} + \bar{m} \neq \text{integer} \quad (40)$$

and the functions (37), called 'profiles' in the following, satisfy the symmetry relation

$$\mathbf{f}^S(\bar{n}\hbar, \Theta + \pi) = (-1)^{2\bar{n}} \mathbf{f}^S(\bar{n}\hbar, \Theta). \quad (41)$$

The change from the discrete variable  $\bar{n}\hbar$  to the continuous variable  $\mathbf{l}$  is achieved by 'smearing out' the profiles sitting on the orbits  $\mathbf{l} = \bar{n}\hbar$  and combining them into a single function

$$\mathbf{F}^S(\mathbf{l}, \Theta) = \sum_{\bar{n}=0}^{\infty} \mathbf{f}^S(\bar{n}\hbar, \Theta) \mathbf{C}_{\bar{n}\hbar}(\mathbf{l} - \frac{1}{2}\hbar). \quad (42)$$

In (42) the functions  $\mathbf{C}_y(x)$  are step functions defined by

$$\mathbf{C}_y(x) = \begin{cases} 1 & \text{for } |x - y| < \hbar/2 \\ 0 & \text{for } |x - y| > \hbar/2. \end{cases} \quad (43)$$

The reason for choosing just these boundaries for the step functions (43) and for shifting the argument by  $\hbar/2$  in (42) is that this choice will allow us to relate the S-functions to approximate matrix elements obtained from the  $W$ -functions (see section 4 later). These conventions, certainly appropriate for the harmonic oscillator, will be made for all symmetric binding potentials; but we do not exclude the possibility that a deeper analysis will finally



lead to a shift of the centres of the step functions which depends on the potential at hand (see also the remarks after equation (128), section 6).

Definition (43) results in

$$\int d\mathbf{l} \mathbf{C}_{\bar{n}\hbar}(\mathbf{l} - \frac{1}{2}\hbar) \mathbf{C}_{\bar{m}\hbar}(\mathbf{l} - \frac{1}{2}\hbar) = \begin{cases} \hbar & \text{for } |\bar{n} - \bar{m}| = 0 \\ \hbar/2 & \text{for } |\bar{n} - \bar{m}| = 1/2 \\ 0 & \text{for } |\bar{n} - \bar{m}| > 1/2. \end{cases} \quad (44)$$

This, together with (40), transforms (30) in (29) when the integration over  $\mathbf{l}$  is carried out. The value of  $\mathbf{F}^S$  on the orbits  $\mathbf{l} = (\bar{n} + \frac{1}{2})\hbar$  is undefined but this is irrelevant since these orbits form a set of measure zero. Equations (42), (43) and (37)–(39) show that the function  $\mathbf{F}^S$  is uniquely determined by the matrix elements  $\langle n' | \hat{F} | n'' \rangle$ ; this mapping of matrices to S-functions is one-to-one because

$$(\bar{n} + \frac{1}{2}M | \hat{F} | \bar{n} - \frac{1}{2}M) = \gamma(2\bar{n} + M) \lim_{\epsilon \rightarrow 0} \mathbf{F}_M^S([\bar{n} + \frac{1}{2}\hbar + \epsilon]). \quad (45)$$

The  $W$ - and the  $S$ -functions are both defined on the phase space  $\mathcal{C}_+$  and both of them are in one-to-one correspondence with the operators of the Hilbert–Schmidt class. The relation between the two sets of functions is determined by the functions which represent the elementary operators  $|n'\rangle\langle n''|$ . In the Wigner–Weyl formalism these operators are represented by functions  $W_{n',n''}(P, X)$  which can be calculated by means of (15) and (16) once the eigenfunctions  $\psi_n(x)$  are known, i.e. the construction of the function  $W_{n',n''}(P, X)$  requires that the eigenvalue problem of the Hamiltonian in  $x$ -representation has been solved completely beforehand. One fact should be noted in this context because it will turn out to be of relevance in the following discussion. The functions  $W_{n,n}(P, X)$  related to the projection operators  $|n\rangle\langle n|$  are uniquely determined by the Hamiltonian alone, but the explicit form of the functions  $W_{n',n''}(P, X)$  with  $n' \neq n''$  depends also on the conventions made for the phases of the eigenfunctions (the signs of  $\psi_n(x)$  and  $\psi'_n(x)$  at  $x=0$ , if they are chosen to be real). Since the operators  $|n'\rangle\langle n''|$  form an orthonormalized basis of the Hilbert–Schmidt operators, the functions  $\mathbf{W}_{n',n''}(\mathbf{l}, \Theta)$ , obtained from the functions  $W_{n',n''}(P, X)$  by a change of variables, form an orthonormalized basis of the Hilbert space  $L^2(\mathcal{C}_+)$ ,

$$\frac{1}{h} \int d\mathbf{l} d\Theta \mathbf{W}_{n',n''}(\mathbf{l}, \Theta)^* \mathbf{W}_{m',m''}(\mathbf{l}, \Theta) = \delta_{n',m'} \delta_{n'',m''} \quad (46)$$

$$\mathbf{F}(\mathbf{l}, \Theta) = \sum_{n',n''} \langle n' | \hat{F} | n'' \rangle \mathbf{W}_{n',n''}(\mathbf{l}, \Theta) \quad (47)$$

$$\langle n' | \hat{F} | n'' \rangle = \frac{1}{h} \int d\mathbf{l} d\Theta \mathbf{W}_{n',n''}(\mathbf{l}, \Theta)^* \mathbf{F}(\mathbf{l}, \Theta). \quad (48)$$

These equations include the relations between scalar products and norms of operators and those of the related  $W$ -functions, equation (20). Relations analogous to (46)–(48) hold for the  $S$ -formalism where the elementary operator  $|n'\rangle\langle n''|$  is represented by the function

$$\mathbf{S}_{n',n''}(\mathbf{l}, \Theta) = C_{\bar{n}\hbar}(\mathbf{l} - \frac{1}{2}\hbar) e^{i\delta n\Theta}. \quad (49)$$

If the argument of the  $S$ -functions can be interpreted as classical action and angle variables (which is by no means obvious, see section 6), the functions (49) are also defined on the classical phase space and uniquely determined by the classical Hamiltonian and the conventions used in the definition of  $\Theta$  (explicit form of the function  $\Theta(P, X) = 0$ ).

$$\frac{1}{h} \int d\mathbf{l} d\Theta \mathbf{S}_{n',n''}(\mathbf{l}, \Theta)^* \mathbf{S}_{m',m''}(\mathbf{l}, \Theta) = \delta_{n',m'} \delta_{n'',m''} \quad (50)$$

$$\mathbf{F}^S(\mathbf{l}, \Theta) = \sum_{n',n''} \langle n' | \hat{F} | n'' \rangle \mathbf{S}_{n',n''}(\mathbf{l}, \Theta) \quad (51)$$

$$\langle n' | \hat{F} | n'' \rangle = \frac{1}{h} \int d\mathbf{l} d\Theta \mathbf{S}_{n',n''}(\mathbf{l}, \Theta) \mathbf{F}^S(\mathbf{l}, \Theta). \tag{52}$$

Because of (50)–(52)

$$h \langle \hat{F}, \hat{G} \rangle = \langle \mathbf{S}^S, \mathbf{G}^S \rangle_2 = \langle \mathbf{F}, \mathbf{G} \rangle_2 \tag{53}$$

and hence  $h \|\hat{F}\|^2 = \|\mathbf{F}^S\|_2^2 = \|\mathbf{F}\|_2^2$ . Equation (53) shows that the mapping  $\mathbf{F} \rightarrow \mathbf{F}^S$  is an isometry. Because there exist infinitely many square integrable functions which are orthogonal to all functions (49), for example, all the functions  $\mathbf{N}_{n',n''}(\mathbf{l}, \Theta) = \mathbf{S}_{n',n''}(\mathbf{l}, \Theta) \exp\{2i\pi\mathbf{l}/h\}$ , the set of all  $S$ -functions forms a proper subspace of  $L^2(\mathcal{C}_+)$ ,

$$L^2(\mathcal{C}_+) = L_S^2(\mathcal{C}_+) \oplus L_\perp^2(\mathcal{C}_+) \tag{54}$$

$$L_S^2(\mathcal{C}_+) = \text{span of the functions } \mathbf{S}_{n',n''}. \tag{55}$$

Since the Fourier components  $\mathbf{F}_M^S(\mathbf{l})$  of the  $S$ -functions are step functions in  $\mathbf{l}$  with a step width of  $h$ , it is clear that the scalar products of these functions with functions, which are oscillating in  $\mathbf{l}$  with frequencies higher than  $2\pi/h$ , are of extremely small magnitude. The transition  $\mathbf{F} \rightarrow \mathbf{F}^S$  is therefore a transition to ‘smoother’ functions, which carry the same physical information as the original functions. Because of equations (46)–(48) and (50)–(52) the  $W$ - and  $S$ -representative of an operator  $\hat{F}$  are related by

$$T\mathbf{F} = \mathbf{F}^S \quad T^\dagger \mathbf{F}^S = \mathbf{F} \tag{56}$$

where the mappings  $T : L^2(\mathcal{C}_+) \rightarrow L_S^2(\mathcal{C}_+)$  and  $T^\dagger : L_S^2(\mathcal{C}_+) \oplus L_\perp^2(\mathcal{C}_+) \rightarrow L^2(\mathcal{C}_+) \oplus \{0\}$  are given by the kernels

$$T(\mathbf{l}, \Theta | \mathbf{l}', \Theta') = \frac{1}{h} \sum_{n',n''} \mathbf{S}_{n',n''}(\mathbf{l}, \Theta) \mathbf{W}_{n',n''}(\mathbf{l}', \Theta')^* \tag{57}$$

$$T^\dagger(\mathbf{l}, \Theta | \mathbf{l}', \Theta') = \frac{1}{h} \sum_{n',n''} \mathbf{W}_{n',n''}(\mathbf{l}, \Theta) \mathbf{S}_{n',n''}(\mathbf{l}', \Theta')^*. \tag{58}$$

It follows from these definitions that

$$T^\dagger T = \mathbf{1} \text{ unity operator in } L^2(\mathcal{C}_+) \tag{59}$$

$$T T^\dagger = P \text{ projection operator onto } L_S^2(\mathcal{C}_+). \tag{59}$$

The effect of applying the projection operator  $P$  with kernel

$$P(\mathbf{l}, \Theta | \mathbf{l}', \Theta') = \frac{1}{h} \sum_{n',n''} \mathbf{S}_{n',n''}(\mathbf{l}, \Theta) \mathbf{S}_{n',n''}(\mathbf{l}', \Theta')^* \tag{60}$$

onto an arbitrary function  $\mathbf{F} \in L^2(\mathcal{C}_+)$  is twofold, as can be seen from the definition of the functions  $\mathbf{S}_{n',n''}(\mathbf{l}, \Theta)$  (cf equations (43), (49) and (34)–(36)). First, the Fourier components  $\mathbf{F}_M(\mathbf{l})$  are transformed into step functions  $\mathbf{F}'_M(\mathbf{l})$  which are constant within intervals of width  $h$ ; second, these step functions are forced to vanish for  $\mathbf{l} < |M|h/2$  (see equations (39) and (42)). Both these effects can be seen as a kind of smoothing; while the first step eliminates rapid oscillations in  $\mathbf{l}$ , the second eliminates rapid oscillations in  $\Theta$  when  $\mathbf{l}$  is small (low energies).

#### 4. Semiclassical matrix elements

The variables  $\mathbf{l}, \Theta$ , which replaced the discrete variables  $\delta n$  and  $\bar{n}$ , were introduced in (37) and in (42) in a purely formal way. The fact that these variables also vary over the range (2) and that equations (30) and (31) yield the same result suggests to interpret them also as

action and angle variables. This interpretation would be more convincing if the  $S$ - and the  $W$ -representatives occurring in (30) and (31) were of similar form but relations (54)–(60) indicate that such a coincidence will be the exception rather than the rule. It is also not difficult to find examples where the two functions representing the same operator look quite different and the norm of their difference is large compared to the (identical) norm of the two functions. Before we present examples of such a discrepancy for two density operators of physical interest, let us first discuss in general terms when the  $S$ - and the  $W$ -representatives of an operator are similar, in a sense to be specified, or even coincide. This problem does not only affect the physical interpretation of the  $S$ -functions, but is closely related to the validity of a well known approximation for the matrix elements  $\langle n' | \hat{F} | n'' \rangle$  and becomes of interest when the quantum evolution of the system is studied (section 6).

Consider the operators for which

$$\mathbf{F} = \mathbf{F}^S. \quad (61)$$

In the following, operators satisfying (61) and the related phase space functions will be called ‘strictly semiclassical’. Note that the meaning of this term depends both on the classical and on the quantum dynamics of the considered system: whether a given operator is semiclassical or not depends on the Hamiltonian. To check whether (61) is satisfied for a given operator  $\hat{F}$ , one first has to calculate its  $W$ -representative  $F(P, X)$  by means of relations which are independent of the dynamics. Then the variables have to be changed to action and angle; this requires knowledge of the classical Hamiltonian, because otherwise the functions  $\mathbf{P}(\mathbf{l}, \Theta)$  and  $\mathbf{X}(\mathbf{l}, \Theta)$  could not be calculated. To find the function on the right-hand side of (61) the eigenfunctions of the Hamilton operator have to be calculated first. In addition conventions enter on both sides: on the right-hand side it is the phase of these eigenfunctions, on the left-hand side the choice of the curve  $\Theta(P, X) = 0$ .

Although we do not know whether equation (61) can be satisfied for other Hilbert–Schmidt operators than  $\hat{F} = \hat{0}$ , other solutions can be found if restriction (18) is dropped. For instance, it is easily verified that the  $W$ - and the  $S$ -representative of any multiple of the unity operator are the same constant function. No matter what the original set of operators or related phase space functions is, equation (61) will in general restrict this set to a proper subset. Relation (61) implies  $\mathbf{P}\mathbf{F} = \mathbf{P}\mathbf{F}^S = \mathbf{F}^S = \mathbf{F}$  but  $\mathbf{P}\mathbf{F} = \mathbf{F}$  is only a necessary condition for (61) to hold true. The necessary and sufficient condition for a  $W$ -function  $\mathbf{F} \in L^2(\mathcal{C}_+)$  to be strictly semiclassical is

$$T\mathbf{F} = \mathbf{F} \quad (62)$$

that for the  $S$ -representative  $\mathbf{F}^S \in L^2_S(\mathcal{C}_+)$  is

$$PT^\dagger \mathbf{F}^S = \mathbf{F}^S \quad (63)$$

and the equivalent condition for the Hilbert–Schmidt operator  $\hat{F}$  reads

$$\langle n' | \hat{F} | n'' \rangle = \sum_{m', m''} \tilde{T}_{n', n''; m', m''} \langle m' | \hat{F} | m'' \rangle \quad (64)$$

where

$$\tilde{T}_{n', n''; m', m''} = \frac{1}{h} \int dl d\Theta \mathbf{W}_{n', n''}(\mathbf{l}, \Theta)^* \mathbf{S}_{m', m''}(\mathbf{l}, \Theta) = \frac{1}{h} \langle \mathbf{W}_{n', n''}, \mathbf{S}_{m', m''} \rangle_2. \quad (65)$$

To determine all solutions of equations (62)–(64) for a given set of functions or matrices is an open problem. The interest in the solutions of these equations stems from the fact that

for strictly semiclassical operators the matrix elements in energy representation are related to the classical functions (more precisely, the  $W$ -functions) by the relation

$$\langle n' | \hat{F}' | n'' \rangle = \frac{1}{\hbar} \langle \mathbf{S}_{n', n''}, \mathbf{F} \rangle_2 = \frac{1}{\hbar} \int_{(n'+n'')\hbar/2}^{(n'+n''+2)\hbar/2} d\mathbf{l} \mathbf{F}_{n'-n''}(\mathbf{l}). \quad (66)$$

This equation can be seen in two ways. On a fundamental level (66) constitutes an alternative quantization scheme which assigns to each phase space function  $\mathbf{F} \in L^2(\mathcal{C}_+)$  a Hilbert–Schmidt operator  $\hat{F}'$  (the related  $W$ - and  $S$ -functions are  $T^1 \mathbf{F}$  and  $P\mathbf{F}$ , respectively). But contrary to the standard quantization scheme given by (17) this is not a one-to-one mapping because all functions in  $L^2_{\perp}(\mathcal{C}_+)$  are mapped onto the null operator. For the elements of  $L^2_S(\mathcal{C}_+)$  the mapping  $\mathbf{F} \rightarrow \hat{F}'$  is bijective but the operators  $\hat{F}'$  obtained this way coincide with the operators  $\hat{F}$  obtained from standard quantization only for functions  $\mathbf{F}$  which are both square integrable and strictly semiclassical (possibly an empty set). From a practical point of view equation (66) constitutes a considerable simplification in calculating for a given classical function the energy representation of the related operator: it is no longer necessary to solve first the eigenvalue problem of the Hamiltonian; all that is needed is to know how the classical function depends on the action and angle variables. However, to obtain the operator one originally had in mind and which one would interpret in the same way as the classical function, one has to take the validity of equations (62)–(64) for granted. These conditions are too restrictive if one is ready to tolerate small errors in the calculation of matrix elements and expectation values. In this case condition (61) may be weakened to

$$\|P\mathbf{F} - \mathbf{F}^S\|_2 < \epsilon \|\mathbf{F}\|_2 \quad (67)$$

where  $\epsilon$  is a small positive constant. Using the triangle and Schwarz inequalities one can show that (67) implies  $\|P\mathbf{F} - \mathbf{F}\|_2 < \sqrt{2}\epsilon \|\mathbf{F}\|_2$ , i.e. the difference between any two of the functions  $\mathbf{F}$ ,  $P\mathbf{F}$ , and  $\mathbf{F}^S$ , is then small (in the sense of  $L^2$ ). Functions for which (67) holds true and the related operators will be called 'semiclassical'. For the matrix elements (67) yields

$$|\langle n' | \hat{F}' | n'' \rangle - \langle n' | \hat{F} | n'' \rangle| < \hbar^{-1/2} \epsilon \|\mathbf{F}\|_2. \quad (68)$$

This shows that  $\epsilon$  should be  $o(\hbar^{1/2})$  if semiclassical arguments are used to derive (67).

Although the set of semiclassical operators is by definition more comprehensive than that of strictly semiclassical ones, it is not evident from these formal considerations whether it contains any operators of physical interest, nor can (66) or (67) be verified for a given operator without calculating, at least approximately, the eigenfunctions of the Hamiltonian. It is only clear that infinite sets of different classical functions are mapped onto the same operator when they are quantized according to (66), or according to the similar equation

$$\langle n' | \hat{F}'' | n'' \rangle = \mathbf{F}_{n'-n''}((n' + n'' + 1)\hbar/2). \quad (69)$$

The belief that (66) and (69) are nevertheless useful formulae originates from the fact that the latter is a well known formula for matrix elements which is claimed to yield good approximations of the true matrix elements in the semiclassical energy range (small  $\hbar$ , high quantum numbers  $n'$  and  $n''$ ). In [4], where (69) was derived, it was claimed that the difference between the true and the approximate matrix elements is of order  $\hbar^2$  and that (69) makes sense for arbitrary operators. The foregoing considerations clearly show that the second assertion cannot be true without restricting the class of considered operators. A hint how this could be done is given in the introduction of [4] where, in contrast to the otherwise claimed generality, it is said that the true matrix elements should be slowly varying functions of the average quantum number  $\bar{n}$ ; a similar statement is found in [7].

There are indications that this requirement, supplemented with a condition on the variation of the matrix elements for fixed average quantum number  $\bar{n}$  and varying difference quantum number  $\delta n$ , might eventually be quantified to yield necessary and sufficient conditions for semiclassical operators, which are more transparent than equations (64) and (65). In [4] it was implicitly assumed in the derivation of (69) that the  $W$ -representative of the operator admits a representation as power series in  $\hbar$ . That this condition is not necessary for (69) to yield good approximations of the true matrix elements, can be seen from the density operators for coherent states which appear in the second example discussed below.

In part II of this work we present a class of operators related to coherent states of high energy which are good candidates for semiclassical operators because their matrix elements are well approximated by (69); their matrix elements are indeed slowly varying functions of  $\bar{n}$ . In paper II we also solve a second problem related to formulae (69) and (66): let  $\hat{F}$  be an operator given by the kernel  $F(x', x'')$  and  $F(P, X)$  its  $W$ -representative calculated according to (16). The corresponding function  $\mathbf{F}(\mathbf{l}, \Theta)$  is then uniquely fixed by  $F(P, X)$  and the conventions used in the definition of  $\Theta(P, X)$ , as are the Fourier components  $\mathbf{F}_M(\mathbf{l})$ . This determines the right-hand side of both (66) and (69). However, the phases of the non-diagonal matrix elements of the operator are not fixed by  $\hat{F}$  and the Hamiltonian  $\hat{H}$  alone but depend on the phase conventions adopted for the eigenfunctions. Except for a common phase factor there exists only one convention that will give matrix elements which, if  $\hat{F}$  is semiclassical, can be approximated by (66) or (69). It is shown in II that for symmetric potentials  $V(X) = V(-X)$  the proper phase conventions are the same as the ones usually chosen for the eigenfunctions of the harmonic oscillator [9].

We close this section with two examples which illustrate the limitations of (66) and (69) and show how different  $W$ - and  $S$ -representatives of operators are in general. In both cases we choose  $\hat{H}$  to be the harmonic oscillator Hamiltonian since this allows us to obtain exact formulae for all quantities of interest. Although this system is special, semiclassical arguments [8] and numerical calculations for anharmonic symmetric potentials indicate that the conclusions drawn from the two examples are valid for a wider class of potentials.

The first example is the operator  $\hat{F} = |n_1\rangle\langle n_2|$  with  $n_1 \geq n_2$ . Its  $W$ -representative is [10]

$$\mathbf{W}_{n_1, n_2}(\mathbf{l}, \Theta) = 2(-1)^{n_2} \sqrt{\frac{n_2!}{n_1!}} \left(\frac{4\mathbf{l}}{\hbar}\right)^{(n_1-n_2)/2} L_{n_2}^{(n_1-n_2)}\left(\frac{4\mathbf{l}}{\hbar}\right) \exp\left\{-\frac{2\mathbf{l}}{\hbar} + i(n_1 - n_2)\Theta\right\} \quad (70)$$

where  $L_n^{(\alpha)}(z)$  is the (generalized) Laguerre polynomial [11]. Note that for  $n_1 = n_2 = n$ , (70) is the Wigner function of the eigenstate  $|n\rangle$  while  $\mathbf{S}_{n,n}$  is essentially what in literature is called the (semi)classical limit of this function [8, 12]. A plot of these functions immediately shows how different the two functions are and this is also seen in the failure of (66) and (69). The true matrix elements are the Kronecker products  $\delta_{n', n_1} \delta_{n'', n_2} = \delta_{2\bar{n}, n_1+n_2} \delta_{\delta n, n_1-n_2}$ ; equation (69) gives instead

$$\langle n' | \hat{F}'' | n'' \rangle = \delta_{\delta n, n_1-n_2} 2(-1)^{n_2} \sqrt{\frac{n_2!}{n_1!}} (4\bar{n}_+)^{\delta n/2} L_{n_2}^{(\delta n)}(4\bar{n}_+) e^{-2\bar{n}_+} \quad (71)$$

where  $\bar{n}_+ = \bar{n} + \frac{1}{2}$ . For fixed  $n_1$  and  $n_2$  and  $\delta n = n_1 - n_2$  the right-hand side oscillates for  $\bar{n} < (n_1 + n_2 + 1)/2$ , the lower boundary of  $\bar{n}$  depending on  $\delta n$ ; its amplitude is much smaller than 1 and vanishes only for  $\bar{n} \gg (n_1 + n_2 + 1)/2$ . This behaviour persists for large quantum numbers  $n_{1,2}$  and is obviously independent of the magnitude of  $\hbar$ . The same features are found if (66) is used instead of (69). In this case it follows from (70) that  $\tilde{\mathbf{T}}_{n_1, n_2; n', n''}$  is diagonal in the differences  $n_1 - n_2$  and  $n' - n''$  but not in the sums of these quantum numbers.

If only the dependence on the average quantum number is considered, the right-hand side of equation (64) is similar to a convolution with an oscillating function. Such a transformation drastically changes the original function, except if the latter is almost constant over many oscillations. This is an indication that the matrix elements of semiclassical operators have to be indeed slowly varying functions of the average quantum number.

The second example is the density operator of a 'cat state' which is a superposition of the two coherent states  $|\mathbf{l}_0, \Theta_0\rangle$  and  $|\mathbf{l}_0, \Theta_0 + \pi\rangle$ ,

$$\hat{F} = c(\hat{F}^+ + \hat{F}^- + \hat{F}^0) \quad (72)$$

$$\hat{F}^+ = |\mathbf{l}_0, \Theta_0\rangle\langle\mathbf{l}_0, \Theta_0| \quad \hat{F}^- = |\mathbf{l}_0, \Theta_0 + \pi\rangle\langle\mathbf{l}_0, \Theta_0 + \pi|$$

$$\hat{F}^0 = |\mathbf{l}_0, \Theta_0\rangle\langle\mathbf{l}_0, \Theta_0 + \pi| + |\mathbf{l}_0, \Theta_0 + \pi\rangle\langle\mathbf{l}_0, \Theta_0|. \quad (73)$$

If  $\hat{F}$  were a mixture of the two coherent states the term  $\hat{F}^0$  would be missing in (72). The scalar products  $\langle n|P, X\rangle$  are well known (see, e.g., [9]); with  $P = -\sqrt{2\mathbf{l}} \sin \Theta$ ,  $X = \sqrt{2\mathbf{l}} \cos \Theta$  they read

$$\langle n|\mathbf{l}, \Theta\rangle = \frac{1}{\sqrt{n!}} \left(\frac{\mathbf{l}}{\hbar}\right)^{n/2} \exp\left\{-\frac{\mathbf{l}}{2\hbar} - in\Theta\right\} = (-1)^n \langle n|\mathbf{l}, \Theta + \pi\rangle. \quad (74)$$

The matrix elements of the three operators (73) are therefore

$$\left\langle \bar{n} + \frac{\delta n}{2} \left| \hat{F}^+ \right| \bar{n} - \frac{\delta n}{2} \right\rangle = Q(\bar{n}, \delta n) \frac{1}{\Gamma(\bar{n} + 1)} \left(\frac{\mathbf{l}_0}{\hbar}\right)^{\bar{n}} \exp\left\{-\frac{\mathbf{l}_0}{\hbar} - i\delta n\Theta_0\right\} \quad (75)$$

with

$$Q(\bar{n}, \delta n) = \frac{\Gamma(\bar{n} + 1)}{\sqrt{\Gamma(\bar{n} + (\delta n/2) + 1)\Gamma(\bar{n} - (\delta n/2) + 1)}} \quad (76)$$

and

$$\left\langle \bar{n} + \frac{\delta n}{2} \left| \hat{F}^- \right| \bar{n} - \frac{\delta n}{2} \right\rangle = \left\langle \bar{n} + \frac{\delta n}{2} \left| \hat{F}^+ \right| \bar{n} - \frac{\delta n}{2} \right\rangle (-1)^{n'+n''} \quad (77)$$

$$\left\langle \bar{n} + \frac{\delta n}{2} \left| \hat{F}^0 \right| \bar{n} - \frac{\delta n}{2} \right\rangle = \left\langle \bar{n} + \frac{\delta n}{2} \left| \hat{F}^+ \right| \bar{n} - \frac{\delta n}{2} \right\rangle [(-1)^{n'} + (-1)^{n''}]. \quad (78)$$

Because of the factor  $1 + (-1)^{n'+n''} + (-1)^{n'} + (-1)^{n''}$  the matrix elements of (72) vanish if  $n'$  and  $n''$  are not both even numbers;  $\langle n'|\hat{F}|n''\rangle$  is therefore rapidly changing when  $\bar{n}$  increases by  $\frac{1}{2}$ . For  $\bar{n} \gg 1$ ,  $|\delta n| \ll \bar{n}$  the Stirling formula gives

$$Q(\bar{n}, \delta n) \approx \exp\{-(\delta n)^2/8\bar{n}\} \quad (79)$$

and the approximation [13]

$$\sum_M e^{-M^2/2x+iM\alpha} \approx (2\pi x)^{1/2} \exp\{-2x \sin^2(\alpha/2)\} \quad (80)$$

valid for  $x \gg 1$ , may be used to calculate the profiles for the operators (73). With

$$g_0(\bar{n}) = \frac{1}{\Gamma(\bar{n} + 1)} \left(\frac{\mathbf{l}_0}{\hbar}\right)^{\bar{n}} \exp\left\{-\frac{\mathbf{l}_0}{\hbar}\right\} \quad g_1(\alpha) = (8\pi\bar{n})^{1/2} \exp\left\{-8\bar{n} \sin^2\left(\frac{\alpha}{2}\right)\right\} \quad (81)$$

one obtains

$$\mathbf{f}^{+S}(\bar{n}\hbar, \Theta) \approx g_0(\bar{n})[g_1(\Theta - \Theta_0) + (-1)^{2\bar{n}}g_1(\Theta - \Theta_0 - \pi)] \quad (82)$$

$$\mathbf{f}^{-S}(\bar{n}\hbar, \Theta) \approx g_0(\bar{n})[g_1(\Theta - \Theta_0 - \pi) + (-1)^{2\bar{n}}g_1(\Theta - \Theta_0)] \quad (83)$$

$$\mathbf{f}^{0S}(\bar{n}\hbar, \Theta) \approx \gamma(2\bar{n})(-1)^{\bar{n}}g_0(\bar{n})[g_1(\Theta - \Theta_0 - \pi/2) + g_1(\Theta - \Theta_0 + \pi/2)]. \quad (84)$$

For the projection operators  $\hat{F}^\pm$  non-vanishing profiles exist on all orbits  $\mathbf{l} = \bar{n}\hbar$ . On Bohr orbits ( $\bar{n}$  integer) they have identical peaks at  $\Theta = \Theta_0$  and  $\Theta = \Theta_0 + \pi$  which reach their maximum height at  $\bar{n} \approx \mathbf{l}_0/\hbar$ . On half-Bohr orbits ( $\bar{n}$  half-integer) the peaks at inverse positions in phase space have different signs. Therefore, if  $\mathbf{f}^{+S}$  is smeared out to form the function  $\mathbf{F}^{+S}$ , a bell shaped peak emerges near  $(\mathbf{l}_0, \Theta_0)$  while the oscillatory contributions around  $(\mathbf{l}_0, \Theta_0 + \pi)$  practically cancel each other. The resulting functions turn out to be good approximations of the corresponding  $W$ -Functions, i.e. each of the two projection operators is a semiclassical operator in the sense of (67). This property persists when they are added to form the density operator of a mixture of the two coherent states, but is lost when the operator  $\hat{F}^0$  is added. The function  $\mathbf{F}^{0S}$  obtained from the profiles (84) assumes its largest values near  $(\mathbf{l}_0, \Theta_0 \pm \pi/2)$  but these values change their sign when  $\mathbf{l}$  is increased by  $\hbar$ . Note that because of the factor  $\gamma(2\bar{n})$  smearing with the step functions (43) does not suffice to cancel these oscillations.

For the Weyl representatives one obtains from (16) and (12)

$$F^\pm(P, X) = 2 \exp \left\{ -\frac{1}{\hbar} [(P \mp P_0)^2 + (X \mp X_0)^2] \right\} \quad (85)$$

$$F^0(P, X) = 4 \exp \left\{ -\frac{1}{\hbar} [P^2 + X^2] \right\} \cos \left\{ -\frac{2}{\hbar} [P_0 X - P X_0] \right\}. \quad (86)$$

It is already clear at this point that the central oscillating part (86) has no counterpart in the  $S$ -function and that the oscillating parts of the latter, which are seen around  $(\mathbf{l}_0, \Theta_0 \pm \pi/2)$ , are missing in the  $W$ -function. When action and angle are used for variables and parameters the functions depending on  $\Theta - \Theta_0$  can be expanded according to [11]

$$\exp(a \cos \alpha) = \sum_M I_M(a) e^{iM\alpha} \quad \cos(b \sin \beta) = \sum_M J_{2M}(b) e^{2iM\beta}. \quad (87)$$

With  $\bar{n}_+ = \bar{n} + \frac{1}{2}$  this gives

$$F_{\delta n}^+(\bar{n}_+\hbar) = I_{\delta n}(4\sqrt{\bar{n}_+\hbar\mathbf{l}_0}) \exp\{-2\mathbf{l}_0/\hbar - 2\bar{n}_+ - i\delta n\Theta_0\} \quad (88)$$

$$F_{\delta n}^-(\bar{n}_+\hbar) = (-1)^{\delta n} F_{\delta n}^+(\bar{n}_+\hbar) \quad (89)$$

$$F_{\delta n}^0(\bar{n}_+\hbar) = \gamma(\delta n) 4J_{\delta n}(4\sqrt{\bar{n}_+\hbar\mathbf{l}_0}) \exp\{-2\bar{n}_+ - i\delta n\Theta_0\}. \quad (90)$$

For  $\mathbf{l}_0 \gg \hbar$  and  $\bar{n} \gg 1$

$$\begin{aligned} F^+(\bar{n}_+\hbar, \Theta) &= 2 \exp \left\{ -(\sqrt{2\bar{n}_+} - \sqrt{2\mathbf{l}_0/\hbar})^2 - 8\sqrt{\bar{n}_+\hbar\mathbf{l}_0} \sin^2 \left( \frac{\Theta - \Theta_0}{2} \right) \right\} \\ &\approx 2 \exp \left\{ -\frac{1}{2\bar{n}_+} (\bar{n}_+ - \mathbf{l}_0/\hbar)^2 \right\} (8\pi\bar{n}_+)^{-1/2} \sum_M \exp \left\{ -\frac{M^2}{8\bar{n}_+} + iM(\Theta - \Theta_0) \right\} \end{aligned} \quad (91)$$

and the normal distribution centred at  $\bar{n}_+ = \mathbf{l}_0/\hbar$  approaches the Poisson distribution  $g_0(\bar{n})$ , equation (81). Under these conditions (88) is a good approximation to (75) which shows that  $\hat{F}^+$  is semiclassical; the same holds for  $\hat{F}^-$  and for mixtures of the two coherent states. On the other hand, this does not hold for the operator (72) since (90) and (78) are quite different functions of the quantum numbers  $n'$  and  $n''$ .

These examples illustrate what was already evident from the general discussion, namely that the following three statements are equivalent. (i) The matrix elements of the operator are well approximated by (66) or (69). (ii) The  $W$ - and the  $S$ -representative of the operator are similar to each other (in the sense of square-integrable functions). (iii) The variables of the  $S$ -representative may be interpreted as classical action and angle variables.

### 5. Quantization of action and angle variables

The advantage of the  $S$ -formalism will become evident when the quantum evolution of the system is taken into account. Before we turn to this point let us briefly discuss how this formalism is related to a quantum theory that derives from a classical theory based on action and angle variables. As there exists a close connection of this theory with the motion of a point particle on the unit circle we discuss this problem first.

For this system the basic variables are the angle  $\Theta$  and the related angular momentum  $\mathbf{L}$ . The phase space is the cylinder

$$\mathcal{C}: \quad -\infty < \mathbf{L} < \infty \quad -\pi \leq \Theta \leq \pi. \quad (92)$$

Here too  $\mathbf{L}$ ,  $\Theta$  and  $\mathbf{L}$ ,  $\Theta + 2\pi$  are considered as the same physical state. It is sufficient to consider only Hamiltonians of the form  $\mathbf{H}(\mathbf{L}, \Theta) = \mathbf{H}(\mathbf{L})$  for which the angular momentum is a conserved quantity. The evolution is then a uniform motion along the circle  $\mathbf{L} = \text{constant}$ , which contains the initial state, the angular velocity being given by  $d\mathbf{H}(\mathbf{L})/d\mathbf{L} > 0$ . If all states with  $\mathbf{L} < 0$  are excluded and  $\mathbf{L}$  is interpreted as an action variable one recovers the classical mechanics of section 2.

One can quantize the system before the anti-clockwise motions are excluded. To this end one considers square integrable functions  $\langle \theta | \psi \rangle$  of the angular variable  $\theta \in (-\pi, \pi)$  (Hilbert space  $\mathcal{H}_{\text{circle}}$ ), and integral operators whose kernels  $\langle \theta' | \hat{F} | \theta'' \rangle$  are periodic functions in both arguments. A natural choice for the operators which replace the functions  $\mathbf{E}(\mathbf{L}, \Theta) = \exp\{i\Theta\}$  and  $\mathbf{L}(\mathbf{L}, \Theta) = \mathbf{L}$  is

$$\langle \theta' | \hat{E} | \theta'' \rangle = \exp\{i\theta'\} \delta^{(2\pi)}(\theta'' - \theta') \quad (93)$$

$$\langle \theta' | \hat{L} | \theta'' \rangle = i\hbar \delta'^{(2\pi)}(\theta'' - \theta') \quad (94)$$

where  $\delta^{(2\pi)}$  and  $\delta'^{(2\pi)}$  are the periodic continuations of the delta function and its derivative. These basic operators satisfy the commutation relations

$$[\hat{L}, \hat{E}^N] = N\hbar \hat{E}^N \quad (95)$$

for all integer values of  $N$ . When these operators are applied to the eigenfunctions of  $\hat{L}$ ,

$$\langle \theta | m \rangle = (2\pi)^{-1/2} e^{im\theta} \quad m \text{ integer} \quad (96)$$

one finds

$$\hat{L} | m \rangle = m\hbar | m \rangle \quad \hat{E}^M | m \rangle = | m + M \rangle. \quad (97)$$

To fix the operators related to functions  $\mathbf{F}(\mathbf{L}, \Theta)$ , whose Fourier components  $\mathbf{F}_M(\mathbf{L})$  are power series in  $\mathbf{L}$ , one has to supplement definitions (93) and (94) with an ordering rule, for example

$$\mathbf{L}^K \exp\{iM\Theta\} \rightarrow \frac{1}{2^K} \sum_N \binom{K}{N} \hat{L}^{K-N} \hat{E}^M \hat{L}^N = \left( \hat{L} - \frac{\hbar}{2} M \right)^K \hat{E}^M. \quad (98)$$

This is equivalent to the quantization rule

$$\langle m' | \hat{F}'' | m'' \rangle = \mathbf{F}_{m'-m''}((m' + m'')\hbar/2) \quad (99)$$

(cf (69)). There are several problems related to this quantization procedure. A minor one is that for a general square-integrable function  $\mathbf{F}_M(\mathbf{L})$  the value at positions  $\mathbf{L} = \bar{m}\hbar$  need not be defined. A more fundamental problem is that all functions which vanish on all circles  $\mathbf{L} = \bar{m}\hbar$  are mapped onto the null operator. As a consequence, (99) relates the two different exponentials  $\mathbf{F}_1(\mathbf{L}, \Theta) = \exp\{-(i/\hbar)\phi\mathbf{L}\}$  and  $\mathbf{F}_2(\mathbf{L}, \Theta) = \exp\{-(i/\hbar)(\phi + 2\pi)\mathbf{L}\}$  to the same unitary operator  $\hat{F} = \exp\{-(i/\hbar)\phi\hat{L}\}$ . In contrast to standard quantum mechanics,



where the relation between (Hilbert–Schmidt) operators and (square-integrable) phase space functions is one-to-one, we are faced here with a serious dequantization problem, which can be traced to the different topology of the configuration space, i.e. the boundary conditions imposed on the analytic wavefunctions.

This fact also becomes evident when one tries to adapt the Wigner–Weyl formalism to a quantum theory with periodic boundary conditions. Various attempts have been made in the past to reformulate quantum mechanics in a phase space language when the configuration space is a circle instead of the real line; for a critical survey see [14] (this paper also covers the case where the configuration space consists of  $N$  points, see also Hannay and Berry [15]). It is a common feature of all these schemes that the ‘phase space’, the domain of the functions which replace the operators, is not the cylinder (92) but a union of circles, for example

$$C' = \{(\bar{m}\hbar, \Theta) | \bar{m} = \dots, -\frac{1}{2}, 0, \frac{1}{2}, 1, \dots; -\pi \leq \Theta \leq \pi\}. \quad (100)$$

Note that in (100) the values assumed by the ‘momentum variable’ are not only the eigenvalues  $m\hbar$  of the momentum operator  $\hat{L}$ , but also the half-integer multiples of  $\hbar$  (for systems with finite configuration space this effect occurs also for the ‘position variable’ [14, 15]). It has been argued in [14] that the closest analogy to the usual Wigner–Weyl formalism is obtained when the phase space functions are related to the operators according to the rule

$$\begin{aligned} \mathbf{f}^S(\bar{m}\hbar, \Theta) &= \int_{-\pi}^{\pi} d\theta \exp\{i\bar{m}(2\Theta - 2\theta)\} \langle \theta | \hat{F} | 2\Theta - \theta \rangle \\ &= \sum_M \gamma(2\bar{m} + M) \exp\{iM\Theta\} \langle \bar{m} + \frac{1}{2}M | \hat{F} | \bar{m} - \frac{1}{2}M \rangle. \end{aligned} \quad (101)$$

It follows from this definition that the profiles (101) satisfy the symmetry relation (41) and that the matrix elements of  $\hat{F}$  are recovered from them according to

$$\mathbf{f}_M^S(\bar{m}\hbar) = \gamma(2\bar{m} + M) \langle \bar{m} + \frac{1}{2}M | \hat{F} | \bar{m} - \frac{1}{2}M \rangle \quad (102)$$

(cf (38)); the only difference to (38) and (41) is that  $\bar{m}$  can also assume negative values. The analogy to the  $S$ -formalism of section 3 can be further extended if the profiles (101) are smeared out and merged into a function defined on the classical phase space (92),

$$\mathbf{F}^S(\mathbf{L}, \Theta) = \sum_{\bar{m}} C_{\bar{m}\hbar}(\mathbf{L}) \mathbf{f}^S(\bar{m}\hbar, \Theta). \quad (103)$$

From this we obtain, in analogy to (53),  $h \langle \langle \hat{F}, \hat{G} \rangle \rangle = \langle \mathbf{F}^S, \mathbf{G}^S \rangle_2$  where the subscript 2 refers to the Hilbert space  $L^2(\mathcal{C})$ . As in section 4 this establishes an isomorphism between  $L_S^2(\mathcal{C})$ , a proper subspace of  $L^2(\mathcal{C})$ , and the Hilbert–Schmidt operators. However, it does not tell us how to quantize phase space functions which, like the ones usually met in classical physics, are not linear combinations of the functions

$$\mathbf{S}_{m', m''}(\mathbf{L}, \Theta) = C_{\bar{m}\hbar}(\mathbf{L}) \exp\{i\delta m \Theta\}. \quad (104)$$

One way to quantize these functions would be to ignore their components orthogonal to  $L_S^2(\mathcal{C})$ ,

$$\langle m' | \hat{F}' | m'' \rangle = \frac{1}{h} \langle \mathbf{S}_{m', m''}, \mathbf{F} \rangle_2 = \frac{1}{h} \int_{(m'+m''-1)\hbar/2}^{(m'+m''+1)\hbar/2} d\mathbf{L} \mathbf{F}_{m'-m''}(\mathbf{L}). \quad (105)$$

This quantization rule is qualitatively similar to rule (99), because it also eliminates in all classical functions those oscillations in  $\mathbf{L}$  which have a wavelength  $\hbar$  or less. But quantitatively there is a difference. Consider, for example, the functions  $\mathbf{F}_K(\mathbf{L}, \Theta) =$

$\mathbf{L}^K \exp(iM\Theta)$ . In both schemes they are mapped onto matrices, whose elements vanish everywhere except along the line  $m' = m'' + M$ . However, for  $m' + m'' = 2\bar{m}$  the non-vanishing element obtained according to (99) is  $\bar{m}^K \hbar^K$ , whereas it is  $(K + 1)^{-1}[(\bar{m} + \frac{1}{2})^{K+1} - (\bar{m} - \frac{1}{2})^{K+1}] \hbar^K$ , if quantization rule (105) is employed. The matrices obtained for the functions  $\mathbf{F}(\mathbf{L}, \Theta) = \mathbf{L}$  and  $\mathbf{F}_{\pm}(\mathbf{L}, \Theta) = \exp(\pm i\Theta)$  coincide in both quantization schemes, but the ordering rule analogous to (98) is

$$\mathbf{L}^K \exp\{iM\Theta\} \rightarrow \frac{1}{K+1} \left[ \left( \hat{L} - \frac{\hbar}{2}(M-1) \right)^{K+1} - \left( \hat{L} - \frac{\hbar}{2}(M+1) \right)^{K+1} \right] \hat{E}^M. \quad (106)$$

If both quantum numbers  $m'$  and  $m''$  are of order  $\hbar^{-1}$ , the difference between the matrix elements obtained from the two quantization rules is of order  $\hbar^2$ . Which of them is the ‘correct’ one and which the ‘semiclassical approximation’ is still a matter of convention.

If we want to proceed in analogy to the Weyl quantization/dequantization scheme and establish a one-to-one correspondence between Hilbert–Schmidt operators in the Hilbert space of square-integrable functions defined on the configuration space (here the interval  $(-\pi, +\pi)$ ) and square-integrable functions defined on the classical phase space (here the cylinder (92)), we have to choose

$$\mathbf{F}(\mathbf{L}, \Theta) = \sum_{m', m''} \langle m' | \hat{F}' | m'' \rangle \mathbf{S}_{m', m''}(\mathbf{L}, \Theta) \quad (107)$$

as the dequantization rule (mapping of operators onto functions) and (105) as the inverse quantization rule. Since the value of the Fourier components  $\mathbf{F}_M(\mathbf{L})$  of the functions (107) is well defined at all positions  $\mathbf{L} = \bar{m}\hbar$ , for which  $2\bar{m} + M$  is even, equation (99) may be considered as a formula which yields approximate matrix elements of the operator  $\hat{F}'$ , which is related to the function  $\mathbf{F} \in L^2_S(\mathcal{C})$  by (105). (The difficulty one would encounter when (99) is chosen as the quantization rule is that dequantization is ambiguous and the status of (105) unclear.)

Two more steps are needed to establish a relation with the discussion of the previous section. First we reduce the set of admissible operators and functions by postulating that

$$\langle m' | \hat{F}' | m'' \rangle = \frac{1}{\hbar} \langle \mathbf{S}_{m', m''}, \mathbf{F} \rangle_2 = 0 \quad \text{for } m' < 0 \text{ or/and } m'' < 0. \quad (108)$$

For functions  $\mathbf{F} \in L^2_S(\mathcal{C})$  this condition implies

$$\mathbf{F}_M(\mathbf{L}) = 0 \quad \text{for } \mathbf{L} < (|M| - 1)\hbar/2 \quad (109)$$

such that all phase space functions of interest vanish on the semicylinder  $\mathbf{L} < -\hbar/2$ . If we now introduce the variable

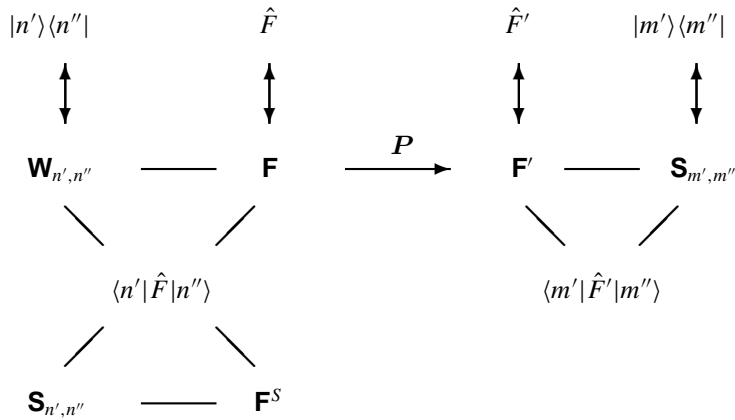
$$\mathbf{I} = \mathbf{L} + \frac{\hbar}{2} \quad (110)$$

instead of  $\mathbf{L}$  we see that all admissible phase space functions vanish for  $\mathbf{I} < 0$  and the space spanned by these functions becomes isomorphic to the space  $L^2_S(\mathcal{C}_+)$  considered in section 3.

The situation may now be summarized as follows: The naive quantization of functions of the classical action and angle variables according to equations (93)–(99) and (110) may be seen as an approximation to the quantization scheme given by (105) and (110). The central question is, whether the matrix assigned to the function by these equations is the same as (or at least similar to) the one, which is obtained according to the following route.  
 (i) Express  $\mathbf{I}$  and  $\Theta$  variables as functions of the original position and momentum variables.  
 (ii) Quantize the function of  $P$  and  $X$  obtained by this substitution of variables according

to the Weyl scheme. (iii) Solve the eigenvalue problem of the Hamilton operator  $\hat{H}$ , fix the phases of the eigenfunctions, and calculate the matrix elements.

The answer to this question can be deduced from the following diagram; here all functions are functions of the classical action and angle variables and symbols labelled by double indices represent sets of functions or the elements of a matrix. The operators on the left-hand side are operators in the usual Hilbert space  $\mathcal{H}_{\text{line}}$  (square-integrable functions of  $x \in (-\infty, +\infty)$ ), while those on the right-hand side are operators in the Hilbert space  $\mathcal{H}_{\text{circle}}$  (square-integrable functions of  $\theta \in (-\pi, +\pi)$ ):



On the left-hand side the one-to-one relation between the function  $\mathbf{F}$  and the operator  $\hat{F}$  is meant to be the Weyl correspondence. It requires explicit knowledge of the functions  $I(P, X)$  and  $\Theta(P, X)$  and evaluation of an integral of the form (16); information on the operator related to the classical Hamiltonian is not needed in this quantization procedure. The functions  $\mathbf{W}_{n',n''}(\mathbf{I}, \Theta)$  are obtained as follows. (i) The function  $H(P, X)$  has to be quantized according to the Weyl scheme. (ii) The eigenfunctions of the operator  $\hat{H}$  obtained in this way have to be determined in  $x$ -representation and their phases have to be fixed by some convention. (These two steps may be approximated by constructing proper WKB wavefunctions, see paper II.) (iii) These (approximate) eigenfunctions have then to be used in (16) to obtain (approximations to) the functions  $W_{n',n''}(P, X)$ . (iv) Finally, the variables  $P$  and  $X$  have to be substituted by  $\mathbf{P}(\mathbf{I}, \Theta)$  and  $\mathbf{X}(\mathbf{I}, \Theta)$ . If the functions  $\mathbf{W}_{n',n''}$  and the  $W$ -representative  $\mathbf{F}$  are known, the matrix elements  $\langle n'|\hat{F}|n''\rangle$  are obtained by integration (equation (48)). Likewise, if the matrix elements and the functions  $\mathbf{W}_{n',n''}$  are known,  $\mathbf{F}$  is determined by the sum (47). In principle this relation is convertible, i.e. if an infinite set of functions  $\mathbf{F}_i$  and the corresponding matrices are known, the functions  $\mathbf{W}_{n',n''}$  could be determined as solutions of linear equations of the form (47). Because any two sets fix the third one, no arrows were used to characterize the relation between general  $W$ -functions, the  $W$ -representatives of the operators  $|n'\rangle\langle n''|$ , and matrix elements. A similar triangular relation holds for  $S$ -representatives of general operators,  $S$ -representatives of the operators  $|n'\rangle\langle n''|$ , and matrix elements; the only difference is, that the functions  $\mathbf{S}_{n',n''}$  are not obtained through the solution of an eigenvalue problem, but are directly given by the defining equation (49) (see also (43)).

The projection operator  $\mathbf{P}$  in the centre of the diagram is the one introduced at the end of section 3 and  $\mathbf{F}' = \mathbf{P}\mathbf{F}$ . The 'smoothing'  $\mathbf{F} \rightarrow \mathbf{F}'$  assigns to each function  $\mathbf{F}$  of

the action and angle variable, another function with the same domain  $\mathcal{C}_+$ . With (110) this function becomes a function of  $\mathbf{L}, \Theta$  and by (109) its domain may be extended to the full cylinder  $\mathcal{C}$ . The scalar products of this function, also denoted by  $\mathbf{F}'$  for simplicity, with the functions  $\mathbf{S}_{m', m''}$  defined in (104) yield then a matrix with elements  $\langle m' | \hat{F}' | m'' \rangle$ ; these elements vanish when one of the two indices becomes negative. To each matrix of this form there corresponds an operator in the Hilbert space  $\mathcal{H}_{\text{circle}}$ . Its kernel follows from (107) and the fact, that the kernels of the operators  $|m'\rangle\langle m''|$  related to the functions  $\mathbf{S}_{m', m''}$  are given by

$$\langle \theta' | m' \rangle \langle m'' | \theta'' \rangle = \frac{1}{2\pi} e^{i(m'\theta' - m''\theta'')} \tag{111}$$

(cf (96)). Note that the relation between matrices of this special form, functions  $\mathbf{S}_{m', m''}$  with  $m', m'' \geq 0$ , and functions  $\mathbf{F}'$  is exactly the same as the triangular relation between the matrices with elements  $\langle n' | \hat{F}' | n'' \rangle$ , functions  $\mathbf{S}_{n', n''}$ , and functions  $\mathbf{F}^S$ . It is therefore evident, that the non-vanishing submatrix of  $\hat{F}'$  coincides with the energy representation of  $\hat{F}$  if, and only if,  $\mathbf{F}' = \mathbf{P}\mathbf{F} = \mathbf{F}^S$ . Since  $\|\mathbf{F}^S\| = \|\mathbf{F}\|$  by definition and  $\mathbf{P}$  is a projection operator, the necessary and sufficient condition for the coincidence of the two matrices is therefore  $\mathbf{F}^S = \mathbf{P}\mathbf{F} = \mathbf{F}$ .

So far, this is only a repetition of the definition of a strictly semiclassical operator. Additional insight can be gained from the comparison of quantization procedures in the first part of this section. If (i) the operator is (strictly) semiclassical; (ii) one is only interested in matrix elements for states of high energy; and (iii) one is ready to tolerate deviations from the true matrix elements which are small compared to their average magnitude, then these approximate elements can also be calculated by (a) quantizing the 'classical' function according to the substitution

$$\mathbf{F}(\mathbf{L}, \Theta) \rightarrow \mathbf{F}\left(-\frac{i}{\hbar} \left[ \frac{\partial}{\partial \theta} + \frac{1}{2} \right], \theta\right) \tag{112}$$

(b) adopting the ordering rule (98) and (c) using the exponentials (96) as eigenfunctions of the Hamilton operator. Up to the constant term in the definition of the action operator, which is a technical detail, this is exactly the semiclassical Hilbert space formalism introduced by Marcus [16] and later on applied to a number of physical problems. Its success indicates that there exist many operators of physical interest, which are 'semiclassical' in the sense of section 4. This is well illustrated by an example: let the system be the harmonic oscillator with classical Hamiltonian  $H(P, X) = (1/2)(P^2 + X^2) = I(P, X)$  and consider the function  $F(P, X) = (1/2)(X + iP)^2$ . Under Weyl quantization this function is mapped onto  $\hat{F} = \hat{A}^2$  where  $\hat{A}$  is the usual destruction operator. The only non-vanishing matrix elements are therefore of the form  $\langle n - 1 | \hat{F} | n + 1 \rangle$ ; they have modulus  $\hbar\sqrt{n(n+1)}$  and are real, if the standard phase convention is adapted for the oscillator eigenfunctions [9]. Quantization of the corresponding function in action and angle variables,  $\mathbf{F}(\mathbf{L}, \Theta) = \mathbf{l} \exp(-2i\Theta)$ , yields the same selection rules for the matrix elements and the non-vanishing elements are also real, if the eigenfunctions (96) with  $m' = n - 1, m'' = n + 1, n \geq 0$ , are used. Their magnitude is  $\hbar(n - \frac{1}{2})$  in Marcus' quantum theory (quantization rule (112) plus ordering rule (98)) and equal to  $\hbar(2/3)[(n + 1)^{3/2} - n^{3/2}]$  if (106) is used.

Examples like this exhibit quite clearly under which conditions a quantum theory based on the Hilbert space  $\mathcal{H}_{\text{circle}}$  may lead to similar results as the standard quantum mechanics based on  $\mathcal{H}_{\text{line}}$ . However, they do not reveal the fundamental difficulty in dequantizing the operators of  $\mathcal{H}_{\text{circle}}$  (or those of the subspace spanned by the functions (96) with  $m \geq 0$ ). This problem is related to the fact that, here too, two variables may be found, which label the elements of an operator basis in  $\mathcal{H}_{\text{circle}}$  [14]; however, contrary to what one is used

to from the Weyl formalism for  $\mathcal{H}_{\text{line}}$ , the ‘mock phase space’ spanned by these variables does not coincide with the classical phase space (cylinder or semicylinder) but only with a discrete subset thereof. This leaves an ambiguity, or freedom, when the domain of functions is extended; hence the physical meaning of these ‘classical’ functions has to be inferred from that of the related operators in  $\mathcal{H}_{\text{circle}}$ . The physical meaning of these operators is in turn determined by comparing their matrix representation with respect to the basis (96) with the energy representation of operators in  $\mathcal{H}_{\text{line}}$ : if the matrix of the operator  $\hat{F}$  in  $\mathcal{H}_{\text{line}}$  coincides with the matrix of the operator  $\hat{F}'_1$  in  $\mathcal{H}_{\text{circle}}$ , or the two are at least similar to each other, the meaning of  $\hat{F}$  is transferred to  $\hat{F}'_1$ . Finally, the physical meaning of the operator  $\hat{F}$  derives from the related  $W$ -representative. Physical interpretation therefore proceeds along the line  $F \rightarrow \hat{F} \rightarrow \hat{F}'_1 \rightarrow \mathbf{F}'_1$ ; this is compatible with the route  $F \rightarrow \mathbf{F} \rightarrow P\mathbf{F} = \mathbf{F}'$  if, and only if,  $\hat{F}$  is a semiclassical operator ( $\mathbf{F}'_1 = \mathbf{F}'$ ).

## 6. Evolution in time

As already stated, the advantage of using  $S$ -functions instead of  $W$ -functions only becomes evident when the quantum mechanical evolution of the system is considered. We first discuss how this evolution and two approximations to it are seen in the  $S$ -,  $W$ -, and  $QP$ -formalism. Next we consider the implications of the assumption that the Hamiltonian  $\hat{H}$  is a semiclassical operator, i.e. that the numbers  $\mathbf{H}([n + \frac{1}{2}]\hbar)$ ,  $n = 0, 1, 2, \dots$ , are good approximations to the true eigenvalues  $\langle n | \hat{H} | n \rangle = E(n)$ . Finally, we assume that not only the Hamiltonian but also the observable and the density operator are, at a given instant, semiclassical operators.

The evolution of the quantum system may be described either by a continuous change of the observables or by the corresponding change of the state symbol. In analogy to the classical evolution, equation (10), we choose the second option,

$$\langle n' | \hat{Z}_t | n'' \rangle = \langle n' | \hat{Z}_0 | n'' \rangle \exp\{-i\Phi(n', n'')t\} \quad (113)$$

$$\Phi(n', n'') = (1/\hbar)[E(n') - E(n'')] = \Omega(\bar{n}, \delta n). \quad (114)$$

The eigenvalues of  $\hat{H}$  are of interest only in a certain energy range which is fixed by the initial state  $\hat{Z}_0$ . If in this range the spectrum can be approximated by a slowly varying smooth function  $E(v)$  the phases of the exponentials in (113) become approximately

$$\Omega(\bar{n}, M) = (1/\hbar)[E(\bar{n} + M/2) - E(\bar{n} - M/2)] \approx (1/\hbar)E'(\bar{n})M. \quad (115)$$

In a cruder approximation

$$E(n) \approx E(n_0) + E'(n_0)(n - n_0) + \frac{1}{2}E''(n_0)(n - n_0)^2 \quad (116)$$

where the reference quantum number  $n_0$  is fixed by the average energy of the considered state, and

$$\Omega(\bar{n}, M) \approx (1/\hbar)[E'(n_0) + E''(n_0)(\bar{n} - n_0)]M. \quad (117)$$

Depending on the phase space formalism that is used, the function which represents the state of the system is

$$\begin{aligned} \mathbf{Z}^S(\mathbf{l}, \Theta) &= \sum_{\bar{n}} \mathbf{Z}_{\bar{n}}^S(\mathbf{l}, \Theta) \\ \mathbf{Z}_{\bar{n}}^S(\mathbf{l}, \Theta) &= \sum_{\delta n}^{(\bar{n})} \langle \bar{n} + \frac{1}{2}\delta n | \hat{Z} | \bar{n} - \frac{1}{2}\delta n \rangle \mathbf{S}_{\bar{n}+\delta n/2, \bar{n}-\delta n/2}(\mathbf{l}, \Theta) \\ \mathbf{Z}(\mathbf{l}, \Theta) &= \sum_{\bar{n}} \mathbf{Z}_{\bar{n}}(\mathbf{l}, \Theta) \end{aligned} \quad (118)$$

$$\mathbf{Z}_{\bar{n}}(\mathbf{l}, \Theta) = \sum_{\delta n}^{(\bar{n})} \langle \bar{n} + \frac{1}{2}\delta n | \hat{Z} | \bar{n} - \frac{1}{2}\delta n \rangle \mathbf{W}_{\bar{n}+\delta n/2, \bar{n}-\delta n/2}(\mathbf{l}, \Theta) \quad (119)$$

or

$$\begin{aligned} \mathbf{Z}^Q(\mathbf{l}, \Theta) &= \sum_{\bar{n}} \mathbf{Z}_{\bar{n}}^Q(\mathbf{l}, \Theta) \\ \mathbf{Z}_{\bar{n}}^Q(\mathbf{l}, \Theta) &= \sum_{\delta n}^{(\bar{n})} \langle \bar{n} + \frac{1}{2}\delta n | \hat{Z} | \bar{n} - \frac{1}{2}\delta n \rangle \mathbf{Q}_{\bar{n}+\delta n/2, \bar{n}-\delta n/2}(\mathbf{l}, \Theta) \end{aligned} \quad (120)$$

where

$$\mathbf{Q}_{n', n''}(\mathbf{l}, \Theta) = \langle \mathbf{l}, \Theta | n' \rangle \langle n'' | \mathbf{l}, \Theta \rangle. \quad (121)$$

As time proceeds each of the functions which represent the operators  $|n'\rangle\langle n''|$  is multiplied by a phase factor  $\exp\{-i\Phi(n', n'')t\}$ . Therefore, the real and imaginary parts of these functions behave like standing waves in phase space, each of which oscillates with its own characteristic frequency. The state function is a superposition of these waves with time-independent coefficients and its form at a given instant results from the interference of all these waves. The same holds for the constituents  $\mathbf{Z}_{\bar{n}, t}^S$ ,  $\mathbf{Z}_{\bar{n}, t}$ , and  $\mathbf{Z}_{\bar{n}, t}^Q$  which evolve independently of each other because of (34)–(36). Another consequence of this method of performing the double summation is that all three functions satisfy the symmetry relation  $\mathbf{F}_{\bar{n}}(\mathbf{l}, \Theta) = (-1)^{2\bar{n}} \mathbf{F}_{\bar{n}}(\mathbf{l}, \Theta + \pi)$ . When the phase factor is approximated according to (115) or (117) each of these functions evolves, either exactly or approximately, according to

$$\mathbf{F}_{\bar{n}, t}(\mathbf{l}, \Theta) = \mathbf{F}_{\bar{n}, 0}(\mathbf{l}, \Theta - \omega(\bar{n})t) \quad (122)$$

the angular frequency depending on the approximation employed

$$\omega_1(\bar{n}) = (1/\hbar)E'(\bar{n}) \quad \omega_2(\bar{n}) = (1/\hbar)[E'(n_0) + E''(n_0)(\bar{n} - n_0)]. \quad (123)$$

That for  $\mathbf{Z}_{\bar{n}, t}^S$  the evolution reduces to a translation in  $\Theta$  follows directly from the fact that the functions  $\mathbf{S}_{n', n''}$  are proportional to  $\exp\{i(n' - n'')\Theta\}$ . As is shown in paper II the same factor is found in the asymptotic form of  $\mathbf{Q}_{n', n''}$  valid for high quantum numbers  $n', n''$ . From this and the asymptotic form of the smoothing kernel (23), obtained in II for large values of  $H(P, X)$  and  $H(P', X')$ , it may be further concluded that  $\mathbf{W}_{n', n''}$  is also asymptotically proportional to  $\exp\{i(n' - n'')\Theta\}$ ; this result may also directly derived from (16) if WKB wavefunctions are used in the kernel  $\langle x' | n' \rangle \langle n'' | x'' \rangle = \psi_{n'}(x') \psi_{n''}(x'')^*$ . For the approximations (115) or (117) the evolution of all three functions,  $\mathbf{Z}_{\bar{n}, t}^S$ ,  $\mathbf{Z}_{\bar{n}, t}$ , and  $\mathbf{Z}_{\bar{n}, t}^Q$ , is therefore simply a ‘rotation’, the shift in  $\Theta$  depending on the average quantum number  $\bar{n}$ . The total state representative at a given instant is obtained by adding all contributions from the energetically relevant average quantum numbers  $\bar{n}$ . It is the interference of these contributions where the essential difference between the three schemes shows up. For the *S*-formalism the function  $\mathbf{Z}_{\bar{n}, t}^S$  interferes only with its nearest neighbours which both have a different parity; therefore, the interaction of these functions is easily perceived. For the *QP*-formalism the situation is similar since for large values of  $\bar{n}$  the  $\mathbf{l}$ -dependence of the function  $\mathbf{Z}_{\bar{n}, t}^Q$  can be approximated by a Gaussian centred at the orbit  $\mathbf{l} = \bar{n}\hbar$ . Put in a different way, these functions may be obtained by smoothing the functions  $\mathbf{Z}_{\bar{n}, t}^S$ , which are extremely localized in  $\mathbf{l}$ , with respect to this variable. The most complex interference patterns are seen in the *W*-formalism because each of the functions  $\mathbf{Z}_{\bar{n}, t}$ , which rotate with different angular velocities, has an oscillatory structure within the region  $\mathbf{l} < \bar{n}\hbar$ , and  $\mathbf{Z}$  is obtained as superposition of a large number of rapidly oscillating functions. This is just another way of seeing the inherent complexity of the evolution of Wigner functions; if the quantum Liouville equation [3] is used to describe it, it is the partial derivatives of high

order which transform an initially smooth function within short time into a function with rich oscillatory structure.

It is clear from these considerations that the most transparent picture of the evolution related to the approximations (115) or (117) is obtained when the profiles

$$\mathbf{z}_t^S(\bar{n}\hbar, \Theta) = \mathbf{z}_0^S(\bar{n}\hbar, \Theta - \omega(\bar{n})t) \quad (124)$$

are considered. These functions, forming the skeleton of the functions  $\mathbf{z}_n^S$  and  $\mathbf{z}_n^Q$ , contain all the information about the state at time  $t$  but do not interfere with each other since they are strictly bounded to the corresponding Bohr or half-Bohr orbits.

The difference between the two approximations (115) and (117) is seen at time

$$T_0 = h/E''(n_0) \quad (125)$$

and multiples thereof. It follows from (124) and (125), the symmetry relation (41), and  $(2\bar{n})^2 - 2\bar{n} = 2\bar{n}(2\bar{n} - 1) \equiv 0 \pmod{2}$ , that

$$\mathbf{z}_{T_0}^S(\bar{n}\hbar, \Theta) = \mathbf{z}_0^S(\bar{n}\hbar, \Theta - \Theta_0 - 2\bar{n}\pi) = \mathbf{z}_0^S(\bar{n}\hbar, \Theta - \Theta_0 - \pi) \quad (126)$$

if approximation (117) is employed. In this case all profiles and hence the original state is completely restored after a period  $T_0$ , except for a shift in  $\Theta$  by an amount  $\Theta_0 + \pi$ ,  $\Theta_0 = 2\pi E'(n_0)/E''(n_0)$ ; these ‘full revivals’ of the original state are seen at all integer multiples of  $T_0$ . At rational multiples of  $T_0$  ‘fractional revivals’ can be observed where adjacent profiles are shifted against each other by rational multiples of  $\pi$ , thereby forming superpositions of several copies of the original state which are shifted against each other along the classical orbit  $\mathbf{l} = n_0\hbar$  and are equidistant in  $\Theta$ . This effect was first explained within standard quantum mechanics by Averbukh and Perelman [17]; an explanation in terms of the smoothed profiles  $\mathbf{z}_n^Q$  was given in [18]. If the more accurate approximation (115) is used instead of (117) fractional and full revivals are still seen in the expectation values but no longer occur in perfect form; with increasing time they are more and more blurred by effects which have their origin in the neglected higher-order terms of the Taylor expansion (116). After a while the origin of the pattern, according to which amplitude and frequency of an oscillating expectation value change in time, can no longer be recognized. The period, where time-dependent expectation values are in excellent agreement with the exact result, is by far longer if approximation (115) is used instead of (117); however, this approximation is also bound to fail in the long run when the higher-order terms neglected in (115) become important. For these extremely long time intervals the exact frequencies (114) have to be used for each term that contributes to a profile.

If  $\hat{H}$  is a semiclassical operator, then

$$\begin{aligned} E(n) &= \langle n | \hat{H} | n \rangle \\ &\approx \frac{1}{\hbar} \int_{n\hbar}^{(n+1)\hbar} d\mathbf{l} \mathbf{H}(\mathbf{l}) \end{aligned} \quad (127)$$

$$\approx \mathbf{H}([n + \frac{1}{2}]\hbar) \quad (128)$$

where (127) expresses what the term ‘semiclassical’ means for the Hamiltonian and (128) is the Maslov quantization condition. For both conditions to be essentially equivalent, the derivatives  $d^k \mathbf{H}(\mathbf{l})/d\mathbf{l}^k$ ,  $k = 2, 3, 4, \dots$ , have to be small compared to the values  $\mathbf{H}(\mathbf{l})$  in the energy range under consideration. If (128) is a good approximation at high energies, as it is generally believed, one could think of shifting the integration range in (127) by a small amount such that agreement between (128) and (127) becomes optimal in the considered energy range. Such a shift would imply a slightly different definition of the step functions  $\mathbf{C}_y(x)$ , equation (43), and hence of the  $S$ -representatives of the operators. These

are technical details which can become of interest in explicit calculations of expectation values, but as they do not affect the general line of our arguments we do not pursue this point here.

Accepting the function  $\mathbf{H}([\nu + \frac{1}{2}]\hbar)$  as the function  $E(\nu)$  whose values at the points  $\nu = n$  approximate the eigenvalues  $E(n)$  we have

$$\omega_1(\bar{n}) \approx \omega([\bar{n} + \frac{1}{2}]\hbar) \quad (129)$$

and

$$\omega_2(\bar{n}) \approx \omega(\mathbf{l}_0) + \omega'(\mathbf{l}_0)([\bar{n} + \frac{1}{2}]\hbar - \mathbf{l}_0) \quad (130)$$

where  $\omega(\mathbf{l})$  is the classical angular velocity (10) and  $\mathbf{l}_0 = (n_0 + \frac{1}{2})\hbar$ . If in the relevant range of the action

$$(\hbar/2)|\omega'(\mathbf{l})| \ll \omega(\mathbf{l}) \quad (131)$$

(as is the case for anharmonic oscillators at sufficiently high energies) then (129) may be replaced by the classical angular velocity along the (half-)Bohr orbit  $\mathbf{l} = \bar{n}\hbar$  and (130) becomes the corresponding classical velocity, when the Hamiltonian  $\mathbf{H}(\mathbf{l})$  is approximated by a polynomial of second order. The evolution of profiles is then determined by classical mechanics, except that the Hamiltonian flow is restricted to a discrete set of orbits and the functions transported along these orbits have non-classical symmetry properties. If the considered time interval is so short that the relative shift of adjacent profiles  $\mathbf{z}_t^S(\bar{n}\hbar, \Theta)$  remains very small for all  $t \in (0, T)$ , the interference of the smeared out profiles  $\mathbf{z}_{\bar{n},t}^S(\mathbf{l}, \Theta)$  results in functions of similar form. The evolution is then seen in a shift of the minima and maxima of the original function  $\mathbf{z}_0^S$  and a distortion in the neighbourhood of these extrema; this is in agreement with the classical evolution of  $\mathbf{z}_0^S$ , no matter whether or not this function admits a classical interpretation. The same holds for the related Husimi function  $\mathbf{z}_0^Q$ , which is non-negative by construction, and seems to evolve within the short time interval  $(0, T)$  according to the classical Liouville equation. This is also true for the the Wigner function  $\mathbf{z}_0$ , but in general only for a much shorter time interval after which already existing rapidly oscillating parts of  $\mathbf{z}_0$  decay and new ones emerge.

Finally, let us assume that not only the Hamilton operator is a semiclassical operator but so are the observable  $\hat{A}$  and the density operator  $\hat{Z}_t$  at a certain instant  $t_0$ ; this instant may be chosen as a reference value for the evolution ( $t_0 = 0$ ). Regardless of whether the corresponding  $W$ -functions admit a classical interpretation (as, e.g. the Wigner function of a coherent state) or not (as the Wigner function of a cat state) the definition of semiclassical operators implies that the two  $W$ -functions may be interpreted as  $S$ -functions. The evolution of the expectation value may then be calculated in the  $S$ -formalism, i.e. it can be deduced from the evolution of the profiles contained in  $\mathbf{z}_0^S \approx \mathbf{z}_0$  (cf equations (36)–(42)),

$$\mathbf{z}_0^S(\bar{n}\hbar, \Theta) \approx \frac{1}{2}[\mathbf{z}_0(\bar{n}\hbar, \Theta) + (-1)^{2\bar{n}}\mathbf{z}_0(\bar{n}\hbar, \Theta + \pi)]. \quad (132)$$

These profiles are then propagated according to classical mechanics. To calculate the expectation value for the propagated profiles one can either reconstruct the function  $\mathbf{z}_t^S$  by means of (42) or calculate the profiles  $\mathbf{a}^S(\bar{n}\hbar, \Theta)$  from  $\mathbf{A}(\mathbf{l}, \Theta)$  analogous to (132). If  $\mathbf{A}$  and  $\mathbf{z}_0$  admit a classical interpretation all ingredients of this approximation stem from classical mechanics, except for the magnitude of  $\hbar$  which fixes the set of classical orbits to which the Hamiltonian flow is restricted. Examples of time-dependent expectation values calculated in this way were presented in [19] and compared to their exact quantum evolution. Excellent agreement was found over time intervals of length  $T \approx 2T_0$ , during which two (imperfect) full revivals of the initial coherent state and several (increasingly imperfect) fractional ones could be clearly recognized.



We close this section with a warning: the approximation described above will yield good results only if both the observable and the density operator are semiclassical. It is not sufficient if only one of them has this property at a given instant. If, for example, the initial Wigner function  $\mathbf{Z}_0$  is a semiclassical phase space function, then  $\mathbf{Z}_0 \approx \mathbf{Z}_0^S = P\mathbf{Z}_0^S$  and  $\mathbf{A}$ , the  $W$ -representative of the observable, could be replaced by its projection  $P\mathbf{A}$  without changing the magnitude of the expectation value. In other words, the rapid oscillations of  $\mathbf{A}$ , which would be smoothed by the projection  $P$ , do not contribute to the expectation value. However, this holds only for  $t = 0$  if the observable is not semiclassical ( $\mathbf{A} \not\approx \mathbf{A}^S = P\mathbf{A}^S$ ). Even if  $\mathbf{Z}_t \approx \mathbf{Z}_t^S$  at  $t = 0$ , the functions  $\mathbf{Z}_t$  and  $\mathbf{Z}_t^S$  will strongly deviate from each other after a short time, as can be seen from the evolution of a coherent state in an anharmonic potential, and there is therefore no more reason to consider  $P\mathbf{A}$  as  $S$ -representative of the observable.

## 7. Conclusions

In sections 3 and 6 of this paper we presented a scheme of how to calculate time-dependent quantum mechanical expectation values from phase space functions, which are either classical functions or can be obtained from the matrices of the operators in energy representation. In the first case Planck's constant is the only quantum mechanical ingredient of the scheme, all other objects deriving from classical (statistical) mechanics. The evolution in time depends on the employed approximation of the spectrum of the Hamiltonian, but is in any case non-classical and leads to well known interference effects (e.g. revivals). The scheme covers part of a full quantum mechanical description of classically periodic motion in one dimension and is based on several approximations, which are not related and can be employed independently of each other (the approximation of the spectrum of the Hamiltonian, approximations of matrix elements of the observable and the density operator).

The starting point is the so-called  $S$ -formalism introduced in section 3. This is a new phase space reformulation of quantum mechanics, which is similar to the Wigner–Weyl formalism but makes use of ‘action’ and ‘angle’ variables instead of the usual momentum and position variables. In fact the two variables, which constitute the mock phase space in the  $S$ -formalism, can be identified with the action and angle variables of classical mechanics only if the set of considered operators is sufficiently restricted (‘semiclassical operators’). For operators not belonging to this set the similarity of the general form of the expectation values in the  $S$ -formalism and in classical statistical mechanics is purely formal and there is no obvious relation between the phase space functions representing the same physical objects (observables, states) in the two theories. The necessary and sufficient condition that the  $S$ -symbol of an operator has to satisfy, such that it admits a classical interpretation, is that the function is similar to (or even coincides with) the corresponding Weyl representative, when the latter is expressed in terms of the classical action and angle variables. This is equivalent to the postulate that the matrix elements of the related operator in energy representation, where rows and columns refer to the eigenstates of the Hamiltonian, are well approximated by formula (66). In this relation each matrix element is identified with one of the Fourier components of the  $W$ -function, averaged in the action variable over an interval of width  $\hbar$ , which is centred at a position given by the average of the two quantum numbers. A very similar formula, equation (69), is often used in semiclassical calculations to obtain approximate matrix elements. It is pointed out that this relation, the so-called ‘Heisenberg correspondence principle’, is not valid in general and can give qualitatively wrong results even at high energies where equation (69) is believed to be asymptotically correct for all operators (see, e.g., [4]). To illustrate this point we discussed in section 4 two examples

where (69) fails to give a meaningful result. It is also emphasized that both (66) and (69) imply a phase convention for the eigenfunctions of the Hamiltonian, a problem which is solved in paper II of this series.

In section 5 we discussed how the Heisenberg correspondence principle and the  $S$ -formalism is related to the following approach. First the classical problem is reformulated in terms of action and angle variables and then the new dynamical system is quantized in a naive way, where the action variable is treated like an angular momentum conjugate to the angle and anti-clockwise rotations are excluded after quantization. Formulated as Hilbert space formalism this quantum theory was first introduced by Marcus [16] and is now a well established semiclassical approximation. The corresponding phase space formalism, the  $S$ -formalism of the present paper with the variables interpreted as classical action and angle, seems to be hardly known although it has been used implicitly in the past in several specific examples (see [14] for references). Our approach is similar in spirit to the phase space formalism introduced by Berman and Kolovsky [20, 21] but it has to be emphasized that none of the functions introduced there corresponds to any of the functions defined in this paper. This is most easily seen from the fact that their phase space is of the form  $\{0, \hbar, 2\hbar, \dots\} \times (-\pi, +\pi)$ ; in addition, their phase space functions do not satisfy the symmetry relation (41). The lack of these non-classical constraints on the phase space functions in [21] is related to the absence of half-Bohr orbits in their formalism; in the  $S$ -formalism both these features are a consequence of the algorithm used to calculate the trace of the product of two matrices (see section 3).

The considerations of sections 4 and 5 may also be seen as a contribution to a discussion started by Dirac 70 years ago [22]. It is centred around the following questions: (i) Which of the many canonically equivalent forms of classical mechanics should be quantized to obtain the ‘true’ quantum mechanics? (ii) What are the ‘right’ quantization rules for a given set of canonically conjugate classical variables? (iii) What is the counterpart of a nonlinear canonical transformation in quantum mechanics?

For the harmonic oscillator, in particular, these questions have been extensively discussed in the past, see [23–26] and the references therein. One reason for studying this system is the fact that harmonic oscillators allow for an exact treatment, both in classical and in quantum mechanics; another reason is the importance of these systems in quantum optics. The problem of which operator  $\hat{F}$  in  $\mathcal{H}_{\text{line}}$  should be assigned to a given phase space function  $\mathbf{F}(\mathbf{l}, \Theta)$ , has been recently discussed at length and with full mathematical rigor in [25, 26] for a number of examples. Since the Hilbert space is the usual one and the function  $F(P, X)$  can be explicitly obtained from  $\mathbf{F}(\mathbf{l}, \Theta)$ , the only question left is which ordering scheme one should use in the series expansion of  $F(P, X)$ . Royer [26] studied functions with the asymptotic behaviour

$$\mathbf{F}(\mathbf{l}, \Theta) \rightarrow \mathbf{f}(\Theta) \quad \text{for } \mathbf{l} \rightarrow \infty \quad \hbar = \text{constant} \quad (133)$$

i.e. functions whose variation in  $\mathbf{l}$  becomes negligible for high energies  $\mathbf{H} = \mathbf{l}$ . Using the explicit form of the overlap integrals  $\langle \mathbf{l}, \Theta | \mathbf{l}', \Theta' \rangle$ , equation (13) with  $P = -\sqrt{2\mathbf{l}} \sin \Theta$ ,  $X = \sqrt{2\mathbf{l}} \cos \Theta$ , and  $\langle n | \mathbf{l}, \Theta \rangle$  he was able to show that the expectation values of an operator related to (133) for a coherent state  $|\mathbf{l}, \Theta\rangle$  approaches  $\mathbf{f}(\Theta)$  for  $\mathbf{l} \rightarrow \infty$ , no matter which ordering rule is used in the definition of  $\hat{F}$ . He also showed that  $\langle n' | \hat{F} | n'' \rangle \rightarrow \mathbf{f}_{n'-n''}$  for  $\bar{n} \rightarrow \infty, \delta n = \text{constant}$ , when the function  $\mathbf{F}(\mathbf{l}, \Theta)$  in (133) is the Weyl symbol of the operator. This means that  $W$ -functions with asymptotic behaviour (133) are semiclassical. These are asymptotic results; for large but finite energies the difference in the operators resulting from different ordering rules can be seen in matrix elements and expectation values, which should give rise to experimentally observable effects [25].

Ordering problems in the quantization of functions  $\mathbf{F}(\mathbf{I}, \Theta)$  with  $\mathbf{I} = \frac{1}{2}(P^2 + X^2)$ ,  $\Theta = \arctan(-P/X)$ , when the Hilbert space is  $\mathcal{H}_{\text{line}}$ , are also of interest in a different context. Classical systems which exhibit soft chaos can be approximated by integrable systems, if the energy is well below a critical value. The construction of approximate Hamiltonians, known as Birkhoff–Gustavson normal forms, makes use of action and angle coordinates of a many-dimensional harmonic oscillator, which is related to an approximation of the original Hamiltonian in the neighbourhood of a stable point (potential minimum). Every Birkhoff–Gustavson normal form is a function of the form  $\mathbf{F}(\mathbf{I}_1, \mathbf{I}_2, \dots, \Theta_1, \Theta_2, \dots)$  where the indices refer to the degrees of the oscillator. One can express the action and angle coordinates of the normal form according to  $\mathbf{I}_i = \frac{1}{2}(P_i^2 + X_i^2)$ ,  $\Theta_i = \arctan(-P_i/X_i)$ , map the new function by Weyl’s quantization rule onto an operator in  $\mathcal{H} = \mathcal{H}_{\text{line}} \otimes \mathcal{H}_{\text{line}} \otimes \dots$ , and solve the eigenvalue problem of this operator, hoping to get by this procedure an approximation of the spectrum of the original Hamiltonian (in the relevant energy region). However, the first two steps (change of variables, Weyl ordering of terms) become extremely tedious when normal forms of higher order are considered. For this reason Robnik [27] proposed an alternative (‘algebraic’) quantization scheme which differs from Weyl’s in the ordering rules (but not in the Hilbert space) and makes use of the action and angle coordinates of the oscillators. When the normal form is mapped onto an operator in  $\mathcal{H}_{\text{circle}} \otimes \mathcal{H}_{\text{circle}} \otimes \dots$ , a possibility briefly mentioned in [28], one would face similar ordering problems, as can be seen from the discussion in section 5. (we note in passing that for the non-resonant case Robnik’s rule coincides with the quantization rule defined by (110) and (99)). From section 5 one might conjecture that a change of the underlying Hilbert space and/or the employed ordering rules has little effect on the form of the spectrum at high energies (see also [27, 28]). However, small differences of the spectra at high energies are of little interest here, because the normal form approximates the original Hamiltonian only at low energies.

In [27] eigenvalues obtained by Robnik’s algebraic quantization were compared to the eigenvalues of the Hamilton operator  $\hat{H}^0$ , related to the original classical Hamiltonian  $H^0(P_i^0, X_i^0)$  by the Weyl correspondence. Approximate eigenvalues of this system, either obtained by second-order perturbation theory or by numerical diagonalization, were found to be in excellent agreement with those obtained from Robnik’s scheme. This is a remarkable result, not only because of the ordering problems mentioned above, but even more for the following fact: the momentum and position variables related to the action and angle variables of the normal form by  $P_i = -\sqrt{2\mathbf{I}_i} \sin \Theta_i$ ,  $X_i = \sqrt{2\mathbf{I}_i} \cos \Theta_i$  are not identical to the corresponding variables  $P_i^0$ ,  $X_i^0$  occurring in the original Hamiltonian, but related to them by a nonlinear canonical transformation. In contrast to linear canonical transformations, a nonlinear one cannot be represented by a unitary operator in the original Hilbert space  $\mathcal{H}^0 = \mathcal{H}_{\text{line}} \otimes \mathcal{H}_{\text{line}} \otimes \dots$ , hence the Hilbert space used in the (Weyl or algebraic) quantization of the normal form is only isomorphic to the original one but not identical (the same oscillator eigenfunction has a different physical meaning in the two spaces). The agreement of eigenvalues found in [27] shows that the original Hamiltonian is obviously ‘robust’ in the following sense: whether it is directly quantized (in the standard way) or after a nonlinear canonical transformation (in the same or a similar way) has hardly an influence on the eigenvalues. This property is analogous to the notion ‘semiclassical’ introduced in the present paper to characterize a certain set of phase space functions: whether the matrix elements in energy representation of the Weyl-related operators are calculated directly, or are derived from a (nonlinear) canonical transformation to action and angle variables ( $F(P, X) = \mathbf{F}(\mathbf{I}, \Theta)$ ) followed by a quantization scheme appropriate to these variables (section 5), does not make much difference (at high energies).

If one is interested in properties of this sort one has to restrict both the set of phase space functions, which make sense in classical mechanics, and the set of operators, which satisfy the formal rules for observables and density operators in quantum mechanics. The condition imposed on the two sets is that the mapping ‘dequantization followed by a change of variables induced by a nonlinear canonical transformation’ yields essentially the same phase space function as a mapping of the form ‘isometric transformation followed by dequantization’. For further information on the relation between unitary (isometric) transformations in quantum mechanics and canonical transformations in classical mechanics we refer the reader to [29–31]. For the case discussed in this paper the first dequantization rule is that of Weyl, while the second dequantization rule is given by equation (107); the nonlinear canonical transformation is the mapping  $P, X \rightarrow \mathbf{l}, \Theta$ , which depends on the Hamiltonian at hand. The isometry maps an operator in  $\mathcal{H}_{\text{line}}$  onto an operator in  $\mathcal{H}_{\text{circle}}$  in such a way that the energy representation of the first operator coincides with the matrix representation of the second operator with respect to the exponentials (96) with  $m \geq 0$ , all other elements of this operator being equal to zero. Both the general constraints semiclassical operators have to satisfy, and the examples studied in section 4 indicate that their energy representations have to be essentially banded (i.e.  $\langle n' | \hat{F} | n'' \rangle$  becomes negligibly small when  $|\delta n|$  exceeds a certain value) and slowly varying along the diagonal. Note that the first condition is satisfied if the  $W$ -function is analytical in  $P$  and  $X$ ; this ensures analyticity of  $\mathbf{F}(\mathbf{l}, \Theta)$  and hence rapid decay of the Fourier components  $\mathbf{F}_M(\mathbf{l})$  [4]. The assumed analyticity does not imply slow variation in  $\mathbf{l}$  and hence, by the Heisenberg principle, in the average quantum number. If mentioned at all, the required form of the matrices is taken for granted for all operators of physical interest (see [7] or the introduction of [4]) but this need not be the case as the examples of section 4 show. For the phase space functions representing the operators in the  $W$ - or the  $S$ -formalism the corresponding requirement is that they are slowly varying functions of both variables.

The question of whether a given observable or density operator is semiclassical, in the sense of section 4, has practical consequences when it comes to the calculation of time-dependent expectation values. If both operators are semiclassical, it is possible to identify their  $W$ -representatives (which in many cases have an obvious physical meaning) with the almost identical  $S$ -representatives and to consider the evolution of these objects. It is at this point where the importance of the profiles, which form the skeleton of the  $S$ -formalism, becomes evident. These profiles are functions of the angle variable, each of them being assigned to a Bohr orbit ( $\mathbf{l} = \bar{n}\hbar$ ,  $\bar{n}$  integer) or a half-Bohr orbit ( $\mathbf{l} = \bar{n}\hbar$ ,  $\bar{n}$  half-integer). The set of profiles, which can be merged into a single function defined on the classical phase space, contains the full information on the operator in question. For the density operator the evolution in time is therefore given by that of the corresponding profiles which, due to their definition, evolve independently of each other. If no approximation is made, each profile evolves similar to a wave in a dispersive medium: each of the oscillating functions in the angular variable which contributes to the considered profile, propagates in a clockwise direction with a characteristic angular velocity and the change of the profile in time results from the interference of these propagating waves. If the eigenvalues of the Hamiltonian vary slowly with the quantum number, at least in the range of energy fixed by the initial state, the characteristic angular velocities of the propagating waves become proportional to the number of their nodes. The evolution of the profile is then similar to that of a wave in a non-dispersive medium, i.e. a mere translation along the classical orbit which carries the profile. If the Hamiltonian is a semiclassical operator, as is usually assumed in literature, approximate eigenvalues can be obtained from the classical Hamiltonian and the translation of a profile may be considered as being induced by the Hamiltonian flow

along the corresponding orbit. Seen from classical mechanics, this semiclassical scheme is obtained by (i) a modification of the dynamics given by the classical Hamiltonian and (ii) modifications of phase space functions caused by the symmetry properties of the profiles.

The most localized profiles which are shifted along (half-)Bohr orbits as time proceeds, are the functions

$$\delta_{\bar{n}, \Theta}^S(\bar{n}'\hbar, \Theta') = \delta_{\bar{n}, \bar{n}'} \delta_{\bar{n}}^S(\Theta - \Theta') \quad (134)$$

$$\begin{aligned} \delta_{\bar{n}}^S(\Theta - \Theta') &= \frac{1}{2} [s(2\bar{n}, \Theta - \Theta') + (-1)^{2\bar{n}} s(2\bar{n}, \Theta - \Theta' - \pi)] \\ s(N, \theta) &= \frac{\sin(2N + 1)(\theta/2)}{\sin(\theta/2)} \end{aligned} \quad (135)$$

which correspond to the operators

$$\hat{\Delta}_{\bar{n}, \Theta} = \sum_{M=-2\bar{n}}^{2\bar{n}} \gamma(2\bar{n} + M) e^{-iM\Theta} |\bar{n} + \frac{1}{2}M\rangle \langle \bar{n} - \frac{1}{2}M|. \quad (136)$$

Since the identity

$$\mathbf{f}^S(\bar{n}\hbar, \Theta) = \frac{1}{2\pi} \int d\Theta' \mathbf{f}^S(\bar{n}\hbar, \Theta') \delta_{\bar{n}, \Theta}^S(\bar{n}, \Theta') \quad (137)$$

is valid for any profile  $\mathbf{f}^S$ , the translation in time may be transferred from the profiles  $\mathbf{f}^S$  to the functions (134). This enhances the similarity with classical mechanics where every phase space function may be represented as superposition of delta functions. When time proceeds these delta spikes move along the classical trajectories in accordance with Hamilton's equation of motion. However, this analogy is limited. First, the operators (136) are not positive and therefore do not represent quantum states, whereas the delta functions of classical mechanics represent states of the system. Second, the functions (134) are not single spikes but twin peaks located at inverse points in phase space, both of them positive if  $\bar{n}$  is integer and of opposite sign if  $\bar{n}$  is half-integer. These features are always present, no matter how small Planck's constant may be. They also persist when the profiles are thickened by multiplication with step functions defined on the classical phase space and sets of profiles are merged into a single function (equations (42) and (43)). They are also seen in a  $PQ$ -formalism where the  $Q$ -representatives of the operators (136) consist of two peaks at inverse points in phase space, each of them having half the diameter of the  $Q$ -representative of a coherent state.

To explain the quantum evolution of distribution functions and expectation values by studying the classical motion of localized objects is an idea that has been considered before by several authors. Based on heuristic ideas developed by Heller [32], Takahashi and Shudo [33] introduced an ensemble of weighted delta functions moving along Bohr orbits and used it to approximate the quantum evolution of the Husimi function and to calculate from it the expectation values  $\langle \hat{X} \rangle$  and  $\langle \hat{X}^2 \rangle$ . The considered system was a quartic oscillator and the initial state a coherent state; note that in this example the Hamiltonian  $\hat{H}$ , the density operator  $\hat{Z}_{t=0}$ , and the observables  $\hat{X}$  and  $\hat{X}^2$  are all semiclassical operators. Excellent agreement between the expectation values obtained from their classical ensemble and those obtained from a full quantum mechanical treatment was found in [33], but this does not imply that half-Bohr orbits and twin peaks are redundant. In contrast, as was already noticed by Nauenberg *et al* [34], a theory which makes only use of delta spikes on Bohr orbits yields the correct revival time for a wavepacket (cf equation (125) and the following discussion) but this revival occurs at a position in phase space which is inverse to the one predicted by quantum theory. The difference between the present theory and the classical analogues discussed in [33, 34] shows up in all fractional revivals of odd order where discrepancies in

the location in phase space and related small shifts in the time dependence of expectation values are observed. The inclusion of half-Bohr orbits and implementation of the proper symmetry properties of the profiles (twin peaks instead of delta spikes) removes these flaws and puts the ‘classical’ calculation of time-dependent quantum mechanical expectation values on a better theoretical grounding.

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