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# Semiclassical mechanics in one dimension: II. Approximate matrix elements

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**Abstract.** The semiclassical formula for matrix elements, sometimes called the Heisenberg correspondence principle, relates matrix elements (operators in energy representation) to phase space functions (Weyl representatives). The formula does not make sense for arbitrary operators; when it is valid it implicitly fixes the relative phases of the eigenfunctions of the Hamiltonian. The conventions, which have to be used for the wavefunctions in position or momentum representation, are given here in explicit form, and we present a class of operators related to coherent states of high energy for which the Heisenberg correspondence principle holds.

## 1. Introduction

In the preceding paper (henceforth referred to as paper I) a scheme was presented which allows one to calculate time-dependent quantum mechanical expectation values by methods borrowed from classical mechanics (action and angle variables, Hamiltonian flow). Two independent approximations were employed. In the first, the quantum frequencies associated with matrix elements in the energy representation are replaced by quantities derived from a classical Hamiltonian. This approximation is unavoidable if one wants to reformulate quantum dynamics in a form where the Hamiltonian flow of classical mechanics is still visible on a set of selected classical orbits. In the second approximation, the matrix elements of the density operator and/or the observable are related to classical phase space functions (more precisely, to the Weyl representatives of these operators). Such a relation is needed to obtain the matrices of these operators in energy representation without having to calculate the eigenfunctions of the Hamiltonian first; this matrix representation is of interest because it is the one where the time dependence of the density operator assumes its simplest form.

In both approximations the validity of the semiclassical formula for matrix elements is taken for granted. In the notation of paper I this formula reads as follows

$$\begin{aligned} &\langle n'|\hat{F}|n''\rangle \approx \mathsf{F}_{\delta n}(\bar{n}_+\bar{h}) \\ &\delta n = n' - n'' \qquad \bar{n}_+ = \tfrac{1}{2}(n' + n'' + 1). \end{aligned} \tag{1}$$

Here $\hat{F}$ is the operator in question, $|\, n\, \rangle$ is a normalized eigenstate of the Hamiltonian, and

$$\mathsf{F}(\mathsf{I}, \Theta) = \sum_M \mathsf{F}_M(\mathsf{I})\, \mathrm{e}^{\mathrm{i}M\Theta} \tag{2}$$

is the Fourier series of the Weyl representative of the operator $\hat{F}$, where action and angle coordinates are chosen as variables instead of the usual position and momentum coordinates (see section 2 of paper I).

Formula (1) seems to be so well known that it is difficult to trace its first appearance. A detailed derivation was given recently in [1]; for special cases see [2] and the references in [1]. There are two facts related to the application of this formula which must have been known to people using it in specific problems, but were ignored, or at most mentioned, in passing in general discussions. The first is that the formula does not make sense for arbitrary operators. In [1] it is stated that the 'matrix elements are slow functions of the average of the quantum numbers and are sensitive functions of the difference' (see also [3] for a similar statement). However, the slow variation of $\langle n'|\hat{F}|n''\rangle$ in $\bar{n}$ is not a general feature which is always met but a condition imposed on the admissible operators $\hat{F}$ (these operators were called 'semiclassical' in paper I). It seems to have the status of a necessary condition since it is not satisfied for the two operators presented in section 4 of paper I as examples where the semiclassical matrix elements differ substantially from the true ones. The second peculiarity of (1) is that this formula implicitly fixes the relative phases of the eigenstates $|n\rangle$, once the function $\Theta(P, X)$ is completely defined. This definition involves a convention on the curve $\Theta(P, X) = 0$, whereas the function $I(P, X)$ is uniquely determined by the Hamiltonian. When both functions $I(P, X)$ and $\Theta(P, X)$ are given, the inverse functions $\mathbf{P}(\mathbf{I}, \mathbf{\Theta})$, $\mathbf{X}(\mathbf{I}, \mathbf{\Theta})$ are uniquely determined and so is the right-hand side of (1), because the Weyl representative $F(P, X)$ is uniquely related to the operator $\hat{F}$. Accordingly, for the left-hand side of (1) to coincide with the right-hand side (up to small errors), the phases of the eigenstates have to be properly chosen. However, it is not obvious from (1) what this phase convention implies for $\psi_n(x) = \langle x|n\rangle$ or $\tilde{\psi}_n(p) = \langle p|n\rangle$, the eigenfunctions of the Hamiltonian in the $x$- and the $p$-representation, respectively.

The observed limitations of equation (1) and the inherent phase convention therefore raise two questions. (i) What are the necessary and sufficient conditions, which characterize the set of semiclassical operators? (ii) What is the explicit form of the phase convention used in (1) and the consistent convention used in the definition of the function $\Theta(P, X)$? The second question has been briefly discussed by Morehead [1] but the answer he gives is incomplete (see the discussion at the end of section 2).

In section 2 a partial answer to (i) is given by showing that all operators of the form $|\mathbf{I}, \mathbf{\Theta}\rangle\langle\mathbf{I}', \mathbf{\Theta}'|$ with $\mathbf{I} \approx \mathbf{I}' \gg \hbar$ and $\mathbf{\Theta} \approx \mathbf{\Theta}'$ are semiclassical, if the Hamiltonian meets certain requirements and the considered energy is sufficiently high. We hope that this result will stimulate further investigations which finally result in a complete answer. As a by-product of this investigation a number of new semiclassical approximations were obtained for scalar products of wavefunctions (coherent states, energy eigenfunctions) and phase space representatives of operators ($W$- and $Q$-functions). In addition it was possible to give a complete answer to question (ii); it should have a bearing on the phases of the WKB eigenfunctions which are used in the general derivation of relation (1). In the derivation of these results no attempt was made to quantify the various approximations by means of rigorous error bounds. The approximations finally obtained were instead tested in several examples, partly by analytical methods, partly by numerical ones. It is intended to present this material together with examples which illustrate the methods described in paper I in a future publication.

Finally, in section 3 we speculate on possible extensions of the class of semiclassical operators found in section 2. The appendix on anharmonic oscillators is added to show that two inequalities used in the derivation of section 2 are satisfied for these systems if the energies of the coherent states are sufficiently high.

Throughout this paper the notation and terminology of paper I is used.

## 2. Semiclassical operators

For many operators $\hat{F}$ the problem in checking relation (1) is not the calculation of the $W$-representative $F(P, X)$ but the following. First, this function has to be expressed in terms of action and angle variables whose definition depends on the Hamiltonian of the system and which are therefore not explicitly known in general. Second, one has to calculate the matrix elements $\langle n'|\hat{F}|n''\rangle$ which requires knowledge of the eigenvectors $|n\rangle$, at least in approximate form. In the following we show how to overcome these problems for operators of the form

$$\hat{F}_{\mathbf{I}_0,\mathbf{\Theta}_0;\delta\mathbf{I},\delta\mathbf{\Theta}} = \left|\mathbf{I}_0 + \frac{\delta\mathbf{I}}{2}, \mathbf{\Theta}_0 + \frac{\delta\mathbf{\Theta}}{2}\right\rangle\left\langle\mathbf{I}_0 - \frac{\delta\mathbf{I}}{2}, \mathbf{\Theta}_0 - \frac{\delta\mathbf{\Theta}}{2}\right| \tag{3}$$

when $|\delta\mathbf{I}| \ll \mathbf{I}_0$ and $|\delta\mathbf{\Theta}| \ll 2\pi$, and the energy $\mathbf{H}(\mathbf{I}_0)$ is sufficiently high. In the following derivation of approximations for the quantities of interest ($W$-functions, scalar products of wavefunctions, matrix elements, expectation values) it will be assumed that in this energy range the Hamiltonian satisfies the conditions formulated in equations (10) and (19); the validity of these inequalities for anharmonic oscillators is discussed in the appendix.

Let $P_0 \pm \delta P/2$ and $X_0 \pm \delta X/2$ be related to $\mathbf{I}_0 \pm \delta\mathbf{I}/2$ and $\mathbf{\Theta}_0 \pm \delta\mathbf{\Theta}/2$ by the canonical transformation $\mathbf{I}, \mathbf{\Theta} \to P, X$ [4]. Then

$$F_{P_0,X_0;\delta P,\delta X}(P, X) = 2\exp\left\{-\frac{(P-P_0)^2 + (X-X_0)^2}{\hbar} - \mathrm{i}\frac{(2P-P_0)\delta X - (2X-X_0)\delta P}{2\hbar}\right\}. \tag{4}$$

Assuming $\delta\mathbf{I}, \delta\mathbf{\Theta}$ to be sufficiently small we can linearize the canonical transformation in a neighbourhood of $(P_0, X_0) \equiv (\mathbf{I}_0, \mathbf{\Theta}_0)$

$$\begin{pmatrix} P - P_0 \\ X - X_0 \end{pmatrix} = \alpha_0 \begin{pmatrix} \mathbf{I} - \mathbf{I}_0 \\ \mathbf{\Theta} - \mathbf{\Theta}_0 \end{pmatrix} \tag{5}$$

$$\begin{pmatrix} \mathbf{I} - \mathbf{I}_0 \\ \mathbf{\Theta} - \mathbf{\Theta}_0 \end{pmatrix} = \alpha_0^{-1} \begin{pmatrix} P - P_0 \\ X - X_0 \end{pmatrix} \tag{6}$$

where

$$\alpha = \begin{pmatrix} \dfrac{\partial\mathbf{P}}{\partial\mathbf{I}} & \dfrac{\partial\mathbf{P}}{\partial\mathbf{\Theta}} \\ \dfrac{\partial\mathbf{X}}{\partial\mathbf{I}} & \dfrac{\partial\mathbf{X}}{\partial\mathbf{\Theta}} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \tag{7}$$

$$\alpha^{-1} = \begin{pmatrix} \dfrac{\partial I}{\partial P} & \dfrac{\partial I}{\partial X} \\ \dfrac{\partial\Theta}{\partial P} & \dfrac{\partial\Theta}{\partial X} \end{pmatrix} = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \tag{8}$$

$$\det\alpha = \det\alpha^{-1} = 1 \tag{9}$$

and the subscript 0 means that the partial derivatives have to be taken at $(P_0, X_0) \equiv (\mathbf{I}_0, \mathbf{\Theta}_0)$. The isolines $I(P, X) = \text{constant}$ and $\Theta(P, X) = \text{constant}$ passing $(P_0, X_0)$ are almost orthogonal if

$$\left(\frac{u_0 - v_0}{2w_0}\right)^2 \gg 1 \tag{10}$$

where $u, v, w$ are the elements of the symmetric matrix

$$\beta = \alpha^{\mathrm{T}}\alpha = \begin{pmatrix} u & w \\ w & v \end{pmatrix}. \tag{11}$$

For anharmonic oscillators it can be shown that (10) can be satisfied for every angle $\mathbf{\Theta}_0$ by choosing a sufficiently high value of $\mathbf{I}_0$. We therefore assume that this relation also holds true for the system under consideration and the energy range of interest. Note that (10) allows one to approximate $\beta_0$ by a diagonal matrix with elements $u_0$ and $v_0 = u_0^{-1}$,

$$u = a^2 + c^2 = \left(\frac{\partial \mathbf{P}}{\partial \mathbf{I}}\right)^2 + \left(\frac{\partial \mathbf{X}}{\partial \mathbf{I}}\right)^2. \tag{12}$$

We now split the phase in (4) into two parts, namely $-(1/\hbar)[(P - P_0)\delta X - (X - X_0)\delta P]$ and $+(1/2\hbar)(P_0\delta X - X_0\delta P)$. Using (5) we obtain for the first term

$$(P - P_0)\delta X - (X - X_0)\delta P \approx (\mathbf{I} - \mathbf{I}_0)\delta\mathbf{\Theta} - (\mathbf{\Theta} - \mathbf{\Theta}_0)\delta\mathbf{I} \tag{13}$$

(this is the invariance of the symplectic form under canonical transformations). The term $(1/2)(P_0\delta X)$ appearing in the second part of the phase is the area of a triangle with corners $(0, 0)$ and $(P_0, X_0 \pm \delta X/2)$. Without change of this area the latter two points may be shifted parallel to the (locally straight) isoline $\Theta(P, X) = \mathbf{\Theta}_0$ until they meet the (approximately orthogonal) isoline $I(P, X) = \mathbf{I}_0$, and the coordinates of the new points $(\mathbf{I}, \mathbf{\Theta}) = (\mathbf{I}_0, \mathbf{\Theta}_0 \pm \delta\mathbf{\Theta}')$ may be calculated by means of (6). The same can be done for the second term, and when the two areas are subtracted one obtains

$$(1/2)(P_0\delta X - X_0\delta P) \approx \mathbf{I}_0\delta\mathbf{\Theta}. \tag{14}$$

Since the isolines of $\Theta(P, X)$ and $I(P, X)$ were assumed to be approximately orthogonal, we also have in the neighbourhood of $(P_0, X_0) \equiv (\mathbf{I}_0, \mathbf{\Theta}_0)$

$$(P - P_0)^2 + (X - X_0)^2 \approx u_0(\mathbf{I} - \mathbf{I}_0)^2 + u_0^{-1}(\mathbf{\Theta} - \mathbf{\Theta}_0)^2. \tag{15}$$

When these expressions are inserted into (4) one obtains the Weyl representative as a function of the variables $\mathbf{I}, \mathbf{\Theta}$ and the parameters $\mathbf{I}_0, \mathbf{\Theta}_0$. The result is, however, not periodic in the two angles, since equations (13)–(15) were derived from a local approximation of the canonical transformation $P, X \to \mathbf{I}, \mathbf{\Theta}$. To restore the periodicity we require that

$$\delta\mathbf{I}/\hbar = \text{integer} \tag{16}$$

and modify the Gaussian in $\mathbf{\Theta} - \mathbf{\Theta}_0$ according to

$$\exp\left\{-\frac{(\mathbf{\Theta} - \mathbf{\Theta}_0)^2}{\hbar u_0}\right\} \to \exp\left\{-\frac{4}{\hbar u_0}\sin^2\left(\frac{\mathbf{\Theta} - \mathbf{\Theta}_0}{2}\right)\right\}. \tag{17}$$

For the Fourier decomposition of this periodic function we use the formula [5]

$$\exp\left\{-2x\sin^2\frac{\phi}{2}\right\} \approx \frac{1}{\sqrt{2\pi x}}\sum_M \mathrm{e}^{-M^2/2x + \mathrm{i}M\phi} \tag{18}$$

which is a good approximation for

$$x = 2/\hbar u_0 \gg 1. \tag{19}$$

Putting things together we therefore arrive at

$$(\mathbf{F}_{\mathbf{I}_0,\mathbf{\Theta}_0;\delta\mathbf{I},\delta\mathbf{\Theta}})_{\delta n}(\bar{n}_+\hbar) \approx \left(\frac{\hbar u_0}{\pi}\right)^{1/2} \exp\left\{-\frac{u_0}{\hbar}(\mathbf{I}_0 - \bar{n}_+\hbar)^2 - \frac{\hbar u_0}{4}\left(\delta n - \frac{\delta\mathbf{I}}{\hbar}\right)^2 - \mathrm{i}(\bar{n}_+\delta\mathbf{\Theta} + \delta n\mathbf{\Theta}_0)\right\}. \tag{20}$$

We now turn to the matrix elements of the operator (3). For the eigenfunctions $\psi_n(x)$ we use the simplest WKB approximations [6]. Like the true eigenfunctions these functions can be chosen to be real and to have definite parity,

$$\psi_{\mathbf{I}_n}(x) = \left[\frac{2}{\pi}\frac{\partial^2 S(\mathbf{I}_n, x)}{\partial \mathbf{I}\partial x}\right]^{1/2} \cos\left[\frac{S(\mathbf{I}_n, x)}{\hbar} - \frac{n\pi}{2}\right] \qquad \text{for} \quad |x| < x_{\mathbf{I}_n} \tag{21}$$

$$= 0 \qquad \text{for} \quad |x| > x_{\mathbf{I}_n}. \tag{22}$$

In (21) $S(\mathbf{I}, x)$ is the generating function of the canonical transformation $P, X \to \mathbf{I}, \mathbf{\Theta}$,

$$S(\mathbf{I}, x) = \int_0^x \mathrm{d}x'\, p_+(\mathbf{I}, x') = -S(\mathbf{I}, -x) \tag{23}$$

$$p_+(\mathbf{I}, x) = \sqrt{2\mathbf{H}(\mathbf{I}) - 2V(x)} \geqslant 0 \tag{24}$$

$$p_{\mathbf{I}} = p_+(\mathbf{I}, 0). \tag{25}$$

In (24) $\mathbf{H}(\mathbf{I})$ is the inverse function of

$$\mathbf{I}(\mathbf{H}) = \frac{1}{2\pi}\int_{H(p,x)<\mathbf{H}} \mathrm{d}p\, \mathrm{d}x \tag{26}$$

and in (23) and (24) it is assumed that $x \in (-x_{\mathbf{I}}, x_{\mathbf{I}})$ where $\pm x_{\mathbf{I}}$ are the turning points

$$x_{\mathbf{I}} = x_+(\mathbf{I}, 0) \tag{27}$$

$$x_+(\mathbf{I}, p) = \text{non-negative solution of } V(x) = \mathbf{H}(\mathbf{I}) - \tfrac{1}{2}p^2. \tag{28}$$

The partial derivatives of (23) are

$$\frac{\partial S(\mathbf{I}, x)}{\partial x} = p_+(\mathbf{I}, x) = p_+(\mathbf{I}, -x) \tag{29}$$

$$\frac{\partial S(\mathbf{I}, x)}{\partial \mathbf{I}} = \theta(\mathbf{I}, x) = -\theta(\mathbf{I}, -x) \tag{30}$$

where $\theta(\mathbf{I}, x)$ is an angle measured with respect to the positive $p$-axis (not to be confused with the angle $\Theta(p, x)$ which is defined in (32) later). Because of (29) and (30)

$$\frac{\partial^2 S(\mathbf{I}, x)}{\partial \mathbf{I}\partial x} = \frac{\partial \theta(\mathbf{I}, x)}{\partial x} = \frac{\partial p_+(\mathbf{I}, x)}{\partial \mathbf{I}} = \frac{\omega(\mathbf{I})}{p_+(\mathbf{I}, x)} \geqslant 0 \qquad \text{for} \quad |x| \leqslant x_{\mathbf{I}}. \tag{31}$$

Given the functions $H(P, X)$, $\mathbf{I}(\mathbf{H})$, and $\theta(\mathbf{I}, x)$ the action variable is then defined by $I(P, X) = \mathbf{I}(H(P, X))$, while the conjugate angle variable $\Theta(P, X)$ is defined by the equation

$$(\text{sign } P)\Theta(P, X) = \theta(\mathbf{I}(H(P, X)), X) - \pi/2. \tag{32}$$

Note that $\theta(\mathbf{I}, x)$ varies between $-\pi/2$ and $\pi/2$ whereas $\Theta(P, X)$ varies between $-\pi$ and $\pi$, assuming the value 0 on the positive $X$-axis.

The integer $n = 0, 1, 2, \ldots$ in (21) fixes the parity of the function; it also counts the number of nodes of the true eigenfunction and labels the eigenvalues in increasing order. The dependence of $\mathbf{I}_n$, the value of the action $\mathbf{I}$ used in (21), on the number $n$ is usually fixed by the Maslov (Einstein, Brillouin, Keller, ...) quantization condition

$$\mathbf{I}_n = (n + \tfrac{1}{2})\hbar = n_+\hbar \tag{33}$$

which also follows from Langer's modification of the simple WKB approximation (21) near the turning points $x = \pm x_{\mathbf{I}}$ [6]. This result is also obtained in the following, provided that the potential does not confine the particle's motion to a finite interval, which does not depend on the considered energy (infinitely deep square well, Pöschl–Teller potential). The function (21) diverges at the classical turning points $\pm x_{\mathbf{I}}$. This is unphysical and one should keep in mind that the true eigenfunction is well approximated by equations (21) and (22) only in the case where $x$ is sufficiently far away from the turning points.

The next step is to calculate the scalar product $\langle n|P, X\rangle$ where $|n\rangle$ is given by (21)–(28) and $|P, X\rangle$ by equation (12) of paper I. It is sufficient to consider only the case $P > 0$, $X > 0$ because

$$\langle n|P, X\rangle = \langle n| - P, X\rangle^* = (-1)^n \langle n|P, -X\rangle^* = (-1)^n \langle n| - P, -X\rangle. \quad (34)$$

The integration over $x$ is performed only in an approximate way, essentially by the method of steepest descent. Since $\langle x|P, X\rangle$ has a sharp peak at $x = X$ we substitute in (21)

$$\begin{aligned} S(\mathbf{I}_n, x) &\to S(\mathbf{I}_n, X) + (x - X)p_+(\mathbf{I}_n, X) \\ \frac{\partial^2 S}{\partial \mathbf{I} \partial x}(\mathbf{I}_n, x) &\to \frac{\partial p_+}{\partial \mathbf{I}}(\mathbf{I}_n, X). \end{aligned} \quad (35)$$

If the remaining integral is evaluated by means of

$$\int_{-\infty}^{\infty} \mathrm{d}x \, \exp\{-ax^2 + \mathrm{i}bx\} = \left(\frac{\pi}{a}\right)^{1/2} \exp\left\{-\frac{b^2}{4a}\right\} \quad (36)$$

one arrives at

$$\begin{aligned} \langle n|P, X\rangle \approx \left(\frac{\hbar}{\pi}\right)^{1/4} \left[\frac{\partial p_+}{\partial \mathbf{I}}(\mathbf{I}_n, X)\right]^{1/2} \mathrm{e}^{\mathrm{i}PX/2\hbar} \\ \times \exp\left\{-\frac{[P - p_+(\mathbf{I}_n, X)]^2}{2\hbar} - \mathrm{i}\left[\frac{S(\mathbf{I}_n, X)}{\hbar} - \frac{n\pi}{2}\right]\right\}. \end{aligned} \quad (37)$$

In equation (37) the second term has been omitted because it is proportional to $\exp\{-(1/2\hbar)[P + p_+(\mathbf{I}_n, X)]^2\} \ll 1$. It should be noted that the right-hand side of (37) approximates the scalar product only for $|X| < x_{\mathbf{I}_n} - \sqrt{2\hbar}$; for $|X| > x_{\mathbf{I}_n} + \sqrt{2\hbar}$ one obtains $\langle n|P, X\rangle \approx 0$ because the overlap of the two functions becomes negligibly small in this case. Moreover, it is only for coherent states lying near the $P$-axis ($X \approx 0$) that (37) can be expected to be a reliable approximation since the quality of the WKB approximation (21) decreases as one moves away from $x = 0$.

Considered as a function of the coherent state parameters $P, X$ the modulus of the right-hand side of (37) reaches its maximum value when $P = p_+(\mathbf{I}_n, X)$ or $I(P, X) = \mathbf{I}_n$. If we keep this value of $I(P, X)$ fixed and vary the centre of the coherent state with $\mathbf{\Theta}$, i.e. $P = \mathbf{P}(\mathbf{I}_n, \mathbf{\Theta})$ and $X = \mathbf{X}(\mathbf{I}_n, \mathbf{\Theta})$, then the phase of (37) varies according to

$$\frac{1}{2\hbar} p_+(\mathbf{I}_n, \mathbf{X}(\mathbf{I}_n, \mathbf{\Theta}))\mathbf{X}(\mathbf{I}_n, \mathbf{\Theta}) - \frac{1}{\hbar} S(\mathbf{I}_n, \mathbf{X}(\mathbf{I}_n, \mathbf{\Theta})) + n\frac{\pi}{2} = -\frac{1}{\hbar}\mathbf{I}_n \left(\mathbf{\Theta} + \frac{\pi}{2}\right) + n\frac{\pi}{2}. \quad (38)$$

That the both sides of (38) are equal follows from definitions (23) and (24) and $\mathrm{d}P\,\mathrm{d}X = \mathrm{d}\mathbf{I}\,\mathrm{d}\mathbf{\Theta}$. For $\mathbf{\Theta} = -\pi/2$ (positive $P$-axis) (38) assumes the value $n\pi/2$, which is in agreement with $\langle n|P, 0\rangle = (-1)^n \langle n|P, 0\rangle^*$ (cf equation (34)). For $\mathbf{\Theta} \to 0$ (positive $X$-axis) the phase (38) would approach the value zero, if $\mathbf{I}_n$ were equal to $n\hbar$. While this would be acceptable for (34), which requires $\langle n|0, X\rangle = \langle n|0, X\rangle^*$, it would contradict the quantization condition (33). This discrepancy has two reasons. First, the WKB function (21) is only a poor approximation of the true eigenfunction when $x$ approaches the turning point ($X \to x_{\mathbf{I}_n}$, $\mathbf{\Theta} \to 0$). Second, when the coherent state is centred in this region, it is no longer meaningful to neglect second-order terms in the expansion (35) and to extend the range of integration to the full real line as it was done in (36). To improve the approximation one has to include the second-order term and to choose $x = x_{\mathbf{I}_n}$ as upper bound in the integration over $x$. For anharmonic oscillators

$$\frac{\partial^2 S}{\partial X^2}(\mathbf{I}, X) < 0 \qquad \text{for} \quad 0 < X < x_{\mathbf{I}} \tag{39}$$

while this quantity vanishes identically for the infinitely deep square well. If we restrict the discussion to Hamiltonians for which (39) holds true, we are left with expressions of the form $(a, b, c > 0)$

$$\lim_{c\to 0}\int_{-\infty}^{c} \mathrm{d}x \ \exp\{-ax^2 + \mathrm{i}bx^2\} = \frac{\sqrt{\pi}}{2(a^2+b^2)^{1/4}}\,\mathrm{e}^{\mathrm{i}\Phi} \qquad \Phi = \frac{1}{2}\arctan\left(\frac{b}{a}\right). \tag{40}$$

When $X$ approaches the turning point, $b$ tends to $+\infty$ and the phase $\Phi$ tends to $+\pi/4$. From this we conclude that

$$\text{phase of } \langle n|\mathbf{I}_n, \boldsymbol{\Theta}\rangle \approx -\frac{1}{\hbar}\mathbf{I}_n\left(\boldsymbol{\Theta} + \frac{\pi}{2}\right) + n\frac{\pi}{2} + \Phi(\boldsymbol{\Theta}) \tag{41}$$

where $\Phi(\boldsymbol{\Theta})$ is a function which varies slowly from $\Phi(-\pi/2) = 0$ to $\Phi(0) = +\pi/4$.

To gain further insight into the phase of the scalar product $\langle n|\mathbf{I}_n, \boldsymbol{\Theta}\rangle$, when $\boldsymbol{\Theta}$ is close to 0 (centre of the coherent state near the positive $X$-axis), we also consider the approximation which is obtained from the momentum representation of the two functions. The formulae corresponding to (21)–(23) and (29)–(32) are of the following form (cf [7])

$$\tilde{\psi}_{\mathbf{I}_n}(p) = \mathrm{i}^{-n}\left[-\frac{2}{\pi}\frac{\partial^2\tilde{S}(\mathbf{I}_n, p)}{\partial\mathbf{I}\partial p}\right]^{1/2}\cos\left[\frac{\tilde{S}(\mathbf{I}_n, p)}{\hbar} - \frac{n\pi}{2}\right] \qquad \text{for} \quad |p| < p_{\mathbf{I}} \tag{42}$$

$$= 0 \qquad \text{for} \quad |p| > p_{\mathbf{I}} \tag{43}$$

$$\tilde{S}(\mathbf{I}, p) = -\int_0^p \mathrm{d}p'\, x_+(\mathbf{I}, p') = -\tilde{S}(\mathbf{I}, -p) \tag{44}$$

$$-\frac{\partial\tilde{S}(\mathbf{I}, p)}{\partial p} = x_+(\mathbf{I}, p) = x_+(\mathbf{I}, -p) \tag{45}$$

$$\frac{\partial\tilde{S}(\mathbf{I}, p)}{\partial\mathbf{I}} = \tilde{\theta}(\mathbf{I}, p) = -\tilde{\theta}(\mathbf{I}, -p) \tag{46}$$

$$-\frac{\partial^2\tilde{S}(\mathbf{I}, p)}{\partial\mathbf{I}\partial p} = -\frac{\partial\tilde{\theta}(\mathbf{I}, p)}{\partial p} = \frac{\partial x_+(\mathbf{I}, p)}{\partial\mathbf{I}} \geqslant 0 \qquad \text{for} \quad |p| \leqslant p_{\mathbf{I}} \tag{47}$$

$$\Theta(P, X) = \tilde{\theta}(\mathbf{I}(H(P, X)), (\operatorname{sign} X)P) - (\operatorname{sign} P)[1 - (\operatorname{sign} X)]\frac{\pi}{2}. \tag{48}$$

The analogue of (37) is

$$\langle n|P, X\rangle \approx \left(\frac{\hbar}{\pi}\right)^{1/4}\left[\frac{\partial x_+}{\partial\mathbf{I}}(\mathbf{I}_n, P)\right]^{1/2}\mathrm{e}^{-\mathrm{i}PX/2\hbar + \mathrm{i}n\pi/2}$$
$$\times \exp\left\{-\frac{[X - x_+(\mathbf{I}_n, P)]^2}{2\hbar} + \mathrm{i}\left[\frac{\tilde{S}(\mathbf{I}_n, P)}{\hbar} - \frac{n\pi}{2}\right]\right\} \tag{49}$$

and the validity of this approximation is similarly limited as that of (37). If we repeat the arguments leading from (37) to (41) we find

$$\text{phase of } \langle n|\mathbf{I}_n, \boldsymbol{\Theta}\rangle \approx -\frac{1}{\hbar}\mathbf{I}_n\boldsymbol{\Theta} + \tilde{\Phi}(\boldsymbol{\Theta}) \tag{50}$$

where $\tilde{\Phi}(\boldsymbol{\Theta})$ is a function which increases slowly from $\tilde{\Phi}(-\pi/2) = -\pi/4$ to $\Phi(0) = 0$. Comparison of (50) and (41) shows that $(-\mathbf{I}_n/\hbar + n)(\pi/2) + \Phi - \tilde{\Phi}$ should vanish for all values of $\boldsymbol{\Theta} \in (-\pi/2, 0)$; this is only possible if the difference $\Phi - \tilde{\Phi}$ is a constant. The value of this constant follows from the value of the two functions at the boundaries of the interval $(-\pi/2, 0)$. At both ends one finds $\Phi - \tilde{\Phi} = \pi/4$, which entails the quantization condition (33). This condition was first obtained from a study of the WKB function (21) and (22) near the turning points; in the present approach, which follows Maslov's ideas [7], the behaviour of the particle near the turning points is taken into account by the inclusion of the WKB function in $p$-representation, equations (42) and (43), which yields a good approximation for this situation. When the quantization condition (33) is inserted into (41) and (50) and the monotonicity of the functions $\Phi$ and $\tilde{\Phi}$ in $\mathbf{\Theta} \in (-\pi/2, 0)$ is taken into account, one obtains

$$\tilde{\Phi}(\mathbf{\Theta}) = \Phi(\mathbf{\Theta}) - \pi/4 = \tfrac{1}{2}\mathbf{\Theta} \tag{51}$$

and $-n\mathbf{\Theta}$ for both phases. We assume that the phase of the scalar products $\langle n|\mathbf{I}, \mathbf{\Theta}\rangle$ can be well approximated by this expression if $\mathbf{I}$ is close to $\mathbf{I}_n$.

To obtain an approximation of the modulus of $\langle n|\mathbf{I}, \mathbf{\Theta}\rangle$ we take into account that approximation (21) is good for $x \approx 0$ and approximation (42) good for $p \approx 0$. Noting that

$$\begin{aligned} &P - p_+(\mathbf{I}_n, X = 0) = \mathbf{P}(\mathbf{I}, \mathbf{\Theta} = -\pi/2) - \mathbf{P}(\mathbf{I}_n, \mathbf{\Theta} = -\pi/2) \\ &\mathbf{X}(\mathbf{I}, \mathbf{\Theta} = -\pi/2) = \mathbf{X}(\mathbf{I}_n, \mathbf{\Theta} = -\pi/2) = 0 \end{aligned} \tag{52}$$

$$\begin{aligned} &X - x_+(\mathbf{I}_n, P = 0) = \mathbf{X}(\mathbf{I}, \mathbf{\Theta} = 0) - \mathbf{X}(\mathbf{I}_n, \mathbf{\Theta} = 0) \\ &\mathbf{P}(\mathbf{I}, \mathbf{\Theta} = 0) = \mathbf{P}(\mathbf{I}_n, \mathbf{\Theta} = 0) = 0 \end{aligned} \tag{53}$$

we expect that for the general position of the coherent state the quadratic term in the exponent of the scalar product is given by

$$[\mathbf{P}(\mathbf{I}, \mathbf{\Theta}) - \mathbf{P}(\mathbf{I}_n, \mathbf{\Theta})]^2 + [\mathbf{X}(\mathbf{I}, \mathbf{\Theta}) - \mathbf{X}(\mathbf{I}_n, \mathbf{\Theta})]^2 \approx u(\mathbf{I} - \mathbf{I}_n)^2 \tag{54}$$

and that the modulus may be approximated by a Gaussian. The final result for the approximation of the scalar product is then

$$\langle n|\mathbf{I}, \mathbf{\Theta}\rangle \approx \left(\frac{\hbar\bar{u}(n_+\hbar)}{\pi}\right)^{1/4} \exp\left\{-\frac{\bar{u}(n_+\hbar)}{2\hbar}(\mathbf{I} - n_+\hbar)^2 - \mathrm{i}n\mathbf{\Theta}\right\} \tag{55}$$

where $\bar{u}(\mathbf{I})$ is defined by

$$\bar{u}(\mathbf{I}) = \frac{1}{2\pi}\int \mathrm{d}\mathbf{\Theta}\, u(\mathbf{I}, \mathbf{\Theta}). \tag{56}$$

The constant on the right-hand side of (55) follows from the normalization condition

$$\frac{1}{h}\int \mathrm{d}\mathbf{I}\,\mathrm{d}\mathbf{\Theta}\,\langle n'|\mathbf{I}, \mathbf{\Theta}\rangle\langle \mathbf{I}, \mathbf{\Theta}|n''\rangle \approx \delta_{n',n''}. \tag{57}$$

The following facts may serve as a test of approximation (55).

(i) The scalar products (55) are the expansion coefficients of a coherent state $|\mathbf{I}, \mathbf{\Theta}\rangle$ of high energy, when it is expanded in the eigenvectors $|n\rangle$ of the Hamiltonian. As is clear from its derivation, (55) should hold for a wide class of binding potentials; these asymptotic expansion coefficients can be compared to the exact ones when the latter are known. For instance, for the harmonic oscillator the exact coefficients are given by equation (74) of paper I; if the Poisson distribution in $\mathbf{I}$ is approximated by a normal distribution one recovers (55) with $\bar{u}(\bar{n}_+\hbar) \approx (2n_+\hbar)^{-1}$. That superpositions of energy eigenstates yield wavepackets similar to coherent states if the moduli of the expansion coefficients are chosen as Gaussians in the quantum number $n$ has been noticed before by other authors [8, 9] but not justified by general considerations. The derivation of equation (55) fills this gap and shows that only those eigenvectors have to be considered in the expansion for which, say, $|n-(\mathbf{I}/\hbar)| < 3/\sqrt{\hbar u}$. This allows one to estimate the relevant energy range when the (initial) state is a superposition or a mixture of coherent states.

(ii) In accordance with (34)

$$\langle n|\mathbf{I},\Theta\rangle = \langle n|\mathbf{I},-\Theta\rangle^* = (-1)^n\langle n|\mathbf{I},\pi-\Theta\rangle^* = (-1)^n\langle n|\mathbf{I},\Theta+\pi\rangle. \tag{58}$$

(iii) We may also use (55) to obtain an approximation of the scalar product of two coherent states (equation (13) of paper I). If $|\Theta'-\Theta''| \ll 2\pi$, $(\mathbf{I}'/\hbar) \approx (\mathbf{I}''/\hbar) \gg 1$, and inequality (19) holds true for these values of the action, the discrete variable $n \geqslant 0$ may be treated like a continuous variable ranging from $-\infty$ to $+\infty$. If in (55) $\bar{u}(n_+\hbar)$ is replaced by $\bar{u}(\mathbf{I})$ the integration over $n$ may be performed in closed form, the result being

$$\langle\mathbf{I}',\Theta'|\mathbf{I}'',\Theta''\rangle \approx \exp\left\{-\frac{\bar{u}}{4\hbar}(\mathbf{I}'-\mathbf{I}'')^2 - \frac{1}{\tilde{u}\hbar}\sin^2\left(\frac{\Theta'-\Theta''}{2}\right) - \frac{\mathrm{i}}{2\hbar}(\mathbf{I}'+\mathbf{I}'')(\Theta'-\Theta'')\right\} \tag{59}$$

where $\tilde{u} = \frac{1}{2}[\bar{u}(\mathbf{I}') + \bar{u}(\mathbf{I}'')]$. If this approximation is used in the exact equations

$$2|\langle\mathbf{I}',\Theta'|\mathbf{I}'',\Theta''\rangle|^4 = h\boldsymbol{K}(\mathbf{I}',\Theta'|\mathbf{I}'',\Theta'') = \mathbf{F}_{\mathbf{I}',\Theta';0,0}(\mathbf{I}'',\Theta'') \tag{60}$$

(cf (4) and equations (13) and (23) of paper I) one obtains approximations of the last two functions which are consistent with equations (18) and (20).

The last step in the calculation of the matrix elements of operator (3) is to multiply $\langle n'|\mathbf{I}_0+\delta\mathbf{I}/2,\Theta_0+\delta\Theta/2\rangle$ by $\langle\mathbf{I}_0-\delta\mathbf{I}/2,\Theta_0-\delta\Theta/2|n''\rangle$ and to rearrange the terms in the exponentials. Doing so we replace $\bar{u}(\bar{n}_+ \pm \delta n/2)$ with $\bar{u}(\bar{n}_+)$ and make use of the identity $(z-x)^2+(z-y)^2 = (1/2)[(2z-x-y)^2+(x-y)^2]$. This gives finally

$$\langle n'|\hat{F}_{\mathbf{I}_0,\Theta_0;\delta\mathbf{I},\delta\Theta}|n''\rangle \approx (\mathbf{F}_{\mathbf{I}_0,\Theta_0;\delta\mathbf{I},\delta\Theta})_{\delta n}(\bar{n}_+\hbar) \tag{61}$$

which proves that (3) is a semiclassical operator in the sense of equation (1), provided that $u$ is slowly varying in the action variable when $\mathbf{I} \approx \mathbf{I}_0$ and that inequality (19) is satisfied there.

The physical meaning of this result is that for systems like (an)harmonic oscillators the density operators related to coherent states of high energy, as well as mixtures and certain superpositions thereof, are all semiclassical operators so that equation (1) may be used to obtain their matrix elements in energy representation. No matter whether their $W$-functions admit an interpretation as classical distribution functions or not, the corresponding (almost identical) $S$-functions may be used to calculate time-dependent expectation values as described in paper I. The operators used as density operators at initial time $t=0$ may also serve as observables in which case the expectation value coincides with the square modulus of the autocorrelation function. Combined with the scheme of paper I relation (61) therefore shows that the quantum mechanical autocorrelation function may be calculated for long time intervals by means of classical mechanics. Results of such a calculation are presented in [10].

We close this section with two remarks. First, equation (55) shows that for $\bar{n} \gg 1$ and $|\delta n| \ll \bar{n}$ the $Q$- representatives of the basic operators $|n'\rangle\langle n''|$ have the form

$$\mathbf{Q}_{n',n''}(\mathbf{I},\Theta) = \langle\mathbf{I},\Theta|n'\rangle\langle n''|\mathbf{I},\Theta\rangle = \int \mathrm{d}\mathbf{I}'\,\mathrm{d}\Theta'\,\boldsymbol{K}(\mathbf{I},\Theta|\mathbf{I}',\Theta')\mathbf{W}_{n',n''}(\mathbf{I}',\Theta') \tag{62}$$

$$\approx \sqrt{\frac{\hbar\bar{u}(\bar{n}_+\hbar)}{\pi}}\exp\left\{-\frac{\bar{u}(\bar{n}_+\hbar)}{\hbar}(\mathbf{I}-\bar{n}_+\hbar)^2 - \frac{\bar{u}(\bar{n}_+\hbar)\hbar}{4}(\delta n)^2 + \mathrm{i}\delta n\Theta\right\} \tag{63}$$

$$\approx] \int \mathrm{d}\mathbf{I}'\,\mathrm{d}\Theta'\,\boldsymbol{K}(\mathbf{I},\Theta|\mathbf{I}',\Theta')\mathbf{S}_{n',n''}(\mathbf{I}',\Theta') \tag{64}$$

(cf equations (21)–(23) and (43), (49) of paper I). The effect of smoothing with the kernel (60) is twofold. (i) The region in $\mathbf{I}$, where the function is essentially different from zero, is widened because of the Gaussian in $\mathbf{I}$. (ii) As is evident from (18) the number of oscillations in $\boldsymbol{\Theta}$ remains unchanged but the amplitudes are more reduced the higher the number of oscillations. Since the number of oscillations is preserved by a kernel of the form (60) we may conclude that not only the angular dependence of $\mathbf{S}_{n',n''}$ is given by $\exp\{\mathrm{i}(n'-n'')\boldsymbol{\Theta}\}$, but also that of $\mathbf{Q}_{n',n''}$ and $\mathbf{W}_{n',n''}$ if the two quantum numbers are sufficiently large and their difference comparatively small. This observation is also confirmed by numerical calculation of the three functions for anharmonic oscillators. Since smoothing does not change the minima and maxima of the real and imaginary parts of the functions $\mathbf{S}_{n',n''}$ it also does not change qualitatively the $\boldsymbol{\Theta}$-dependence of superpositions of these functions, except that extrema are less pronounced after the smoothing. All the arguments used in paper I to explain revivals in terms of the relative motion of profiles can therefore equally well be used for the corresponding constituents of the Husimi function [11].

The second remark refers to the conventions implied by equation (1). In deriving the validity of (1) for the operators (3) we started from the WKB functions (21), (22) and (42), (43). It is therefore clear that a proper phase convention for the eigenfunctions of $\hat{H}$ reads

$$\psi_n(x) \to c_n \cos(n\pi/2) + d_n \sin(n\pi/2)x \qquad \text{for } x \to 0 \tag{65}$$

where $c_n$ and $d_n$ are positive constants. The corresponding condition in momentum representation is

$$\tilde{\psi}_n(p) \to \mathrm{i}^{-n}[\tilde{c}_n \cos(n\pi/2) - \tilde{d}_n \sin(n\pi/2)p] \qquad \text{for } p \to 0 \tag{66}$$

with $\tilde{c}_n, \tilde{d}_n > 0$. Conventions (65) and (66), which might be modified by a common phase factor independent of $n$ without changing the left-hand side of (1), are nothing but the standard phase conventions for the harmonic oscillator eigenfunctions [6]; for WKB functions they were stated in [12].

However, these are not all conventions needed to ensure the validity of (61), a special case of equation (1). We would not have obtained this result, if we had used another definition of the function $\Theta(P, X)$. The definition used here makes use of the convention

$$\lim_{P\to 0} \Theta(P, X) = 0 \qquad \text{for} \quad X > 0. \tag{67}$$

Should we choose another ray, obtained from the positive $X$-axis through a rotation by some constant angle $\boldsymbol{\Theta}'$, as curve $\Theta(P, X) = 0$ it would change all Fourier components $\mathbf{F}_M(\mathbf{I})$ by a phase factor $\exp(\mathrm{i}M\boldsymbol{\Theta}')$; as a consequence (61) would no longer hold true. This sensitivity to the definition of the angle variable was noticed by Morehead in [1]. He claimed that for equation (1) to hold true, the lower limit of the integral, which defines the function $S(\mathbf{I}, x)$ appearing in the WKB functions (21), should be the same for all values of $\mathbf{I}$. This is the case in (23), and the definition of $\Theta(P, X)$ in terms of the function $S(\mathbf{I}, x)$ is completely specified through equations (26), (30) and (32). But while these equations (which are missing in [1]) establish a relation between the functions $\Theta(P, X)$ and $S(\mathbf{I}, x)$, they do in no way fix the phase of the argument of the cosine function in (21). In other words, the shift $-n\pi/2$, which varies from one eigenfunction to the other, is a convention that has to be added to the conventions made in the definitions of the action integral and the angle variable. Similar arguments hold for the eigenfunctions in $p$-representation.

## 3. Conclusion and outlook

Finite linear combinations of operators of the form (3) contain many operators of physical interest such as density operators of coherent states and mixtures thereof. They also contain superpositions of several coherent states, provided that inequalities (10) and (19) are satisfied for all auxiliary coherent states, which are centred at interior points of the simplex spanned by the centres of the components of the superposition, i.e. if these infinitely many auxiliary coherent states all lie in the high energy region. This excludes the cat state considered in section 4 of paper I, but it shows that the density operators of cat states formed of two nearby coherent states are semiclassical. For all these operators the Weyl representative (Wigner function) is a good substitute for the $S$-representative and this may be used to study the time evolution of the state as described in paper I.

However, the class of operators of the form (3) is in any case too restricted to contain all observables of physical interest. A semiclassical theory should at least contain also basic operators like position, momentum, kinetic energy, etc. An extension of the class of semiclassical operators that suggests itself is to make use of the diagonal representation

$$\hat{A} = \frac{1}{h}\int \mathrm{d}\mathbf{I}\,\mathrm{d}\boldsymbol{\Theta}\,\mathbf{A}^P(\mathbf{I},\boldsymbol{\Theta})\hat{F}_{\mathbf{I},\boldsymbol{\Theta}} \tag{68}$$

$$\hat{F}_{\mathbf{I},\boldsymbol{\Theta}} = \hat{F}_{\mathbf{I},\boldsymbol{\Theta};0,0} = |\mathbf{I},\boldsymbol{\Theta}\rangle\langle\mathbf{I},\boldsymbol{\Theta}|. \tag{69}$$

Because of (61) each of the projection operators (69) which appear in the integral (68) is a semiclassical operator if the value of the parameter $\mathbf{I}$ is high enough. For these operators the $L^2$-norm of the difference between the $W$- and the $S$-representatives is small. Moreover, it is to be expected that in the region of the phase space, where the function $\mathbf{F}^S_{\mathbf{I},\boldsymbol{\Theta}}$ derived from the matrix elements and the Weyl representative $\mathbf{F}_{\mathbf{I},\boldsymbol{\Theta}}$ are essentially different from zero, their values do not differ much. This conclusion follows from a comparison of their Fourier decomposition with respect to the variable $\boldsymbol{\Theta}$: The functions $(\mathbf{F}_{\mathbf{I},\boldsymbol{\Theta}})_M(\mathbf{I}')$ are smooth functions which, because of (19), vary slowly when $\mathbf{I}'$ varies over distances of order $\hbar$ (see (20) with $\delta\mathbf{I} = \delta\boldsymbol{\Theta} = 0$); for this reason it should be possible to approximate them well by the step functions $(\mathbf{F}^S_{\mathbf{I},\boldsymbol{\Theta}})_M(\mathbf{I}')$. If these assumptions are correct one only has to impose conditions on the function $\mathbf{A}^P$ which ensure that the similarity of the $S$- and the $W$-functions of the projection operators (69) carries over to the corresponding representatives of $\hat{A}$. To this end we first require $\mathbf{A}^P$ to have a compact support which lies in a region of high energies (usually determined by the state under consideration). This assumption already eliminates the operators presented in section 4 of paper I for which the semiclassical formula for the matrix elements, equation (1), was seen to fail. However, if this were the only postulate, $\mathbf{A}^P$ could still be a tempered distribution consisting, for example, of derivatives of delta functions. As the derivatives of the $W$- and the $S$-representatives of the coherent states can be very different (one being smooth, the other a step function), we require as a second condition that $\mathbf{A}^P$ is also a smooth function. This should ensure that the operator (68) is semiclassical. The class of observables of the form (68) is especially interesting when, as it is often the case, the $P$-representatives of the interesting operators are known as functions of $P$ and $X$. All that is needed is then a change of variables and a cut-off in energy which has to be performed in such a way that it has practically no impact on the value of the expectation value.

These arguments should be at least plausible but it is obvious that a deeper mathematical analysis of these questions is still lacking. We hope that the results of this paper will initiate a more rigorous study of semiclassical operators and the Heisenberg correspondence principle. Since the magnitude of $\hbar$ cannot be varied in nature, we have to make a selection of comparable objects in both theories, i.e. a proper reduction of the phase space functions and operators under consideration, if we want to understand the relation between classical and quantum mechanics.

## Appendix. Anharmonic oscillators

Consider the potential $V(x) = k|x|^\nu$, $k > 0$, $0 < \nu < \infty$. By a canonical transformation $p = \eta P$, $x = \eta^{-1} X$ the Hamiltonian can be brought to the standard form

$$H(P, X) = c(P^2 + |X|^\nu) \qquad c > 0. \tag{A1}$$

The action $\mathbf{I}(\mathbf{H})$ is $2/\pi$ times the area in $P > 0$, $X > 0$ enclosed by the curve $H(P, X) = \mathbf{H}$ (cf (26)). Hence [4]

$$\mathbf{I}(\mathbf{H}) = c_\nu \mathbf{H}^{(\nu+2)/2\nu} \tag{A2}$$

with

$$c_\nu = \frac{2}{\pi\nu} c^{-(\nu+2)/2\nu} \int_0^1 \mathrm{d}\xi\, \xi^{(1/\nu)-1} \sqrt{1-\xi}. \tag{A3}$$

The functional dependence of $P$ and $X$ on the action and angle variables $\mathbf{I}$, $\mathbf{\Theta}$ is given by

$$\mathbf{P}(\mathbf{I}, \mathbf{\Theta}) = (c_\nu/c)^{1/2} \mathbf{I}^{\nu/(\nu+2)} \mathbf{c}(\mathbf{\Theta}) \qquad \mathbf{X}(\mathbf{I}, \mathbf{\Theta}) = (c_\nu/c)^{1/\nu} \mathbf{I}^{2/(\nu+2)} \mathbf{s}(\mathbf{\Theta}) \tag{A4}$$

where $\mathbf{c}$ and $\mathbf{s}$ are generalizations of the cosine and sine functions, respectively.

$$\mathbf{c}(\mathbf{\Theta}) = \mathbf{c}(\mathbf{\Theta} + 2\pi) = \mathbf{c}(-\mathbf{\Theta}) \qquad \mathbf{s}(\mathbf{\Theta}) = \mathbf{s}(\mathbf{\Theta} + 2\pi) = -\mathbf{s}(-\mathbf{\Theta}) \tag{A5}$$

$$\mathbf{c}(0) = \mathbf{s}(\pi/2) = 1. \tag{A6}$$

Since $\mathrm{d}/\mathrm{d}t = \omega(\mathbf{I}) \partial/\partial\mathbf{\Theta}$ and

$$\omega(\mathbf{I}) = \frac{\mathrm{d}\mathbf{H}}{\mathrm{d}\mathbf{I}} = \frac{2\nu}{\nu+2} c_\nu^{(\nu+2)/2\nu} \mathbf{I}^{(\nu-2)/(\nu+2)} \tag{A7}$$

Hamilton's equations of motion become a pair of coupled differential equations for the functions $\mathbf{c}$ and $\mathbf{s}$.

$$\begin{aligned} \mathbf{c}'(\mathbf{\Theta}) &= -\nu \frac{\nu+2}{2\nu} \left(\frac{c}{c_\nu}\right)^{(\nu+2)/2\nu} \mathbf{s}(\mathbf{\Theta})^{\nu-1} \\ \mathbf{s}'(\mathbf{\Theta}) &= 2 \frac{\nu+2}{2\nu} \left(\frac{c}{c_\nu}\right)^{(\nu+2)/2\nu} \mathbf{c}(\mathbf{\Theta}). \end{aligned} \tag{A8}$$

Elimination of $\mathbf{c}$ yields a differential equation for $\mathbf{s}$ (Newton's equation), which is nonlinear if $\nu \neq 2$. It also follows from (A6) and (A8) that

$$\mathbf{c}(\mathbf{\Theta})^2 + \mathbf{s}(\mathbf{\Theta})^\nu = 1. \tag{A9}$$

From (A8) the functional determinant $\alpha$, equation (7), and the related matrix $\beta$, equation (11), can be calculated. The asymptotics for $\mathbf{I} \to \infty$ are

$$\begin{aligned} &u = O(\mathbf{I}^{-x/(\nu+2)}) \qquad v = O(\mathbf{I}^{y/(\nu+2)}) \qquad w = O(\mathbf{I}^{z/(\nu+2)}) \\ &\nu \geqslant 2: \qquad x = 4, \quad y = 2\nu, \quad z = \nu - 2 \\ &\nu \leqslant 2: \qquad x = 2\nu, \quad y = 4, \quad z = 2 - \nu \end{aligned} \tag{A10}$$

which shows that the inequalities (10) and (19) are satisfied at sufficiently high energies.

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