

Semiclassical approximations in phase space with coherent states

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Abstract

We present a complete derivation of the semiclassical limit of the coherent-state propagator in one dimension, starting from path integrals in phase space. We show that the arbitrariness in the path integral representation, which follows from the overcompleteness of the coherent states, results in many different semiclassical limits. We explicitly derive two possible semiclassical formulae for the propagator, we suggest a third one, and we discuss their relationships. We also derive an initial-value representation for the semiclassical propagator, based on an initial Gaussian wavepacket. It turns out to be related to, but different from, Heller’s thawed Gaussian approximation. It is very different from the Herman–Kluk formula, which is not a correct semiclassical limit. We point out errors in two derivations of the latter. Finally we show how the semiclassical coherent-state propagators lead to WKB-type quantization rules and to approximations for the Husimi distributions of stationary states.

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1. Introduction

Semiclassical approximations in phase space using coherent states have been discussed extensively for several decades. This attractive topic, a favourite of many theoretical physicists and chemists, turns out to be very difficult. In this contribution to its literature, we shall attempt to sort out and clarify the web of contradictions and inconsistencies that have characterized the recent state of the field. We shall do so for the simplest possible case, one-dimensional coordinate space, i.e. two-dimensional phase space. This is the case where it is relatively easy to check the semiclassical approximations. We have done work in higher dimensions as well, but we do not include it here, as it would only obscure the basic relationships and further lengthen the paper. The conclusions we have reached are stated in section 7, and the reader who is already familiar with the subject may jump to them now to get an overall view. Because the pitfalls are numerous, however, we shall follow a slower approach, a historical one in this introduction, and then a systematic and detailed one in the body of the paper.

The study of semiclassical methods has two basic motivations. First, it provides approximations to quantum mechanical quantities in terms of classical ingredients. These approximations should be very good if the typical classical actions are much larger than Planck's constant. Interestingly, they are often fairly good even at very low quantum numbers. Second, semiclassical methods also help in understanding the quantum mechanical processes themselves, providing a more intuitive description. This description includes quantum mechanical interference, since both amplitudes and phases can be calculated semiclassically.

The semiclassical approximation for the evolution operator, or propagator, in the coordinate representation has been known for more than 70 years and was first written by Van Vleck [Van28]. It is a complex number with a modulus and a phase. The main part of the phase is the action of a classical trajectory joining a given initial coordinate to a given final coordinate

in a given time. Finding such trajectories is usually not a simple task. It is known as ‘the root search problem’ and it gets more and more complicated as the number of dimensions increases. The modulus of the semiclassical propagator is related to the second derivative of the action with respect to these initial and final points. It measures the dispersal of nearby trajectories. Gutzwiller, among others, revisited this problem around 1970 [Gut71, Gut90], focusing on non-integrable systems and giving birth to the field of quantum chaos. Much progress has been made since then, particularly on the topological properties of Maslov indices [Rob91] and on the scars of periodic trajectories [Hel84, Bog88].

But there is another interesting representation for the evolution operator, which seems at first sight to be more appropriate for comparisons with classical mechanics. This is the representation using the coherent states of a harmonic oscillator. They are Gaussian states, localized in both coordinates and momenta, and therefore they can be thought of as *quantum points* in phase space. Although the exact coordinate propagator and the exact coherent-state propagator are related by a simple change of representation, the semiclassical approximations to them are quite different. One of the differences is that the classical Hamiltonians with which the trajectories are calculated are different. Another is that the classical trajectories for the coherent-state propagator are usually complex. Both semiclassical propagators involve trajectories with mixed initial and final conditions, hence both have the root search problem.

This semiclassical coherent-state propagator first appeared in the work of Klauder [Kla78, Kla79, Kla87a] without a detailed derivation. Weissman [Wei82] extended the old semiclassical correspondence relations to the case of coherent state variables and presented a first derivation of the semiclassical propagator; his derivation was based on the general semiclassical machinery rather than on path integral techniques. The possibility of a rigorous derivation using the latter is mentioned in several papers, but it does not seem to have actually been published, to our knowledge. The properties of the propagator were studied, however, for a number of fundamental quantum processes (see, e.g., [Xav96a, Xav96b, Xav97, Gro98a]). A recent application to the semiclassical quantization of a system with classically mixed regular and chaotic dynamics [Sch98] demonstrated the power of this approach.

There is another important difference between the coordinate and coherent state representations. Due to the overcompleteness of the latter, the path integral for the coherent-state propagator is not at all unique, and this non-unicity reflects itself in a large multiplicity of possible semiclassical propagators. For the quantum mechanical path integral, some good discussion of this variety was given in a review by Klauder and Skagerstam (KS) [Kla85]. Yet more ambiguity arises because coordinates and momenta do not commute in quantum mechanics, and therefore there is no unique general way of associating a quantal Hamiltonian with a classical one. The net result of all this is that many arbitrary decisions need to be made whenever one contemplates making a semiclassical approximation.

Without doubt, semiclassical approximations based on the propagator have been highly successful in chemical, molecular, atomic and nuclear physics. In spite of this, however, problems are turning up more and more often for which these methods are made very hard or inapplicable by the root search difficulty. These are usually problems in which the underlying classical dynamics is chaotic, which means that the number of contributing (real or complex) ‘root trajectories’ can be extremely large. Consequently, people have attempted more and more to avoid mixed initial and final conditions. The ideal method is one in which one is given a coordinate and a momentum *both at the initial time*. Then the classical trajectory is unique, and the wavefunction evolves with time by following this unique thread. Such a method is called an ‘initial-value representation’ or IVR. Much work has been done on IVRs by many people, including Miller *et al* [Mil70, Sun97], Levit and Smilansky [Lev77] and Brumer *et al* [Cam92, Pro95]. These IVRs do not involve coherent states. Klauder [Kla87b] also

struggled with this problem with coherent states. Kay [Kay94a, Kay94b, Kay97] compared several IVRs numerically. A very popular IVR, based on coherent states, is the Herman–Kluk or HK propagator [Her84, Her86, Klu86, Gro97, Gue98, Gro98b]. For recent reviews see the papers by Sepúlveda and Grossmann [Sep96, Gro99].

Finally we should note that the coherent state representation is not the only way to do quantum mechanics in phase space. A fascinating alternative is provided by the Wigner–Weyl representation [Wig32, Hil84, Ber89]. We shall not pursue this approach in this paper and we refer to a recent review article by Ozorio de Almeida [Ozo98].

Contents of this paper: In section 2 we give a very complete derivation of the semiclassical propagator in the coherent state representation. The result is equation (2.63) or (2.72). We have actually two different calculations of the path integral, a step-by-step calculation in section 2 and a more general method in the appendix. The latter is used again (in section 3) to perform a different integral. Section 3 discusses the variety of possible path integrals using coherent states and compares them. Section 4 contains the derivation of our IVR, which is equation (4.29). Our original purpose was to give a solid derivation of the HK formula but, when we were finished, we found a result very different from theirs, and in much better agreement with the expected behaviour of such a formula. Also in section 4, we compare our IVR with Heller’s IVR. Both have equal claims to being a correct semiclassical IVR, but they are different. Section 5 returns to the HK propagator and points out the errors made in two papers where it was derived. It also explains why, in spite of being an incorrect semiclassical formula, HK still works (sometimes poorly) in some situations. In section 6 we Fourier transform the propagator from time to energy, which yields the Green function in the coherent state representation. By looking for the poles of this Green function, we obtain the quantization rule for the energy levels. By looking at the residues of the poles, we obtain approximate Husimi distributions for the stationary states. Finally section 7 contains a summary of our results and our conclusions.

2. The semiclassical coherent-state propagator

In classical mechanics, it is convenient to describe the time evolution by focusing on a trajectory in phase space. One candidate for a similar quantity in quantum mechanics is the operator which describes the time evolution in the coherent state representation, the coherent-state propagator. In this section we shall construct the semiclassical limit of this propagator. The result is equation (2.63). For convenience, we shall confine ourselves here to a single degree of freedom. The extension to higher-dimensional systems will be discussed in the future.

2.1. The path integral

The coherent states $|z\rangle$ of a harmonic oscillator of mass m and frequency ω are defined by

$$|z\rangle = e^{-\frac{1}{2}|z|^2} e^{z\hat{a}^\dagger} |0\rangle \quad (2.1)$$

with $|0\rangle$ the harmonic oscillator ground state and

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}} \left(\frac{\hat{q}}{b} - i \frac{\hat{p}}{c} \right) \quad z = \frac{1}{\sqrt{2}} \left(\frac{q}{b} + i \frac{p}{c} \right). \quad (2.2)$$

In the above \hat{q} , \hat{p} and \hat{a}^\dagger are operators; q and p are real numbers; z is complex. The parameters

$$b = (\hbar/m\omega)^{\frac{1}{2}} \quad \text{and} \quad c = (\hbar m\omega)^{\frac{1}{2}} \quad (2.3)$$

define the length and momentum scales, respectively, and their product is \hbar . We shall need the wavefunction of a coherent state in the position representation, which is

$$\begin{aligned}\langle x|z\rangle &= \pi^{-\frac{1}{4}} b^{-\frac{1}{2}} \exp\left(-\frac{(x-q)^2}{2b^2}\right) \exp\left(\frac{i}{\hbar} p(x-q/2)\right) \\ &= \pi^{-\frac{1}{4}} b^{-\frac{1}{2}} \exp\left[-\frac{1}{2}(x/b - \sqrt{2}z)^2 + \frac{z}{2}(z - z^*)\right].\end{aligned}\quad (2.4)$$

Now we consider a system with Hamiltonian operator $\hat{H}(t)$. We restrict ourselves to 'reasonable' Hamiltonians, i.e. we assume that $\hat{H}(t)$, written as a function of the creation and annihilator operators \hat{a}^\dagger and \hat{a} , can be expanded into a power series of \hat{a}^\dagger , \hat{a} . The matrix elements of the evolution operator from time 0 to time t in the basis of the coherent states (2.1) are

$$K(z'', t; z', 0) = \langle z'' | \hat{T} e^{-\frac{i}{\hbar} \int_0^t \hat{H}(t') dt'} | z' \rangle \quad (2.5)$$

where \hat{T} is the time-ordering operator. For time-independent \hat{H} this is simply

$$K(z'', t; z', 0) = \langle z'' | e^{-\frac{i}{\hbar} \hat{H}t} | z' \rangle. \quad (2.6)$$

In order to write the propagator as a path integral, we divide the time interval $(0, t)$ into N small intervals of length $\tau := t/N$, and we write

$$K(z'', t; z', 0) = \langle z_N | \prod_{j=0}^{N-1} \hat{T} \exp\left\{-\frac{i}{\hbar} \int_{j\tau}^{(j+1)\tau} \hat{H}(t') dt'\right\} | z_0 \rangle \quad (2.7)$$

where, for simplicity of notation, we identify $|z_N\rangle \equiv |z''\rangle$ and $|z_0\rangle \equiv |z'\rangle$. If the time step τ is small enough, the variable $\hat{H}(t')$ in the integral can be replaced by the constant $\hat{H}(t_j)$, with some intermediate time $t_j \in [j\tau, (j+1)\tau]$. Then the time-ordering operator becomes unnecessary and we get, with large N ,

$$K(z'', t; z', 0) \approx \langle z_N | \prod_{j=0}^{N-1} e^{-\frac{i}{\hbar} \hat{H}(t_j)\tau} | z_0 \rangle. \quad (2.8)$$

Now we insert the unit operator, namely

$$\mathbf{1} = \int |z\rangle \frac{d^2z}{\pi} \langle z| \equiv \iint |z\rangle \frac{dx dy}{\pi} \langle z| \equiv \iint |z\rangle \frac{dz^* dz}{2\pi i} \langle z| \quad (2.9)$$

everywhere between adjacent propagation steps. We denoted the real and imaginary parts of z by x and y , respectively. The sign of the last equation member on the right is actually undetermined, because the sign of the Jacobian depends on the order in which the variables are taken. To avoid any possible confusion, we state here that, in all integrations, $dz^* dz/2\pi i$ actually means $dx dy/\pi$. After the insertions, the propagator becomes a $2(N-1)$ -fold integral over the whole phase space

$$\begin{aligned}K(z'', t; z', 0) &= \int \left\{ \prod_{j=1}^{N-1} \frac{d^2z_j}{\pi} \right\} \prod_{j=0}^{N-1} \{ \langle z_{j+1} | e^{-\frac{i}{\hbar} \hat{H}(t_j)\tau} | z_j \rangle \} \\ &= \int \left\{ \prod_{j=1}^{N-1} \frac{dz_j^* dz_j}{2\pi i} \right\} e^{f(z^*, z)}\end{aligned}\quad (2.10)$$

where f is defined by

$$f(z^*, z) := \ln \left[\prod_{j=0}^{N-1} \{ \langle z_{j+1} | e^{-\frac{i}{\hbar} \hat{H}(t_j)\tau} | z_j \rangle \} \right] \quad (2.11)$$

with $z := (z_0, z_1, \dots, z_N)$ and its complex conjugate $z^* := (z_0^*, z_1^*, \dots, z_N^*)$. The reason for writing z^* separately from z as arguments of f is that they must be considered independent variables, because we are integrating over the two variables x_j and y_j for each j . Eventually, when we carry out the stationary-exponent approximation, each of these two real variables will be allowed to become complex, which will result in *four* real variables for each j . Following Klauder [Kla78], we transform the integrand $e^{f(z^*, z)}$ as follows:

$$\begin{aligned} e^{f(z^*, z)} &\approx \prod_{j=0}^{N-1} \langle z_{j+1} | 1 - \frac{i\tau}{\hbar} \hat{H}(t_j) | z_j \rangle \\ &= \prod_{j=0}^{N-1} \langle z_{j+1} | z_j \rangle \left(1 - \frac{i\tau}{\hbar} \frac{\langle z_{j+1} | \hat{H}(t_j) | z_j \rangle}{\langle z_{j+1} | z_j \rangle} \right) \\ &\approx \left[\prod_{j=0}^{N-1} \langle z_{j+1} | z_j \rangle \right] \exp \left\{ \sum_{j=0}^{N-1} -\frac{i\tau}{\hbar} \mathcal{H}_{j+1,j} \right\} \end{aligned} \quad (2.12)$$

with the abbreviation

$$\mathcal{H}_{j+1,j} \equiv \mathcal{H}(z_{j+1}^*, z_j; t_j) := \frac{\langle z_{j+1} | \hat{H}(t_j) | z_j \rangle}{\langle z_{j+1} | z_j \rangle}. \quad (2.13)$$

Using the coherent-state overlap formula

$$\langle z_{j+1} | z_j \rangle = \exp \left\{ -\frac{1}{2} |z_{j+1}|^2 + z_{j+1}^* z_j - \frac{1}{2} |z_j|^2 \right\} \quad (2.14)$$

we write $e^{f(z^*, z)}$ as

$$\begin{aligned} e^{f(z^*, z)} &= \exp \left[\sum_{j=0}^{N-1} \left\{ -\frac{1}{2} |z_{j+1}|^2 + z_{j+1}^* z_j - \frac{1}{2} |z_j|^2 - \frac{i\tau}{\hbar} \mathcal{H}_{j+1,j} \right\} \right] \\ &= \exp \left[\sum_{j=0}^{N-1} \left\{ \frac{1}{2} (z_{j+1}^* - z_j^*) z_j - \frac{1}{2} z_{j+1}^* (z_{j+1} - z_j) - \frac{i\tau}{\hbar} \mathcal{H}_{j+1,j} \right\} \right]. \end{aligned} \quad (2.15)$$

Later the limit $N \rightarrow \infty$ (respectively $\tau \rightarrow 0$) will be taken. Then the above summations will turn into integrals, and expressions (2.8)–(2.12) would appear to be exact, were it not for the well known problems attached to the meaning of such functional integrals. We see, however, that the treatment of time-dependent systems is (almost) identical to that of time-independent ones.

2.2. The stationary-exponent approximation

In the semiclassical limit of small \hbar we can approximate the integral (2.10), with equation (2.15), by looking for the places where the exponent f is stationary and replacing it in their vicinity by a quadratic form of its variables (z^*, z) . We call this the stationary-exponent approximation or the Gaussian approximation. In the literature it is often referred to as the stationary-phase approximation (SPA) or the steepest-descent approximation. Strictly speaking, neither of these two names is quite correct. Our exponent f is complex, therefore it is not a phase, and ‘steepest descent’ refers to a geometrical interpretation for the case of a single complex variable.

Our approximation method involves going into the complex plane for the variables x_j and y_j , which are intrinsically real. Therefore it is important to keep clearly in mind why we go through so many developments where we treat them as complex. The integrals we are after are

over the *real* variables x_j, y_j . Anything else we may do to calculate them is just mathematical tricks. The trick of going into the complex plane works only with analytic functions. Hence, when we have to do an integral over real x_j and y_j , we shall first make sure that the function is analytic, and then we shall see what happens to this analytic function when we let the variables be complex. These words of caution may seem superfluous at this time, but they will turn out to be crucial later, when the need for further simplification arises. As we shall see in section 3, confusion about this point seems to be what led Grossmann and Xavier [Gro98b] into error. As a start, one should test this analyticity requirement for the present integral (2.10). We have already assumed in section 2.1 that the operator \hat{H} could be approximated by a polynomial in the operators \hat{a}^\dagger and \hat{a} . When we take its matrix element between the bra $\langle z_{j+1} |$ and the ket $|z_j\rangle$, we have to do an integral of the type

$$\langle z_{j+1} | \hat{H}(t_j) | z_j \rangle = \int dx \langle z_{j+1} | x \rangle \left(\text{Polynomial in } x \text{ and } \frac{d}{dx} \right) \langle x | z_j \rangle \quad (2.16)$$

where the two wavefunctions are given by (2.4) and its complex conjugate. The integral produces an analytic function of z_{j+1}^* and z_j , with the additional factor

$$\exp \left[-\frac{1}{2} (z_{j+1}^* z_{j+1} + z_j^* z_j) \right] \quad (2.17)$$

which is the only place where the other two variables, z_{j+1} and z_j^* , occur. According to (2.13), this must then be divided by $\langle z_{j+1} | z_j \rangle$, which is given in (2.14), and which contains the same factor (2.17), times another, never vanishing, analytic function of z_{j+1}^* and z_j . When the quotient is taken, the factor (2.17) cancels out. Hence the ‘effective Hamiltonian function’ $\mathcal{H}_{j+1,j}$ or $\mathcal{H}(z_{j+1}^*, z_j; t_j)$ of equation (2.13) is an analytic function of the variables z_{j+1}^* and z_j separately, and *it does not contain the other two variables z_{j+1} and z_j^* at all!*

Thus, the basic idea is to approximate the argument of the exponential in equation (2.15) by a second-order Taylor expansion in the vicinity of the stationary trajectory. The resulting quadratic form in the exponent leads to a Gaussian integral which can be done exactly. There may be more than one classical trajectory between the end points, each with its own contribution, which leads to a sum. For clarity during the derivation, this sum will not be written explicitly. We find the stationary points by requiring the vanishing of the derivatives of f with respect to z and z^* separately, as mentioned earlier

$$\begin{aligned} \frac{\partial f}{\partial z_j} &= z_{j+1}^* - z_j^* - \frac{i\tau}{\hbar} \frac{\partial \mathcal{H}_{j+1,j}}{\partial z_j} = 0 & j = 1, \dots, N-1 \\ \frac{\partial f}{\partial z_{j+1}^*} &= -z_{j+1} + z_j - \frac{i\tau}{\hbar} \frac{\partial \mathcal{H}_{j+1,j}}{\partial z_{j+1}^*} = 0 & j = 0, \dots, N-2. \end{aligned} \quad (2.18)$$

We introduce new integration variables η and η^* which describe the deviations from the points of stationary exponent: $z \rightarrow z + \eta$, $z^* \rightarrow z^* + \eta^*$, with the boundary conditions

$$\eta_0 = \eta_0^* = \eta_N = \eta_N^* = 0. \quad (2.19)$$

Now the exponent in equation (2.15)

$$\begin{aligned} f(z^* + \eta^*, z + \eta) &= \sum_{j=0}^{N-1} \left\{ \frac{1}{2} (z_{j+1}^* + \eta_{j+1}^* - z_j^* - \eta_j^*) (z_j + \eta_j) - \frac{1}{2} (z_{j+1}^* + \eta_{j+1}^*) \right. \\ &\quad \left. \times (z_{j+1} + \eta_{j+1} - z_j - \eta_j) - \frac{i\tau}{\hbar} \mathcal{H}_{j+1,j}(z_{j+1}^* + \eta_{j+1}^*, z_j + \eta_j) \right\} \end{aligned} \quad (2.20)$$

will be expanded into a Taylor series in (η^*, η) around the stationary points (z^*, z) up to second order:

$$f(z^* + \eta^*, z + \eta) \approx \sum_{j=0}^{N-1} \left\{ \frac{1}{2} (z_{j+1}^* - z_j^*) z_j - \frac{1}{2} z_{j+1}^* (z_{j+1} - z_j) \right.$$

$$\begin{aligned}
& -\frac{i\tau}{\hbar}\mathcal{H}_{j+1,j}(z_{j+1}^*, z_j) + \frac{1}{2}(z_{j+1}^* - z_j^*)\eta_j \\
& + \frac{1}{2}(\eta_{j+1}^* - \eta_j^*)z_j - \frac{1}{2}z_{j+1}^*(\eta_{j+1} - \eta_j) \\
& - \frac{1}{2}\eta_{j+1}^*(z_{j+1} - z_j) - \frac{i\tau}{\hbar}\frac{\partial\mathcal{H}_{j+1,j}}{\partial z_j}\eta_j - \frac{i\tau}{\hbar}\frac{\partial\mathcal{H}_{j+1,j}}{\partial z_{j+1}^*}\eta_{j+1}^* \\
& + \frac{1}{2}(\eta_{j+1}^* - \eta_j^*)\eta_j - \frac{1}{2}\eta_{j+1}^*(\eta_{j+1} - \eta_j) \\
& - \frac{i\tau}{2\hbar}\left[\frac{\partial^2\mathcal{H}_{j+1,j}}{\partial z_j^2}\eta_j^2 + 2\frac{\partial^2\mathcal{H}_{j+1,j}}{\partial z_{j+1}^*\partial z_j}\eta_{j+1}^*\eta_j + \frac{\partial^2\mathcal{H}_{j+1,j}}{\partial z_{j+1}^{*2}}\eta_{j+1}^{*2}\right] \Big\} \quad (2.21) \\
= & f(z^*, z) + \sum_{j=0}^{N-1} \left\{ \left(z_{j+1}^* - \frac{1}{2}z_j^* - \frac{i\tau}{\hbar}\frac{\partial\mathcal{H}_{j+1,j}}{\partial z_j} \right) \eta_j - \frac{1}{2}z_{j+1}^*\eta_{j+1} \right. \\
& + \left(z_j - \frac{1}{2}z_{j+1} - \frac{i\tau}{\hbar}\frac{\partial\mathcal{H}_{j+1,j}}{\partial z_{j+1}^*} \right) \eta_{j+1}^* - \frac{1}{2}z_j\eta_j^* \\
& - \frac{1}{2}\eta_{j+1}^*\eta_{j+1} + \eta_{j+1}^*\eta_j - \frac{1}{2}\eta_j^*\eta_j \\
& \left. - \frac{i\tau}{2\hbar}\left[\frac{\partial^2\mathcal{H}_{j+1,j}}{\partial z_j^2}\eta_j^2 + 2\frac{\partial^2\mathcal{H}_{j+1,j}}{\partial z_{j+1}^*\partial z_j}\eta_{j+1}^*\eta_j + \frac{\partial^2\mathcal{H}_{j+1,j}}{\partial z_{j+1}^{*2}}\eta_{j+1}^{*2}\right] \right\}. \quad (2.22)
\end{aligned}$$

The terms of first order (second and third line of equation (2.22)) vanish, when the boundary conditions (2.19) are taken into account, because of the stationary exponent conditions (2.18). Inserting equation (2.22) into (2.10) yields, in view of equation (2.19),

$$\begin{aligned}
K(z'', t; z', 0) = & e^{f(z^*, z)} \int \left\{ \prod_{j=1}^{N-1} \frac{d\eta_j^* d\eta_j}{2\pi i} \right\} \exp \left[\sum_{j=0}^{N-1} \left\{ -\frac{i\tau}{2\hbar} \frac{\partial^2\mathcal{H}_{j+1,j}}{\partial z_j^2} \eta_j^2 \right. \right. \\
& \left. \left. - \frac{i\tau}{2\hbar} \frac{\partial^2\mathcal{H}_{j+1,j}}{\partial z_{j+1}^{*2}} \eta_{j+1}^{*2} - \eta_j^*\eta_j + \left(1 - \frac{i\tau}{\hbar} \frac{\partial^2\mathcal{H}_{j+1,j}}{\partial z_{j+1}^*\partial z_j} \right) \eta_{j+1}^*\eta_j \right\} \right]. \quad (2.23)
\end{aligned}$$

2.3. Performing the integrals

At this point we start to carry out the integrations over the variables η_j, η_j^* . We have two ways of doing this. In the body of the paper, we perform successively $\iint d\eta_1^* d\eta_1, \iint d\eta_2^* d\eta_2, \dots$, deriving eventually a recursion relation, which becomes a nonlinear differential equation when we go to the limit of continuous variables. In the appendix, we do it by writing the multiple integral in terms of the determinant of the quadratic form; we calculate this determinant with a pair of recursion relations, which turn into linear differential equations in the limit. The two methods are quite different, but they give the same result. The reader who wants to save time does not have to study both. In the appendix, then, we go on to use the same method to calculate a different path integral, which arises in section 3.

Here, we calculate the integrals $\iint d\eta_j^* d\eta_j$ by applying the general formula

$$\begin{aligned}
& \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dx dy}{\pi} e^{A_1 x^2 + A_2 y^2 + A_3 xy + B_1 x + B_2 y} \\
& = \frac{1}{\sqrt{A_1 A_2 - A_3^2/4}} \exp \left(\frac{-B_1^2 A_2 - B_2^2 A_1 + B_1 B_2 A_3}{4A_1 A_2 - A_3^2} \right) \quad (2.24)
\end{aligned}$$

which is correct if the integrations are done along the two real axes, as they would be if x and y were the real and imaginary parts of η , respectively. Two comments need to be made here.

First, the integral must converge. If we call $-\mu_1$ and $-\mu_2$ the eigenvalues of the symmetric matrix of the quadratic form in the exponent on the left-hand side, convergence requires that μ_1 and μ_2 both have a non-negative real part. Second, the phase of the square root needs to be defined, since A_1, A_2, A_3 are complex numbers. This square root is also equal to the product $\sqrt{\mu_1}\sqrt{\mu_2}$, and the phase ϕ_i of each $\sqrt{\mu_i}$ must be chosen to satisfy $-\pi/4 \leq \phi_i \leq \pi/4$. This phase rule is extremely important in determining the phase of the semiclassical propagator when one works in configuration space. For the present case of the semiclassical coherent-state propagator, it is less crucial because the phase can usually be determined by appealing to continuity in time.

We must now rewrite this formula in terms of the variables η and η^* rather than x and y . The transformation of variables is simple enough, but the paths of integration are totally changed, and the associated conditions need to be restated. To simplify notations a little, we call the variables u and v instead of η and η^* , respectively. Then the new formula is

$$\iint \frac{du dv}{2\pi i} e^{a_1 u^2 + a_2 v^2 + a_3 uv + b_1 u + b_2 v} = \frac{1}{\sqrt{a_3^2 - 4a_1 a_2}} \exp\left(\frac{b_1^2 a_2 + b_2^2 a_1 - b_1 b_2 a_3}{a_3^2 - 4a_1 a_2}\right). \quad (2.25)$$

The integral is convergent if and only if the two numbers

$$\mu_{1,2} = -a_3 \pm 2\sqrt{a_1 a_2}$$

which are the negatives of the eigenvalues of the symmetric matrix in the exponent on the left-hand side of equation (2.24), *not* (2.25), both have a non-negative real part. The square root in equation (2.25) is again the product $\sqrt{\mu_1}\sqrt{\mu_2}$ and, once again, the phase ϕ_i of each $\sqrt{\mu_i}$ must be chosen to satisfy $-\pi/4 \leq \phi_i \leq \pi/4$.

For the η_1^*, η_1 integration, the parameters are

$$a_1 = -\frac{i\tau}{2\hbar} \frac{\partial^2 \mathcal{H}_{2,1}}{\partial z_1^2} \quad a_2 = -\frac{i\tau}{2\hbar} \frac{\partial^2 \mathcal{H}_{1,0}}{\partial z_1^{*2}} := X_1 \quad a_3 = -1 \quad (2.26)$$

$$b_1 = \left(1 - \frac{i\tau}{\hbar} \frac{\partial^2 \mathcal{H}_{2,1}}{\partial z_2^* \partial z_1}\right) \eta_2^* \quad \text{and} \quad b_2 = 0. \quad (2.27)$$

Convergence is assured since $-a_3$ is real, positive and much larger than a_1 and a_2 (τ is arbitrarily small). The correct branch of the square root is the one whose phase is close to 0. The result is

$$\begin{aligned} K(z_N, t; z_0, 0) &= \frac{e^{f(z^*, z)}}{\sqrt{1 + 2i\frac{\tau}{\hbar} \frac{\partial^2 \mathcal{H}_{2,1}}{\partial z_1^2} X_1}} \int \left[\prod_{j=2}^{N-1} \frac{d\eta_j^* d\eta_j}{2\pi i} \right] \exp \left\{ \frac{\left(1 - \frac{i\tau}{\hbar} \frac{\partial^2 \mathcal{H}_{2,1}}{\partial z_2^* \partial z_1}\right)^2 X_1 \eta_2^{*2}}{1 + 2\frac{i\tau}{\hbar} \frac{\partial^2 \mathcal{H}_{2,1}}{\partial z_1^2} X_1} \right\} \\ &\times \exp \left\{ \sum_{j=2}^{N-1} -\frac{i\tau}{2\hbar} \frac{\partial^2 \mathcal{H}_{j+1,j}}{\partial z_j^2} \eta_j^2 - \frac{i\tau}{2\hbar} \frac{\partial^2 \mathcal{H}_{j,j-1}}{\partial z_j^{*2}} \eta_j^{*2} - \eta_j^* \eta_j \right. \\ &\left. + \left(1 - \frac{i\tau}{\hbar} \frac{\partial^2 \mathcal{H}_{j+1,j}}{\partial z_{j+1}^* \partial z_j}\right) \eta_{j+1}^* \eta_j \right\}. \quad (2.28) \end{aligned}$$

The second set of integrals, $\iint d\eta_2^* d\eta_2$, is done again with equation (2.25), but now a_2 becomes more complicated and is expressed as a function of X_1 . This kind of behaviour continues at each stage of the integrations. If we call X_j the value of a_2 when we do the integrals $\iint d\eta_j^* d\eta_j$

according to equation (2.25), we find the following parameters:

$$\begin{aligned} a_1 &= -\frac{i\tau}{2\hbar} \frac{\partial^2 \mathcal{H}_{j+1,j}}{\partial z_j^2} & a_3 &= -1 \\ b_1 &= \left(1 - \frac{i\tau}{\hbar} \frac{\partial^2 \mathcal{H}_{j+1,j}}{\partial z_{j+1}^* \partial z_j}\right) \eta_{j+1}^* & b_2 &= 0 \end{aligned} \quad (2.29)$$

while the formula for a_2 becomes a recursion relation for X_j

$$\begin{aligned} X_0 &= 0 & (\text{initial condition}) \\ X_j &= -\frac{i\tau}{2\hbar} \frac{\partial^2 \mathcal{H}_{j,j-1}}{\partial z_j^{*2}} + \frac{\left(1 - \frac{i\tau}{\hbar} \frac{\partial^2 \mathcal{H}_{j,j-1}}{\partial z_j^* \partial z_{j-1}}\right)^2}{1 + 2\frac{i\tau}{\hbar} \frac{\partial^2 \mathcal{H}_{j,j-1}}{\partial z_{j-1}^2}} X_{j-1} & j &= 1, \dots, N-1. \end{aligned} \quad (2.30)$$

Once all integrations are done, the result is

$$K(z_N, t; z_0, 0) = e^{f(z^*, z)} \prod_{j=1}^{N-1} \frac{1}{\sqrt{1 + 2i\frac{\tau}{\hbar} \frac{\partial^2 \mathcal{H}_{j+1,j}}{\partial z_j^2} X_j}} \quad (2.31)$$

with X_j satisfying equation (2.30). Once again, the phase of each square root should be chosen close to 0.

2.4. Continuous variables

The time has come to perform the limit $N \rightarrow \infty$ (respectively $\tau \rightarrow 0$). This gets rid of the approximations associated with the time discretization in equation (2.15), and the discrete recursion formula (2.30) becomes a solvable differential equation. The stationary phase conditions (2.18) are in this limit identical to Hamilton's equations

$$\begin{aligned} \dot{z}^* &= \frac{i}{\hbar} \frac{\partial \mathcal{H}}{\partial z} \\ \dot{z} &= -\frac{i}{\hbar} \frac{\partial \mathcal{H}}{\partial z^*} \end{aligned} \quad (2.32)$$

where $\mathcal{H}(z^*, z, t)$ is the limit of $\mathcal{H}_{j+1,j}$, equation (2.13), and is simply given by

$$\mathcal{H}(z^*, z, t) = \langle z | \hat{H}(t) | z \rangle. \quad (2.33)$$

The question of boundary conditions presents us with a grave problem at this point. We have been approximating the propagator going in time t from coherent state (q', p') to coherent state (q'', p'') , and our approximation seems to involve the classical path between the two points in phase space. But there is no such classical path, real or complex, between these two points, generically speaking! The unique classical trajectory which goes through (q', p') at time 0 does not in general go through (q'', p'') at time t . We have too many boundary conditions!

One way out of this quandary was shown by [Wei83]. Actually, z_N and z_0^* do not enter the equations of motion at all. Neither one occurs in equations (2.15) or (2.18). Thus, the problem is really to find a classical path going from z_0 to z_N^* in time t , and such a path does exist, but it is usually complex, in spite of the fact that (q_0, p_0) and (q_N, p_N) are real. The path will be real only if (q_0, p_0) and (q_N, p_N) happen to be on the same classical trajectory. Given that the intermediate values of q and p will now be both complex usually, it makes no sense to retain

the notations z and z^* , which can only lead to confusion. We replace these by the two complex variables u and v , which are now manifestly independent:

$$\begin{aligned} z &\rightarrow u = \frac{1}{\sqrt{2}} \left(\frac{q}{b} + i \frac{p}{c} \right) \\ z^* &\rightarrow v = \frac{1}{\sqrt{2}} \left(\frac{q}{b} - i \frac{p}{c} \right). \end{aligned} \quad (2.34)$$

Note also the inverse formulae

$$\begin{aligned} q &= \frac{b}{\sqrt{2}}(u + v) \\ p &= -\frac{ic}{\sqrt{2}}(u - v). \end{aligned} \quad (2.35)$$

The differential equations (2.32) are now

$$\begin{aligned} i\hbar\dot{u} &= +\frac{\partial\mathcal{H}}{\partial v} \\ i\hbar\dot{v} &= -\frac{\partial\mathcal{H}}{\partial u} \end{aligned} \quad (2.36)$$

with the boundary conditions

$$\begin{aligned} u(0) &= z' & v(t) &= z''^* \\ v(0) &= \text{nothing special} \neq z'^* \\ u(t) &= \text{nothing special} \neq z''. \end{aligned} \quad (2.37)$$

$v(0)$ and $u(t)$ come out of the calculation and do not have any simple relation to z' and z'' , except in the special case when there exists a real trajectory going from z' to z'' in time t . Then and only then do we get $v(0) = z'^*$ and $u(t) = z''$. Otherwise, the end points of the classical path are truly complex in phase space. To complete the definitions, we rename these end points as follows:

$$u(0) \equiv u' \quad v(0) \equiv v' \quad u(t) \equiv u'' \quad v(t) \equiv v''. \quad (2.38)$$

Given the change of variables, we note the following differentiation rules, which follow from equations (2.34) and (2.35) and will be needed later:

$$\begin{aligned} \frac{\partial}{\partial q} &= \frac{\partial v}{\partial q} \frac{\partial}{\partial v} + \frac{\partial u}{\partial q} \frac{\partial}{\partial u} = \frac{1}{\sqrt{2}b} \left(\frac{\partial}{\partial v} + \frac{\partial}{\partial u} \right) \\ \frac{\partial}{\partial p} &= \frac{\partial v}{\partial p} \frac{\partial}{\partial v} + \frac{\partial u}{\partial p} \frac{\partial}{\partial u} = \frac{i}{\sqrt{2}c} \left(-\frac{\partial}{\partial v} + \frac{\partial}{\partial u} \right) \end{aligned} \quad (2.39)$$

$$\begin{aligned} \frac{\partial}{\partial v} &= \frac{1}{\sqrt{2}} \left(b \frac{\partial}{\partial q} + ic \frac{\partial}{\partial p} \right) \\ \frac{\partial}{\partial u} &= \frac{1}{\sqrt{2}} \left(b \frac{\partial}{\partial q} - ic \frac{\partial}{\partial p} \right). \end{aligned} \quad (2.40)$$

Let us rewrite $f(z^*, z)$, equation (2.15), in the continuous limit and in terms of the new variables. Since f can also be written

$$\tau \sum_{j=0}^{N-1} \left\{ \frac{z_{j+1}^* - z_j^*}{2\tau} z_j - z_{j+1}^* \frac{z_{j+1} - z_j}{2\tau} - \frac{i}{\hbar} \mathcal{H}_{j+1,j} \right\} \quad (2.41)$$

one might think that, in the limit $\tau \rightarrow 0$, this would reduce to

$$\int_0^t dt' \left[\frac{1}{2}(\dot{v}u - \dot{u}v) - \frac{i}{\hbar} \mathcal{H}(u, v, t') \right] \quad (2.42)$$

but that would be a mistake. Recalling the earlier discussion, we realize that equation (2.42) assumes that $u(t) = u_N$, which is not equal to z'' , and it also assumes that $v(0) = v_0$, which is not equal to z'^* . But in expression (2.15), u_N or z_N was z'' , and v_0 or z_0^* was z'^* . To correct this mistake, we must take out from the sum the two terms containing u_N and v_0 , namely $-\frac{1}{2}v_N u_N$ and $-\frac{1}{2}v_0 u_0$, and replace them by their correct values, namely $-\frac{1}{2}|z''|^2$ and $-\frac{1}{2}|z'|^2$. Consequently, the value of f in the limit $\tau \rightarrow 0$ should be

$$f = \int_0^t dt' \left[\frac{1}{2}(\dot{v}u - \dot{u}v) - \frac{i}{\hbar} \mathcal{H}(u, v, t') \right] + \frac{1}{2}(v''u'' + v'u') - \frac{1}{2}(|z''|^2 + |z'|^2). \quad (2.43)$$

Next we rewrite the product in equation (2.31), performing the limit $N \rightarrow \infty$ and using $\ln(1+x) = x + O(x^2)$:

$$\begin{aligned} \lim_{N \rightarrow \infty} \prod_{j=1}^{N-1} \left\{ 1 + 2i \frac{\tau}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u_j^2} X_j \right\}^{-\frac{1}{2}} &= \lim_{N \rightarrow \infty} \exp \left\{ -\frac{1}{2} \sum_{j=1}^{N-1} \ln \left(1 + 2i \frac{\tau}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u_j^2} X_j \right) \right\} \\ &= \lim_{N \rightarrow \infty} \exp \left\{ -i \frac{\tau}{\hbar} \sum_{j=1}^{N-1} \frac{\partial^2 \mathcal{H}}{\partial u_j^2} X_j \right\} \\ &= \exp \left\{ -\frac{i}{\hbar} \int_0^t dt' \frac{\partial^2 \mathcal{H}}{\partial u^2}(t') X(t') \right\}. \end{aligned} \quad (2.44)$$

Altogether, the propagator is

$$\begin{aligned} K(z'', t; z', 0) &= \exp \left\{ -\frac{i}{\hbar} \int_0^t dt' \frac{\partial^2 \mathcal{H}}{\partial u^2}(t') X(t') \right\} \exp \left\{ \int_0^t dt' \left[\frac{1}{2}(\dot{v}u - \dot{u}v) - \frac{i}{\hbar} \mathcal{H} \right] \right. \\ &\quad \left. + \frac{1}{2}(v'u' + v''u'') - \frac{1}{2}(|z'|^2 + |z''|^2) \right\}. \end{aligned} \quad (2.45)$$

We still have to write the continuous form of the discrete recursion formula (2.30) for $X(t)$. With $\frac{(1-ax)^2}{1+bx} = 1 - (2a+b)x + O(x^2)$ equation (2.30) gives

$$X_j \approx -\frac{i\tau}{2\hbar} \frac{\partial^2 \mathcal{H}}{\partial v_j^2} + X_{j-1} - \left(2\frac{i\tau}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u_{j-1} \partial v_j} + 2\frac{i\tau}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u_{j-1}^2} X_{j-1} \right) X_{j-1}. \quad (2.46)$$

In the limit $N \rightarrow \infty$ this leads to the nonlinear differential equation

$$\dot{X}(t) = -\frac{i}{2\hbar} \frac{\partial^2 \mathcal{H}}{\partial v^2} - 2\frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u \partial v} X(t) - 2\frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u^2} X^2(t) \quad (2.47)$$

with the initial condition

$$X(0) = 0. \quad (2.48)$$

To solve this, we consider small variations in the solutions of Hamilton's equations (2.36) around a given solution $v(t)$, $u(t)$:

$$\begin{aligned} \delta \dot{u} &= -\frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u \partial v} \delta u - \frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial v^2} \delta v \\ \delta \dot{v} &= +\frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u^2} \delta u + \frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u \partial v} \delta v. \end{aligned} \quad (2.49)$$

It can be seen that the solution of equation (2.47) is $X = \frac{1}{2} \frac{\delta u}{\delta v}$. The time derivative is

$$\begin{aligned} \dot{X} &= \frac{1}{2} \frac{\delta \dot{u}}{\delta v} - \frac{1}{2} \frac{\delta u}{\delta v^2} \delta \dot{v} \\ &= -\frac{i}{2\hbar} \frac{\partial^2 \mathcal{H}}{\partial u \partial v} \frac{\delta u}{\delta v} - \frac{i}{2\hbar} \frac{\partial^2 \mathcal{H}}{\partial v^2} - \frac{1}{2} \frac{\delta u}{\delta v} \left[\frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u^2} \frac{\delta u}{\delta v} + \frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u \partial v} \right] \end{aligned}$$

$$\begin{aligned}
&= -\frac{i}{2\hbar} \frac{\partial^2 \mathcal{H}}{\partial v^2} - \frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u \partial v} \frac{\delta u}{\delta v} - \frac{i}{2\hbar} \frac{\partial^2 \mathcal{H}}{\partial u^2} \left(\frac{\delta u}{\delta v} \right)^2 \\
&= -\frac{i}{2\hbar} \frac{\partial^2 \mathcal{H}}{\partial v^2} - 2 \frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u \partial v} X - 2 \frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u^2} X^2
\end{aligned} \tag{2.50}$$

which agrees with the differential equation (2.47). The initial condition $X(0) = 0$ can be satisfied by picking $\delta u(0) = \delta u' = 0$, $\delta v(0) = \delta v'$ arbitrary. The integrand in the first exponential of equation (2.45) can be transformed with the help of equation (2.49)

$$\frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u^2} X = \frac{i}{2\hbar} \frac{\partial^2 \mathcal{H}}{\partial u^2} \frac{\delta u}{\delta v} = \frac{1}{2} \frac{\delta \dot{v}}{\delta v} - \frac{i}{2\hbar} \frac{\partial^2 \mathcal{H}}{\partial u \partial v} = \frac{1}{2} \frac{d}{dt} \ln \delta v - \frac{i}{2\hbar} \frac{\partial^2 \mathcal{H}}{\partial u \partial v} \tag{2.51}$$

so that the first exponent of equation (2.45) is

$$\begin{aligned}
\exp \left\{ -\frac{i}{\hbar} \int_0^t dt' \frac{\partial^2 \mathcal{H}}{\partial u^2}(t') X(t') \right\} &= \exp \left\{ -\frac{1}{2} \int_0^t dt' \left[\frac{d}{dt'} (\ln \delta v) - \frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial u \partial v} \right] \right\} \\
&= \sqrt{\frac{\delta v'}{\delta v''}} \exp \left\{ \frac{i}{2\hbar} \int_0^t dt' \frac{\partial^2 \mathcal{H}}{\partial u \partial v} \right\}.
\end{aligned} \tag{2.52}$$

It is understood that $\delta v'/\delta v''$ is calculated with the initial condition $\delta u' = 0$. The phase of the square root evolves continuously with time, starting at 0 for $t = 0$. Because all the numbers are generically complex, $\delta v''(t)$ does not usually have zeros; therefore the phase is always well defined, barring an accident. In the end we obtain

$$\begin{aligned}
K(z'', t; z', 0) &= \sqrt{\frac{\delta v'}{\delta v''}} \exp \left\{ \frac{i}{2\hbar} \int_0^t dt' \frac{\partial^2 \mathcal{H}}{\partial u \partial v} \right\} \exp \left\{ \int_0^t dt' \left[\frac{1}{2} (\dot{v}u - \dot{u}v) - \frac{i}{\hbar} \mathcal{H} \right] \right. \\
&\quad \left. + \frac{1}{2} (v''u'' + v'u') - \frac{1}{2} (|z'|^2 + |z''|^2) \right\}.
\end{aligned} \tag{2.53}$$

Just as a plausibility check, consider the limit $t \rightarrow 0$. In this case, the complex path has $u'' = u' = z'$, $v' = v'' = z''^*$, and therefore $K(z'', 0; z', 0) = \exp\{0\} \exp\{0 + \frac{1}{2}v'u' + \frac{1}{2}v''u'' - \frac{1}{2}|z'|^2 - \frac{1}{2}|z''|^2\} = \exp\{-\frac{1}{2}|z'|^2 + z'z'' - \frac{1}{2}|z''|^2\} = \langle z''|z' \rangle$, which is the overlap of two coherent states.

2.5. The complex action

In most discussions of Hamiltonian mechanics, one gains much simplicity and understanding by defining the ‘action’, which is the quantity entering Hamilton’s variational principle and the Hamilton–Jacobi equation. In the present problem, this is true also. The action is complex in most cases, like the trajectories themselves and like the energy. It is given by the formula

$$S(v'', u', t) := \int_0^t dt' \left[\frac{i\hbar}{2} (\dot{u}v - \dot{v}u) - \mathcal{H}(u, v, t') \right] - \frac{i\hbar}{2} (u''v'' + u'v'). \tag{2.54}$$

The independent variables are v'' and u' , the two end variables which define the classical trajectory, and the time t ; u'' and v' must be understood as functions of these three variables. Note that u and v are proportional to $1/\sqrt{\hbar}$, since b and c in equation (2.34) are both proportional to $\sqrt{\hbar}$. Therefore the only term in S which depends on \hbar is $\int_0^t \mathcal{H}(u, v, t') dt'$. We shall show in the following that this S is indeed the correct action for the boundary conditions we have. Given its definition, S should be an analytic function of its variables most of the time, since $\mathcal{H}(u, v)$ is analytic and the velocities \dot{u} and \dot{v} can be written as derivatives of \mathcal{H} using Hamilton’s equations (2.36). It would take an accident in the determination of the classical trajectory from the boundary conditions to produce a singularity. Similarly, the functions u'' and v' should be

analytic in v'' and u' most of the time; in fact, according to equation (2.60), they are essentially the partial derivatives of S .

Suppose that we make small variations $\delta v''$, $\delta u'$, δt in each of the independent variables. This induces variations $\delta u''$, $\delta v'$ in u'' and v' . It also induces variations $\delta u(t')$, $\delta v(t')$ in the trajectory itself. The consequent variation in S is

$$\begin{aligned} \delta S = \int_0^t dt' \left[\frac{i\hbar}{2} (v\delta\dot{u} - u\delta\dot{v} - \dot{v}\delta u + \dot{u}\delta v) - \frac{\partial\mathcal{H}}{\partial v}\delta v - \frac{\partial\mathcal{H}}{\partial u}\delta u \right] \\ - \frac{i\hbar}{2} (v''\delta u'' + u''\delta v'' + v'\delta u' + u'\delta v') + \delta t \left[\frac{i\hbar}{2} (\dot{u}''v'' - \dot{v}''u'') - \mathcal{H}(u'', v'', t) \right]. \end{aligned} \quad (2.55)$$

We do two integrations by parts as follows:

$$\begin{aligned} \int_0^t dt' v\delta\dot{u} &= v''\delta u(t) - v'\delta u(0) - \int_0^t dt' \dot{v}\delta u \\ - \int_0^t dt' u\delta\dot{v} &= -u''\delta v(t) + u'\delta v(0) + \int_0^t dt' \dot{u}\delta v. \end{aligned} \quad (2.56)$$

Since the lower limit 0 of the t' -integral is not changed, we have

$$\delta u(0) = \delta u' \quad \delta v(0) = \delta v'. \quad (2.57)$$

But the upper limit is changed from t to $t + \delta t$, hence

$$\delta u(t) = \delta u'' - \dot{u}''\delta t \quad \delta v(t) = \delta v'' - \dot{v}''\delta t. \quad (2.58)$$

Much simplification occurs when we carry this back into equation (2.55), and we find for the variation in S

$$\delta S = \int_0^t dt' \left[\left(i\hbar\dot{u} - \frac{\partial\mathcal{H}}{\partial v} \right) \delta v + \left(-i\hbar\dot{v} - \frac{\partial\mathcal{H}}{\partial u} \right) \delta u \right] - i\hbar(u''\delta v'' + v'\delta u') - \mathcal{H}(u'', v'', t)\delta t. \quad (2.59)$$

The first line says that paths satisfying Hamilton's equations (2.36) have a stationary action S when the independent variables v'' , u' , t are held fixed. The second line says that, for such a classical trajectory, the derivatives of S with respect to these variables are

$$\frac{\partial S}{\partial v''} = -i\hbar u'' \quad \frac{\partial S}{\partial u'} = -i\hbar v' \quad \frac{\partial S}{\partial t} = -\mathcal{H}(u'', v'', t). \quad (2.60)$$

In the special case of a time-independent Hamiltonian, $\mathcal{H}(u'', v'')$ is the constant energy \mathcal{E} , and the last equality becomes

$$\frac{\partial S}{\partial t} = -\mathcal{E}. \quad (2.61)$$

We are now able to express most of the coherent-state propagator, equation (2.53), in terms of the action function. By equation (2.60) we have

$$\frac{\delta v'}{\delta v''} = \frac{i}{\hbar} \frac{\partial^2 S}{\partial u' \partial v''}. \quad (2.62)$$

Therefore the coherent-state propagator can be written

$$\begin{aligned} K(z'', t; z', 0) &= \sum_v \sqrt{\frac{i}{\hbar} \frac{\partial^2 S_v}{\partial u' \partial v''}} \exp \left\{ \frac{i}{2\hbar} \int_0^t dt' \left(\frac{\partial^2 \mathcal{H}}{\partial u \partial v} \right)_v \right\} \\ &\times \exp \left\{ \frac{i}{\hbar} S_v(v'', u', t) - \frac{1}{2} (|z''|^2 + |z'|^2) \right\}. \end{aligned} \quad (2.63)$$

The sum over v represents the sum over all (complex) classical trajectories satisfying the boundary conditions, since there may be more than one. We have already mentioned (see before equation (2.18)) that we were going to suppress this sum for purposes of clarity, and we shall do so in the future again.

There is one very important caveat. The Hamiltonian function $\mathcal{H}(u, v, t)$ entering equations (2.54) and (2.63) is *not the original classical Hamiltonian* of the problem, the quantal version of which we used when we first wrote the path integral (2.5). As equation (2.33) shows, this ‘script’ Hamiltonian is a smoothed version of the original one, obtained by folding it with a Gaussian in phase space. This is one of the interesting features of formula (2.63). Another interesting feature is the first exponential, which we shall write

$$e^{\frac{i}{\hbar}\mathcal{I}} \quad (2.64)$$

where the quantity \mathcal{I} , with dimensions of action, is defined by

$$\mathcal{I}(v'', u', t) := \frac{1}{2} \int_0^t dt' \left(\frac{\partial^2 \mathcal{H}}{\partial u \partial v} \right). \quad (2.65)$$

Though this \mathcal{I} term was assuredly obtained in the past by various workers in the field, most authors seem to have been in a big hurry to forget its existence. One simple and compelling reason for not doing so is the following: when you calculate the harmonic oscillator (as we do in section 6), you get the exact answer if you keep \mathcal{I} , but you do not if you drop it.

There will be more discussion of \mathcal{I} in sections 3 and 4. This, and only this, is the result of making the standard semiclassical approximations on the coherent state propagator (2.10). As far as we know, no formula equivalent to (2.63) has been in wide use before. Both Herman and Kay [Her86, Kay94a, Kay94b] claim, in words only, that a particular formula follows from a semiclassical treatment of the coherent-state propagator. In both cases the claim is not justified and the formula is incorrect. In the next section, we shall see how other formulae can be derived in which the two special features above are either absent or reversed. In sections 4 and 5 we shall compare with two other formulae in the literature.

For an additional note, we use equations (2.35) to write the integrand of \mathcal{I} in terms of q and p

$$\frac{\partial^2 \mathcal{H}}{\partial u \partial v} = \frac{b^2}{2} \frac{\partial^2 \mathcal{H}}{\partial q^2} + \frac{c^2}{2} \frac{\partial^2 \mathcal{H}}{\partial p^2}. \quad (2.66)$$

Given formulae (2.3), we see that \mathcal{I} is of order \hbar . Whenever q and p are real, \mathcal{H} is real, therefore $\partial^2 \mathcal{H} / \partial u \partial v$ is real. Hence, if the classical trajectory happens to be real, \mathcal{I} is real.

2.6. The tangent matrix

For the applications of our semiclassical formula (2.63) to be developed in sections 4 and 5, we shall have to write the prefactor in terms of the elements of the tangent matrix M , which connects small displacements of the classical trajectory about the initial point at time zero to the evolved displacements at time t . Differentiating in equation (2.60), but keeping the variable t constant, we can obtain the connection between initial and final displacements. In matrix form it is

$$-i\hbar \begin{pmatrix} \delta u'' \\ \delta v' \end{pmatrix} = \begin{pmatrix} A_{uv} & A_{vv} \\ A_{uu} & A_{vu} \end{pmatrix} \begin{pmatrix} \delta u' \\ \delta v'' \end{pmatrix} \quad (2.67)$$

with the notation

$$A_{uv} = \frac{\partial^2 S}{\partial u' \partial v''} \quad A_{vv} = \frac{\partial^2 S}{\partial v'' \partial v''} \quad A_{uu} = \frac{\partial^2 S}{\partial u' \partial u'} \quad A_{vu} = A_{uv}. \quad (2.68)$$

Solving for $\delta u''$ and $\delta v''$ in terms of $\delta u'$ and $\delta v'$ yields

$$\begin{pmatrix} \delta u'' \\ \delta v'' \end{pmatrix} = \frac{1}{A_{uv}} \begin{pmatrix} \frac{i}{\hbar}(A_{uv}^2 - A_{uu}A_{vv}) & A_{vv} \\ -A_{uu} & -i\hbar \end{pmatrix} \begin{pmatrix} \delta u' \\ \delta v' \end{pmatrix}. \quad (2.69)$$

If we call M_{uu}, M_{uv}, \dots the matrix elements of the tangent matrix (note: unlike A_{uu}, A_{uv}, \dots , these are *not* second derivatives) this last equation should also be

$$\begin{pmatrix} \delta u'' \\ \delta v'' \end{pmatrix} = \begin{pmatrix} M_{uu} & M_{uv} \\ M_{vu} & M_{vv} \end{pmatrix} \begin{pmatrix} \delta u' \\ \delta v' \end{pmatrix}. \quad (2.70)$$

Therefore we have

$$\frac{i}{\hbar} \frac{\partial^2 \mathcal{S}}{\partial u' \partial v''} = \frac{1}{M_{vv}} \quad (2.71)$$

and we rewrite the propagator (2.63) as

$$K(z'', t; z', 0) = \sum_v \frac{1}{\sqrt{(M_v)_{vv}}} e^{\frac{i}{\hbar} \mathcal{I}} \exp \left\{ \frac{i}{\hbar} S_v(v'', u', t) - \frac{1}{2}(|z''|^2 + |z'|^2) \right\}. \quad (2.72)$$

The square root in the prefactor has an undetermined sign. To know which sign is correct, one must start from $t = 0$ when the square root is simply unity, and proceed by continuity along the trajectory, which can be done since M_{vv} never vanishes. We shall meet an important example of this in section 6.1.

Another useful representation of the tangent matrix is in terms of the scaled variables q/b and p/c :

$$\begin{pmatrix} \delta q''/b \\ \delta p''/c \end{pmatrix} = \begin{pmatrix} m_{qq} & m_{qp} \\ m_{pq} & m_{pp} \end{pmatrix} \begin{pmatrix} \delta q'/b \\ \delta p'/c \end{pmatrix}. \quad (2.73)$$

The relation between the matrix elements above and those in equation (2.70) is

$$\begin{aligned} M_{uu} &= \frac{1}{2}(m_{qq} + m_{pp} + im_{pq} - im_{qp}) \\ M_{uv} &= \frac{1}{2}(m_{qq} - m_{pp} + im_{pq} + im_{qp}) \\ M_{vu} &= \frac{1}{2}(m_{qq} - m_{pp} - im_{pq} - im_{qp}) \\ M_{vv} &= \frac{1}{2}(m_{qq} + m_{pp} - im_{pq} + im_{qp}). \end{aligned} \quad (2.74)$$

3. Ambiguities in the choice of path integral

There is more than one way of representing the propagator by a path integral in phase space in terms of coherent states. The way we chose in section 2 is just the one adopted by most workers in the field. Although each one of these different path integrals would give the same answer in an exact quantum mechanical calculation, they may differ when semiclassical approximations are made. In this section we shall discuss a number of such alternatives, and the implications of these ambiguities for the validity of the approximations.

We begin with a qualitative remark. We introduced the path integral by splitting the propagator (2.5) into many segments, each with infinitesimal time-interval τ , and then introducing the unit operator (2.9) between each pair of adjacent segments. But the basis $|z\rangle$ in terms of which the unit operator is written is vastly overcomplete (see [Vou97] for a recent discussion with references), and therefore there is an infinite number of ways of writing the unit operator in terms of the $|z\rangle$. The way chosen for equation (2.9) is only one of them. We shall not pursue this approach to the ambiguous choice, but it does demonstrate the existence of an enormous arbitrariness. Instead, we shall discuss two other aspects of the problem. The first of these, through a different derivation of the path integral, leads to a different 'effective

Hamiltonian'. The second deals with the arbitrariness in operator ordering when one goes from a classical Hamiltonian to a quantum mechanical one. It will turn out that both of them will lead us to reconsider the significance of the first exponential (2.64) in the semiclassical propagator (2.63).

3.1. Alternative forms of the path integral

In their introduction to their overview of coherent states [Kla85], KS discuss two ways of arriving at a path integral, which they call 'path integral—first form' (p 60) and 'path integral—second form' (p 69). The first form is the one we gave in section 2.1. The second form starts from the 'diagonal representation' of the Hamiltonian operator, namely

$$\hat{H} = \int |z\rangle h(z) \frac{d^2z}{\pi} \langle z|. \tag{3.1}$$

Given that we assumed (see second paragraph of section 2.1) that \hat{H} was either a polynomial in p and q or a converging sequence of such polynomials, this diagonal representation always exists. The notation $h(z)$ for the function in equation (3.1) is that of KS; we shall change it to $H_2(z^*, z)$. This will be contrasted with the first-form Hamiltonian function which we called \mathcal{H} in equation (2.33), and which in this section we are going to call $H_1(z^*, z)$, assuming no explicit time dependence. Equation (3.1) is now rewritten

$$\hat{H} = \int |z\rangle H_2(z^*, z) \frac{d^2z}{\pi} \langle z|. \tag{3.2}$$

According to KS, the connection between H_1 and H_2 is

$$H_1(z^*, z) = \int \frac{d^2z'}{\pi} |\langle z|z'\rangle|^2 H_2(z'^*, z') = \int \frac{d^2z'}{\pi} e^{-|z-z'|^2} H_2(z'^*, z') \tag{3.3}$$

$$H_2(z^*, z) = \left(\exp -\frac{\partial^2}{\partial z^* \partial z} \right) H_1(z^*, z). \tag{3.4}$$

In addition to these two effective Hamiltonian functions, there is also the original classical Hamiltonian $H_C(z^*, z)$. All three are different.

A very common type of classical Hamiltonian is $H_C(q, p) = p^2/2m + V(q)$, where, once again, we assume that the function $V(q)$ can be approximated by a polynomial. For such a Hamiltonian, the choice of quantum mechanical operator \hat{H} is straightforward. Then we can work out the connection between H_C , H_1 and H_2 for simple monomials. If we call x and y the real and imaginary parts of z , respectively, this connection is given by the table

H_2	H_C	H_1	
1	1	1	
x	x	x	
$x^2 - \frac{1}{4}$	x^2	$x^2 + \frac{1}{4}$	(3.T)
$x^3 - \frac{3}{4}x$	x^3	$x^3 + \frac{3}{4}x$	
$x^4 - \frac{3}{2}x^2 + \frac{3}{16}$	x^4	$x^4 + \frac{3}{2}x^2 + \frac{3}{16}$	
...	

with an identical table for monomials of y . We see that, up to cubic terms, we have $H_C = \frac{1}{2}(H_1 + H_2)$, but this does not remain true for higher powers. In a qualitative way,

one can think of H_1 as a smoothing of H_C , and of H_2 as an unsmoothing. This idea becomes precise for monomials containing purely x or purely y . In the first case, we have

$$\begin{aligned} H_C(x) &= \sqrt{\frac{2}{\pi}} \int dx' e^{-2(x-x')^2} H_2(x') \\ H_1(x) &= \sqrt{\frac{2}{\pi}} \int dx' e^{-2(x-x')^2} H_C(x') \end{aligned} \quad (3.5)$$

showing that H_C is a smoothing of H_2 , and H_1 a smoothing of H_C . The relations for pure functions of y are identical. If the monomial in H_C contains both x and y , then the problem of operator ordering arises; we shall discuss it in the next subsection.

We shall now sketch the derivation of the semiclassical propagator for the second form of path integral. For simplicity, we exclude an explicit time dependence in \hat{H} . With fewer details, we repeat the steps of sections 2.1–2.3. We use the notation K_1 for the propagator of the first form and K_2 for that of the second form. The starting point is equation (2.8). Following KS (their equation (6.11)), we write each of the N exponentials as

$$e^{-\frac{i}{\hbar} \hat{H} \tau} \approx \int |z_j\rangle e^{-\frac{i\tau}{\hbar} H_2(z_j^*, z_j)} \frac{d^2 z_j}{\pi} \langle z_j|. \quad (3.6)$$

To facilitate the comparison between K_2 and K_1 , it is convenient to write $e^{-\frac{i}{\hbar} \hat{H} t}$ as the product of $N - 1$ factors like (3.6) rather than N . In other words, we take $(N - 1)\tau = t$, which makes no difference in the limit of large N and infinitesimal τ . Then j in equation (3.6) goes from 1 to $N - 1$. The complete propagator is

$$\begin{aligned} K_2(z_N, t; z_0, 0) &= \langle z_N | (N - 1) \text{ factors similar to (3.6)} | z_0 \rangle \\ &= \int \prod_{j=1}^{N-1} \frac{d^2 z_j}{\pi} e^{-\frac{i\tau}{\hbar} H_2(z_j^*, z_j)} \prod_{j=0}^{N-1} \langle z_{j+1} | z_j \rangle. \end{aligned} \quad (3.7)$$

Contrast this with the first-form propagator, obtained from equations (2.10) and (2.12)

$$K_1(z_N, t; z_0, 0) = \int \prod_{j=1}^{N-1} \frac{d^2 z_j}{\pi} \prod_{j=0}^{N-1} e^{-\frac{i\tau}{\hbar} H_1(z_{j+1}^*, z_j)} \langle z_{j+1} | z_j \rangle. \quad (3.8)$$

Whereas in K_1 the two arguments of H_1 belong to two adjacent times in the mesh, the two arguments of H_2 in K_2 belong to the same time. This difference is important and results in different semiclassical propagators after one does the stationary-exponent approximation. The stationarity conditions are found to be

$$\begin{aligned} z_{j+1}^* - z_j^* - \frac{i\tau}{\hbar} \frac{\partial}{\partial z_j} H_2(z_j^*, z_j) &= 0 & j = 1, 2, \dots, N - 1 \\ -z_j + z_{j-1} - \frac{i\tau}{\hbar} \frac{\partial}{\partial z_j^*} H_2(z_j^*, z_j) &= 0 & j = 1, 2, \dots, N - 1. \end{aligned} \quad (3.9)$$

Contrast this with the stationarity conditions for K_1 , which are

$$\begin{aligned} z_{j+1}^* - z_j^* - \frac{i\tau}{\hbar} \frac{\partial}{\partial z_j} H_1(z_{j+1}^*, z_j) &= 0 & j = 1, 2, \dots, N - 1 \\ -z_j + z_{j-1} - \frac{i\tau}{\hbar} \frac{\partial}{\partial z_j^*} H_1(z_j^*, z_{j-1}) &= 0 & j = 1, 2, \dots, N - 1. \end{aligned} \quad (3.10)$$

The differences are subtle, but real. In the continuum limit, both sets of equations become the classical equations of motion, but for Hamiltonian H_1 in the case of K_1 , and for Hamiltonian H_2 in the case of K_2 . In both cases, neither z_0^* nor z_N appear in the equations, hence the

trajectory is determined purely by z_0 and z_N^* and is complex. The two actions S_1 and S_2 , coming from different Hamiltonians, are different.

Now we must calculate the prefactor. As in section 2.2, the exponent in (3.7) is taken at the points $z_j^* + \eta_j^*$, $z_j + \eta_j$ and expanded to second order in the vicinity of the stationary points z_j^* , z_j . The zeroth order gives an expression calculated on the classical trajectory, the first order vanishes by the stationarity conditions and the second order is a quadratic form leading to a Gaussian integration. The quadratic form for K_2 is

$$-\frac{i\tau}{\hbar} \sum_{j=1}^{N-1} \left[\frac{1}{2} \eta_j^2 \frac{\partial^2}{\partial z_j^2} + \eta_j^* \eta_j \frac{\partial^2}{\partial z_j^* \partial z_j} + \frac{1}{2} \eta_j^{*2} \frac{\partial^2}{\partial z_j^{*2}} \right] H_2(z_j^*, z_j) - \sum_{j=1}^{N-1} \eta_j^* \eta_j + \sum_{j=1}^{N-2} \eta_{j+1}^* \eta_j. \quad (3.11)$$

According to equation (2.23) the quadratic form for K_1 is

$$-\frac{i\tau}{\hbar} \sum_{j=1}^{N-1} \frac{1}{2} \left[\eta_j^2 \frac{\partial^2}{\partial z_j^2} H_1(z_{j+1}^*, z_j) + \eta_j^{*2} \frac{\partial^2}{\partial z_j^{*2}} H_1(z_j^*, z_{j-1}) \right] \\ - \frac{i\tau}{\hbar} \sum_{j=1}^{N-2} \eta_{j+1}^* \eta_j \frac{\partial^2}{\partial z_{j+1}^* \partial z_j} H_1(z_{j+1}^*, z_j) - \sum_{j=1}^{N-1} \eta_j^* \eta_j + \sum_{j=1}^{N-2} \eta_{j+1}^* \eta_j. \quad (3.12)$$

The comparison of K_2 with K_1 is easy if this Gaussian integration is performed by the determinant method presented in the appendix of this paper. The details are given there and the result is the following. The semiclassical K_2 is given by equation (2.63) again, with two changes: (i) of course, H_1 is replaced by H_2 , and S_1 by S_2 ; (ii) the first exponent is $-\frac{i}{\hbar}\mathcal{I}$ instead of $+\frac{i}{\hbar}\mathcal{I}$.

In those cases where the semiclassical approximation is expected to be good, one can then hope that the two changes cancel each other approximately. Both path integrals are exact originally and therefore they should give the same propagator. But one semiclassical propagator contains H_1 and the other contains H_2 , which necessarily leads to different results unless the Hamiltonians are purely quadratic. If both approximations are good, it must mean that the difference is cancelled by another one: the change in sign of the first exponent.

Out of these considerations comes the justification for a procedure which has been used in some of the past literature: leave out the first exponential in (2.63), or replace it by unity, and do the classical calculations using the original classical Hamiltonian H_C instead of H_1 (or \mathcal{H}). This follows from the fact that, as equations (3.5) demonstrate, H_C can be thought of as more or less half-way between H_1 and H_2 . It should then be associated with a first exponent which is also half-way between first form and second form, and that means zero. Another justification was given in [Kur89], where it is shown that this is the way of getting the exact first-correction term in an expansion in powers of \hbar . Hence the procedure is correct in the extreme semiclassical limit, the limit of high quantum numbers. It may not be as good for low energies, comparable to the energies of low excited states. We shall return to this question in a future publication. In our opinion, the best procedure for low energies is to take at face value the result (2.63) of the first-form path integral, using Hamiltonian H_1 and including the first exponential. This is because H_1 is the smoothest of the three Hamiltonians, and therefore the stationary-exponent approximation has the best chance of being good in this case. There is one final question one might ask: besides the first form and the second form of path integrals, can one find a continuum of integrals which interpolate smoothly between these two? The answer is yes. Instead of the diagonal form (3.6) for the infinitesimal propagator, one can write it in non-diagonal form thus:

$$e^{-\frac{i}{\hbar}\hat{H}\tau} = \iint |z''\rangle \frac{d^2 z''}{\pi} \langle z'' | e^{-\frac{i}{\hbar}\hat{H}\tau} | z'\rangle \frac{d^2 z'}{\pi} \langle z' |. \quad (3.13)$$

We can approximate the matrix element as in section 2.1, which gives

$$e^{-\frac{i}{\hbar}\hat{H}\tau} \approx \iint |z''\rangle \frac{d^2 z''}{\pi} \langle z''|z'\rangle e^{-\frac{i\tau}{\hbar}H_1(z'',z')} \frac{d^2 z'}{\pi} \langle z'|. \quad (3.14)$$

After multiplying together many such expressions, one has to perform many integrals, twice as many as before. But half of the variables do not occur in the H_1 functions, and the integrations over them are straightforward, the stationary exponent method being exact. This leads back to the first form of path integral. However, nothing prevents us from mixing the two recipes (3.6) and (3.14) in any proportions whatever, generating all possible interpolations between the first and the second form. We shall not pursue this approach further.

3.2. Ambiguities in operator ordering

In the above discussion, many of the statements were precise only if each monomial in the Hamiltonian contained only q or only p . We shall now generalize to arbitrary monomials, which brings up the question of operator ordering. Given a classical $H_C(q, p)$, there are many corresponding \hat{H} , because q and p do not commute and their order matters. Hence there are many quantum mechanical problems and therefore many different results, the differences becoming smaller as \hbar becomes smaller. The number of possible orderings, or combinations of orderings, is infinite, but three of them stand out. *The normal ordering* consists in rewriting H_C in terms of z and z^* , replacing in each monomial z by a and z^* by a^\dagger (see equation (2.2)), and writing all creation operators a^\dagger to the left of all annihilation operators a , making each monomial look like $c_{mn}a^{\dagger m}a^n$. *The antinormal ordering* does the same thing, but it writes the creation operators to the right of the annihilation operators, thus $c_{mn}a^n a^{\dagger m}$. The third kind, called *Weyl ordering or symmetric ordering*, has several equivalent definitions. One says to write all possible orderings of the monomial, and then take the average of them all. Another definition of the Weyl operator \hat{A}_W corresponding to a classical function $A(q, p)$ is as follows. First, write $A(q, p)$ as a double Fourier transform

$$A(q, p) = \iint d\alpha d\beta B(\alpha, \beta) e^{i(\alpha q + \beta p)}. \quad (3.15)$$

Then the Weyl operator is obtained by changing q and p into operators in this formula

$$\hat{A}_W = \iint d\alpha d\beta B(\alpha, \beta) e^{i(\alpha \hat{q} + \beta \hat{p})}. \quad (3.16)$$

Some easily read references are [Hil84, Kur89] and [Vor89].

Thus we have three different ways of associating an operator with a function in classical phase space. We can call them \hat{A}_N , \hat{A}_A and \hat{A}_W . Of the three, \hat{A}_W is the most 'reasonable' one in the classical limit. Conversely, there are three ways of associating a classical function with an arbitrary operator \hat{A} , which are the inverses of the three transformations above. The most interesting one (see [Hil84]) turns out to be the inverse of the Weyl transformation. It is

$$A_C(q, p) = \int ds e^{\frac{i}{\hbar}ps} \left\langle q - \frac{s}{2} \left| \hat{A} \right| q + \frac{s}{2} \right\rangle. \quad (3.17)$$

This is called the Wigner transformation. $A_C(q, p)$ is called the Weyl symbol of the operator \hat{A} and is often denoted by $A_W(q, p)$. The other two inverse transformations also have names. For the transformation which associates a normal-ordered operator with a classical function, the inverse transformation is called the Q -transformation, and the classical function is called the Q -symbol of the operator

$$\begin{aligned} A(q, p) &\implies \text{normal ordering} \implies \hat{A}_N \\ A_Q(q, p) &\longleftarrow Q\text{-transformation} \longleftarrow \hat{A}. \end{aligned} \quad (3.18)$$

Similarly, the inverse of antinormal ordering is called the P -transformation, and the classical function is the P -symbol of the operator

$$\begin{aligned} A(q, p) &\implies \text{antinormal ordering} \implies \hat{A}_A \\ A_P(q, p) &\longleftarrow P\text{-transformation} \longleftarrow \hat{A}. \end{aligned} \quad (3.19)$$

There is a very simple explicit expression for the Q -symbol

$$A_Q(q, p) = \langle z | \hat{A} | z \rangle. \quad (3.20)$$

For the P -symbol there is nothing as easy, but it is given implicitly by the requirement

$$\hat{A} = \int |z\rangle A_P(q, p) \frac{d^2z}{\pi} \langle z|. \quad (3.21)$$

Of the three symbols, the Q -symbol, which is analytic in both z and z^* , is the smoothest. The P -symbol is the most likely to be singular. The Weyl symbol is in between.

Coming back to our subject, we see now that H_1 is the Q -symbol associated with the operator \hat{H} , H_2 is the P -symbol and the function which we have called $H_C(q, p)$ in the past should be the Weyl symbol H_W . As we had defined it for the pure monomials of q or p , it is indeed the Weyl symbol. Moreover, everything we have said about H_C so far will remain true in general, provided we define H_C as the Weyl symbol H_W of \hat{H} .

Let us summarize the results. We have three effective classical Hamiltonians associated with the quantum mechanical \hat{H} . Their smoothness decreases in the order H_1, H_W, H_2 . This is evident from the relations

$$\begin{aligned} H_1(q, p) &= \sqrt{\frac{2}{\pi}} \int d^2z' e^{-2|z-z'|^2} H_W(q', p') \\ H_W(q, p) &= \sqrt{\frac{2}{\pi}} \int d^2z' e^{-2|z-z'|^2} H_2(q', p'). \end{aligned} \quad (3.22)$$

Going in the opposite direction, the relations are

$$\begin{aligned} H_2(q, p) &= \exp\left(-\frac{1}{2} \frac{\partial^2}{\partial z^* \partial z}\right) H_W(q, p) \\ H_W(q, p) &= \exp\left(-\frac{1}{2} \frac{\partial^2}{\partial z^* \partial z}\right) H_1(q, p). \end{aligned} \quad (3.23)$$

In the extreme semiclassical limit, i.e. for large quantum numbers, the best formula for the propagator is (2.63) calculated with H_W throughout and omitting the first exponential (2.64). For low energy, the best formula is (2.63) as it stands, i.e. calculated with H_1 and with the first exponential. The third formula, (2.63) calculated with H_2 and with \mathcal{I} replaced by $-\mathcal{I}$ (see after equation (3.12) and also the last sentence of the appendix), is valid too, though we do not know in what circumstances it might be expected to be better. All three propagators have claims to being called 'the' semiclassical propagator in phase space, although there is no simple derivation of the propagator with the Weyl Hamiltonian from path integrals. They are all different since the classical Hamiltonians are different. All three are exact for the harmonic oscillator and the free particle. But it would be wrong to calculate with H_1 without including the \mathcal{I} term, or with H_2 without including $-\mathcal{I}$, or with H_W including \mathcal{I} .

3.3. Powers of \hbar

In the following sections we shall use our semiclassical formula for the coherent-state propagator in a number of different situations. In particular, we shall derive an initial-value representation for the propagator in section 4 and the Green function in section 6. In order to

perform these calculations consistently, we must state precisely what is the ‘philosophy’ of our approximation, i.e. what terms must be kept and what terms can be discarded in calculations involving this semiclassical propagator. In order to do so, we have to understand the difference between calculations with the Weyl Hamiltonian, which does not involve \hbar explicitly, and those with $H_1 \equiv \mathcal{H}$ or H_2 . The discussion boils down to understanding the semiclassical formulae in terms of powers of \hbar .

We start by recalling the nature of the SPA for a simple one-dimensional integral. Let

$$A = \int_{-\infty}^{+\infty} g(x) e^{\frac{i}{\hbar} f(x)} dx. \quad (3.24)$$

Assume that f has a single stationary point at $x = x_0$ and that $g(x)$ is a slowly varying function of x . The SPA can be applied if \hbar is small. It amounts to expanding $f(x)$ to second order about x_0 while keeping $g(x)$ constant in the vicinity of x_0 . The integration is then reduced to that of a Gaussian, which is straightforward. The result is

$$A \approx A_0 := \sqrt{\frac{2\pi\hbar}{|f^{(2)}|}} g(x_0) \exp\left(\frac{i\pi s}{4} + \frac{i}{\hbar} f(x_0)\right) \quad (3.25)$$

where $f^{(2)}$ is the second derivative of f and s is its sign. This approximation neglects third and higher derivatives of f , as well as all derivatives of g .

By keeping more derivatives, we can calculate the next non-zero contribution to the integral. This is done in appendix B. The result is that A can be written as

$$A = A_0 [1 + i\hbar R(x_0) + \mathcal{O}(\hbar^2)] \quad (3.26)$$

where $R(x_0)$, given explicitly in equation (B.10), involves the first and second derivatives of g and the third and fourth derivatives of f , all computed at $x = x_0$. If instead we were to write these corrections in the exponential, the result would look like this:

$$A = \sqrt{\frac{2\pi\hbar}{|f^{(2)}|}} g(x_0) \exp\left(\frac{i\pi s}{4}\right) \exp\left(\frac{i}{\hbar} [f(x_0) + \hbar^2 R(x_0) + \mathcal{O}(\hbar^3)]\right). \quad (3.27)$$

Therefore, since what we do all along is a quadratic exponent approximation, we do not have any hope of being able to calculate completely and accurately either the terms of order \hbar in the integrals themselves, as (3.26) shows, or the terms of order \hbar^2 in quantities occurring in an exponent with overall coefficient i/\hbar , as shown in (3.27). However, since we actually do have terms of this sort in our results, more discussion needs to take place.

The path integral calculation of the semiclassical propagator involves many integrals similar to (3.24), which are evaluated by an appropriate quadratic exponent approximation. The role of $f(x)$ is played by the action and that of x_0 by the stationary trajectory. In the coordinate or momentum representations, neither the action nor the stationary trajectory depend on \hbar . In these cases, as in the one-dimensional integral (3.24), corrections beyond the SPA are of order \hbar with respect to the semiclassical formula, as in equation (3.26). In the coherent state representation, however, both the action *and* the stationary trajectory depend on Planck’s constant via \mathcal{H} . Therefore, the quadratic approximation already involves ‘nonclassical’ \hbar -dependent terms, and an expansion of the propagator in powers of \hbar similar to (3.26) becomes somewhat confusing. Interestingly, it is shown in appendix C that the non-classical terms in the action S cancel those in \mathcal{I} up to first order in \hbar . Therefore, the non-classical terms in the ‘effective phase’ $S + \mathcal{I}$ are of order \hbar^2 , which is beyond the precision of the approximation. It is not clear at this point whether these extra terms improve or not the semiclassical formula with respect to a pure ‘Weyl’ calculation. We shall come back to this point in section 6 when we discuss semiclassical quantization rules.

In view of these results, this is what we should do in future calculations to be consistent with our semiclassical procedure. We must distinguish two parts to the integrand. One is the exponent that we make stationary. This is always multiplied by a factor i/\hbar , and it usually consists of some kind of action. The other part, which is everything else, we call the prefactor. Then:

- (i) In the stationary exponent, we can drop terms containing third- or higher-order derivatives of \mathcal{H} or S with respect to u and v , since they have not been taken into account in the quadratic approximation. We should keep all terms of order \hbar . They are the ones that are expected to cancel out. All terms of order \hbar^2 can be discarded.
- (ii) In the prefactor, we do not need to expand at all. Improving the result by expanding the prefactor is an illusion. In addition, the prefactor may have a phase, which of course we should keep.

4. An initial-value representation

The biggest difficulty in numerical applications using the coherent-state propagator is the root-searching problem. This explains the recent popularity of the initial-value representations (IVRs), which avoid this problem. In this section we shall transform the propagator (2.63) into a semiclassical IVR propagator with the same initial and final states as the Herman–Kluk (HK) propagator [Her84]. We had expected that the result would be the HK propagator itself, but it did not turn out that way: our IVR propagator differs radically from HK's. Along the way, we shall point out the mistake made by Grossmann and Xavier [Gro98b] in their attempt at a similar derivation. We shall return to the HK propagator in section 5, where we compare it with our IVR and point out that its original derivation in [Her84] also contains a mistake very similar to that made by Grossmann and Xavier.

The basic purpose of an IVR formula is the following. We are given at time 0 a wavefunction $\langle x|\psi(0)\rangle$ in the usual configuration-space representation. We want to calculate its evolution, i.e. we want to know

$$\langle x|\psi(t)\rangle = \langle x|K(t)|\psi(0)\rangle \quad (4.1)$$

again in configuration-space representation, $K(t)$ being the usual Feynman propagator. We want to do this semiclassically, in terms of integrals over classical trajectories, *and we want these trajectories to be specified purely in terms of the initial values of their coordinates*. The alternative, mixed values of the coordinates, some being initial and some final, leads to unacceptable 'root-search' difficulties. Among the many IVR formulae that have been proposed, it has been reported [Kay94b] that the HK expression [Klu86] is particularly easy to use and gives particularly good results. To use this formula, one must first transform the initial wavefunction to the coherent-state representation (a.k.a. the Bargmann representation) by doing the integral

$$\langle z'|\psi(0)\rangle = \int \langle z'|x\rangle dx \langle x|\psi(0)\rangle. \quad (4.2)$$

Then the propagation is carried out with a mixed propagator, which has coherent-state coordinates initially and configuration coordinates finally,

$$\langle x|\psi(t)\rangle = \int \langle x|K(t)|z'\rangle \frac{d^2 z'}{\pi} \langle z'|\psi(0)\rangle. \quad (4.3)$$

The mixed propagator $\langle x|K(t)|z'\rangle$ is the quantity calculated by HK. Our purpose is also to calculate it, but we obtain a different result (sections 4.1 and 4.2). Our result is the one

that follows naturally when one makes the type of semiclassical approximation that was made in section 2. Moreover, it has the essential property of conserving the normalization of the initial wavefunction, which the HK propagator does not have, as we shall see. Since the HK propagator has been so popular in the past, it is obviously desirable to make some numerical comparisons between the two formulae. In section 5 we shall discuss the HK propagator in some detail and show some simple one-dimensional comparisons, for which the new formula is far superior. More tests are needed, including some for two-dimensional problems.

It should be clear that the mixed propagator $\langle x|K(t)|z'\rangle$ is simply a description of the time-evolution of a Gaussian wavepacket. But a semiclassical approximation for this was proposed long ago by Heller [Hel75]. Obviously we need to compare it with our result. We do this in section 4.3. Once again the two formulae are different, but this time there is a strong resemblance, which we discuss in the light of the ambiguities encountered in section 3. Neither result is 'better' than the other: they have different regions of validity.

Finally, let us recall that the research on IVR formulae was originally motivated by the fact that the semiclassical propagator in coordinate space, long known as the Van Vleck formula, led to unpleasant root-search problems. In section 4.4 we examine the relationship between our and Heller's IVR with the Van Vleck propagator.

4.1. A mixed representation

Our starting point is the coherent-state propagator of equation (2.63). Our expression for the mixed propagator is then

$$\begin{aligned} \langle x|K(t)|z'\rangle &= \int \langle x|z''\rangle \frac{d^2z''}{\pi} \langle z''|K(t)|z'\rangle \\ &= \int \frac{dp'' dq''}{2\pi\hbar} \pi^{-\frac{1}{4}} b^{-\frac{1}{2}} \exp\left\{-\frac{(x-q'')^2}{2b^2} + \frac{i}{\hbar} p'' \left(x - \frac{q''}{2}\right)\right\} \\ &\quad \times e^{\frac{i}{\hbar} \mathcal{I}(v'', z', t)} \sqrt{\frac{i}{\hbar} \frac{\partial^2 S}{\partial u' \partial v''} \Big|_{u'=z', v''=z''^*}} \exp\left\{\frac{i}{\hbar} S(v'', z', t) - \frac{1}{2}(|z''|^2 + |z'|^2)\right\}. \end{aligned} \quad (4.4)$$

Before one does the integration over $dp'' dq''$, it is good to remind oneself of the philosophy spelled out in the second paragraph of section 2.2. The integrals to be done are actually two real integrals over dp'' and dq'' , and if the functions are analytic in p'' and q'' , then it is all right to deform the contour into the four-dimensional space of complex p'' and complex q'' . But there are still two integrals and, therefore, in this four-dimensional space the integration runs over a two-dimensional surface. Applying these thoughts to the last member of equation (4.4), we see that the argument of the exponential in the first line is obviously analytic, and we can rewrite it in terms of u'' and v'' without problem. In the second line we have

$$|z''|^2 = \frac{1}{2} \left(\frac{q''^2}{b^2} + \frac{p''^2}{c^2} \right) \quad (4.5)$$

which is analytic and can also be written $u''v''$. Also in the second line, we have the function $S(v'', z', t)$ and its second derivative. For them, the argument of analyticity and change of variables was made at an earlier stage, when the coherent-state propagator was derived in section 2. Recall that $S(v'', u', t)$ is a complex function of the real variables p'', q'', p', q' which depends on these variables only through the combinations v'' and u' . The fact that it is an action calculated along a complex trajectory is really not relevant to doing the integrals. The thing which *is* relevant is that it is analytic in v'' and u' , and therefore, if we have to

do integrals over p'' , q'' , p' or q' , we may continue them into the complex planes of these variables. Everything that was just said about $S(v'', u', t)$ can be repeated word for word about $\mathcal{I}(v'', u', t)$, which also occurs in the last line of (4.4). Finally, another very relevant thing is that we may wish to talk about the derivatives of S , and therefore we give them names as follows:

$$\begin{aligned}\frac{i}{\hbar} \frac{\partial S}{\partial v''} &= U''(v'', u', t) \\ \frac{i}{\hbar} \frac{\partial S}{\partial u'} &= V'(v'', u', t).\end{aligned}\quad (4.6)$$

Then, in terms of u'' and v'' , which are more convenient variables than p'' and q'' , here are the integrals we have to perform:

$$\begin{aligned}\langle x|K(t)|z'\rangle &= \int \frac{du'' dv''}{2\pi i} \pi^{-\frac{1}{4}} b^{-\frac{1}{2}} e^{\frac{i}{\hbar} \mathcal{I}(v'', z', t)} \sqrt{\frac{i}{\hbar} \frac{\partial^2 S}{\partial u' \partial v''} \Big|_{u'=z', v''=z'^*}} \\ &\times \exp \left\{ -\frac{x^2}{2b^2} + \frac{\sqrt{2}}{b} x u'' - \frac{1}{2} u''^2 - u'' v'' + \frac{i}{\hbar} S(v'', z', t) - \frac{1}{2} |z'|^2 \right\}.\end{aligned}\quad (4.7)$$

We are going to do these integrals by the stationary-exponent approximation. First, we must look for the stationary point of the exponent. We do not include the \mathcal{I} term in the exponent, because that would involve calculating third-order derivatives of \mathcal{H} (see section 3.3). To find a point in four dimensions, one needs four real equations, or two complex ones. If we call the exponent in the second line of equation (4.7) Γ , these two complex equations are

$$\begin{aligned}\frac{\partial \Gamma}{\partial v''} &\equiv -u'' + U''(v'', u', t) = 0 \\ \frac{\partial \Gamma}{\partial u''} &\equiv \frac{\sqrt{2}}{b} x - u'' - v'' = 0.\end{aligned}\quad (4.8)$$

There are two crucial comments to be made here. One is that S does not depend on u'' at all, and therefore the second equation does not contain any derivative of S . In fact the second equation, according to equation (2.34), says very simply

$$q'' = x. \quad (4.9)$$

The second crucial comment is that u'' and U'' are not the same. One is the independent variable u'' . The other, U'' , is a function of the other independent variable v'' . The fact that U'' is obtained by calculating a certain complex trajectory is interesting, but irrelevant to the integration problem: it is some function of v'' . On the other hand, u'' is an independent variable; it can be anything, irrespective of the values of v'' and u' . Therefore the first equation, taken by itself, defines a two-dimensional surface in four-dimensional complex space. One of the points on this surface, and only one, is the end point of the real trajectory which begins at p' , q' . To find the stationary point, one must combine this equation with the second one. These two important facts are the ones that were missed by Grossmann and Xavier [Gro98b]. They totally ignored the existence of the second equation, and they claimed that the first equation said that the end point of the real trajectory was the stationary point. This is not so, unless one happens to pick x equal to the value of q for this end point. For all other choices of x , the stationary point is the end point of a *complex* trajectory. Its q'' is real and equal to x . But its p'' is complex. We give its value in equation (4.13).

We could take this result and use the stationary-exponent approximation in the vicinity of the complex stationary trajectory. There are two defects to this approach. One is that finding this complex trajectory is once again a root-search problem, since it is specified by one initial

coordinate z' and one final coordinate x . The other defect is the inconvenience of having to do classical mechanics in the complex domain. It is obviously preferable, if one can, to set up the practical applications in a way that involves the actual calculation only of real trajectories. This can be done, and at the same time the wished-for IVR character is recovered. The idea is that the complex trajectories which are in the vicinity of a real trajectory are a little bit like the Gaussian which is in the vicinity of a stationary point when you do stationary-phase or steepest-descent integration. In the latter case, most of the contribution to the integral comes from the vicinity of the stationary point, so that you can approximate the exponent in this vicinity by a quadratic, even though it is not really a quadratic. You do a Taylor expansion of the exponent near the stationary point and you keep only the first two terms (actually, the first term vanishes). Similarly, when summing over the whole bunch of classical trajectories, we expect most of the contribution to the integral to come from the vicinity of the real trajectory, so that we can approximate the complex trajectories nearby by doing some sort of Taylor expansion to second order. The assumption is that the contribution of a complex trajectory falls off in a Gaussian-like manner as it gets farther away from the real trajectory. This assumption is correct at least for simple systems like the free particle and the harmonic oscillator and it has been shown numerically to hold for the quartic oscillator as well [Xav96a].

Returning to equation (4.7), we see that three terms in it prevent us from doing the integral exactly: the two terms containing the function S , one in the exponential and one in the prefactor, and the term containing \mathcal{I} . In accordance with the ideas expressed above, the S in the exponential, which is the value of the action for the complex classical trajectory, will be expanded to second order in powers of $v'' - v_r$, where v_r (or z_r^*) refers to the final point of the *real* classical trajectory issued from z' , thus

$$\frac{i}{\hbar} S(v'', z', t) \approx \frac{i}{\hbar} S(v_r, z', t) + u_r(v'' - v_r) + \frac{1}{2} \gamma (v'' - v_r)^2 \quad (4.10)$$

with

$$u_r = \left. \frac{i}{\hbar} \frac{\partial S}{\partial v''} \right|_{u'=z', v''=v_r} = v_r^* \quad (4.11)$$

and

$$\gamma = \left. \frac{i}{\hbar} \frac{\partial^2 S}{\partial v''^2} \right|_{u'=z', v''=v_r} = \frac{M_{uv}}{M_{vv}} = \frac{m_{qq} + im_{qp} + im_{pq} - m_{pp}}{m_{qq} + im_{qp} - im_{pq} + m_{pp}}. \quad (4.12)$$

Here we have used equations (2.69) and (2.74) relating second derivatives of the action and elements of the tangent matrix. A similar expansion to first order in $v'' - v_r$ can be done in the first equation (4.8), which allows us to calculate p'' , the momentum at the end point of the complex trajectory

$$p'' \approx p_r + i \frac{1 - \gamma}{1 + \gamma} \frac{c}{b} (x - q_r). \quad (4.13)$$

As for the second derivative of S under the square root in the prefactor, it presents us with a bit of a problem. We know it (with its factor i/\hbar) to be equal to the inverse of M_{vv} , taken at $u' (= z')$ and v'' . If we were to expand this in the vicinity of the real trajectory, we would be taking derivatives of the tangent matrix, which is itself made up of second derivatives of S , and going to higher order than anyone ever goes in this kind of semiclassical argument. Common practice would say: just replace it by its value at the stationary point. Unfortunately, as we already know, the stationary point is *not* the real trajectory. It is a complex trajectory, hopefully rather close to the real one but not simple. Moreover, if we tried to do that, we would be back into the pitfall of mixed initial and final conditions. Hence the only reasonable thing to do for this presumably weakly varying term is to use its value for the real trajectory, which

is the place that will turn out to give the maximum contribution anyway. (Of course there are phase-space points q'' and p'' for which the difference $v'' - v_r$ is not small. But at these points the propagator itself should be negligible.) The very same argument holds for the \mathcal{I} term, since it already involves second derivatives of \mathcal{H} . Hence we shall replace it by the value it takes for the real classical trajectory issued from (q', p') , and we shall call it \mathcal{I}_r .

Here is the complete formula now, in terms of the variables u'' and $w'' := v'' - v_r$:

$$\langle x|K(t)|z'\rangle = \pi^{-\frac{1}{4}} b^{-\frac{1}{2}} e^{\frac{i}{\hbar}\mathcal{I}_r} M_{vv}^{-\frac{1}{2}} \exp\left[-\frac{x^2}{2b^2} + \frac{i}{\hbar}S(z_r^*, z', t) - \frac{1}{2}|z'|^2\right] \int \frac{du'' dw''}{2\pi i} \times \exp\left[-\frac{1}{2}u''^2 + \frac{1}{2}\gamma w''^2 - u''w'' + \left(\frac{\sqrt{2}}{b}x - v_r\right)u'' + u_r w''\right] \quad (4.14)$$

where it is understood that M_{vv} is taken for the real trajectory. The integral is now a pure Gaussian and we can do it using formula (2.25), with

$$\begin{aligned} a_1 &= -\frac{1}{2} & a_2 &= \frac{1}{2}\gamma & a_3 &= -1 \\ b_1 &= \frac{\sqrt{2}}{b}x - v_r & b_2 &= u_r & a_3^2 - 4a_1a_2 &= 1 + \gamma. \end{aligned} \quad (4.15)$$

The two quantities

$$\mu_{1,2} = -a_3 \pm 2\sqrt{a_1a_2} = 1 \pm i\sqrt{\gamma} \quad (4.16)$$

must have a non-negative real part, which requires

$$|\text{Im } \sqrt{\gamma}| \leq 1. \quad (4.17)$$

We have shown, with a fair amount of algebra, that this condition is indeed satisfied. According to equation (2.25), the value of the Gaussian integral, i.e. the second line of equation (4.14), is

$$\frac{1}{\sqrt{1+\gamma}} \exp \frac{1}{1+\gamma} \left[-\frac{u_r^2}{2} + u_r \left(\frac{\sqrt{2}}{b}x - v_r \right) + \frac{\gamma}{2} \left(\frac{\sqrt{2}}{b}x - v_r \right)^2 \right]. \quad (4.18)$$

All we need to do now is to simplify the result.

The new prefactor $(1 + \gamma)^{-1/2}$, multiplied together with the other prefactor $(M_{vv})^{-1/2}$, yields $(M_{vv} + M_{uv})^{-\frac{1}{2}}$, which is the same as $(m_{qq} + im_{qp})^{-\frac{1}{2}}$. Now let us rewrite $S(z_r^*, z', t)$ in terms of the usual action of Hamilton. Equation (2.54) says

$$\frac{i}{\hbar}S(z_r^*, z', t) - \frac{1}{2}|z'|^2 = \int_0^t dt' \left[\frac{1}{2}(\dot{v}u - \dot{u}v) - \frac{i}{\hbar}H(u, v, t') \right] + \frac{1}{2}|z_r|^2. \quad (4.19)$$

We rewrite the first term in the bracket in terms of p and q :

$$\begin{aligned} (\dot{v}u - \dot{u}v) &= \frac{1}{2} \left(\frac{\dot{q}}{b} - i\frac{\dot{p}}{c} \right) \left(\frac{q}{b} + i\frac{p}{c} \right) - \text{complex conjugate} \\ &= i \left(\frac{\dot{q}p}{bc} - \frac{q\dot{p}}{bc} \right) = \frac{i}{\hbar}(\dot{q}p - \dot{p}q) \end{aligned} \quad (4.20)$$

since $bc = \hbar$. With an integration by parts we have

$$\begin{aligned} \int_0^t dt' (\dot{q}p - \dot{p}q) &= 2 \int_0^t dt' \dot{q}p - pq \Big|_0^t \\ &= 2 \int_0^t pdq - p_r q_r + p'q' \end{aligned} \quad (4.21)$$

where q_r and p_r are the final points of the real trajectory starting at (q', p') . As for the last term $\frac{1}{2}|z_r|^2$ of equation (4.19), it will be convenient to write it $\frac{1}{2}u_r v_r$. Expression (4.19) is therefore

$$\frac{i}{\hbar} S(z_r^*, z', t) - \frac{1}{2}|z'|^2 = \frac{i}{\hbar} S_H - \frac{i}{2\hbar} p_r q_r + \frac{i}{2\hbar} p' q' + \frac{1}{2} u_r v_r \quad (4.22)$$

where S_H is Hamilton's action

$$S_H = \int_i^f (p dq - \mathcal{H} dt') \quad (4.23)$$

for the real trajectory. Carrying this into equation (4.14), whose second line is equation (4.18), we find for the complete exponent in $\langle x|K(t)|z' \rangle$, in addition to the \mathcal{I}_r term,

$$\begin{aligned} & -\frac{x^2}{2b^2} + \frac{i}{\hbar} S_H - \frac{i}{2\hbar} p_r q_r + \frac{i}{2\hbar} p' q' + \frac{1}{2} u_r v_r \\ & + \frac{1}{1+\gamma} \left[-\frac{u_r^2}{2} - u_r v_r + \frac{\gamma}{2} v_r^2 + \frac{\sqrt{2}}{b} x(u_r - \gamma v_r) + \gamma \frac{x^2}{b^2} \right]. \end{aligned} \quad (4.24)$$

This is where the serious work of simplification begins.

We start by gathering all the terms containing x and we complete the square in x , which gives

$$-\frac{x^2}{2b^2} \frac{1-\gamma}{1+\gamma} + \frac{x}{b\sqrt{2}} \frac{2(u_r - \gamma v_r)}{1+\gamma} = -\frac{1-\gamma}{1+\gamma} \times \left(\frac{x}{b\sqrt{2}} - \frac{u_r - \gamma v_r}{1-\gamma} \right)^2 + \frac{(u_r - \gamma v_r)^2}{1-\gamma^2}. \quad (4.25)$$

The first term on the right-hand side of equation (4.25), written in terms of p_r and q_r , becomes

$$\begin{aligned} & -\frac{1-\gamma}{1+\gamma} \left(\frac{x}{b\sqrt{2}} - \frac{q_r}{b\sqrt{2}} - i \frac{1+\gamma}{1-\gamma} \frac{p_r}{c\sqrt{2}} \right)^2 \\ & = -\frac{1}{2} \frac{1-\gamma}{1+\gamma} \left(\frac{x - q_r}{b} \right)^2 + \frac{i}{\hbar} p_r (x - q_r) + \frac{1}{2} \frac{1+\gamma}{1-\gamma} \frac{p_r^2}{c^2}. \end{aligned} \quad (4.26)$$

Return now to expression (4.24) and gather all terms quadratic in (u_r, v_r) , or in (q_r, p_r) , including the last term on the right-hand side of (4.25):

$$-\frac{i}{2\hbar} q_r p_r + \frac{1}{1+\gamma} \left[-\frac{u_r^2}{2} - u_r v_r + \frac{1+\gamma}{2} u_r v_r + \frac{\gamma}{2} v_r^2 + \frac{(u_r - \gamma v_r)^2}{1-\gamma} \right]. \quad (4.27)$$

When this is written solely in terms of q_r and p_r , much simplification occurs and one is left with the single term

$$-\frac{1}{2} \frac{1+\gamma}{1-\gamma} \frac{p_r^2}{c^2} \quad (4.28)$$

which cancels the last term of (4.26).

This is the end of the simplifications. The final formula is

$$\begin{aligned} \langle x|K(t)|z' \rangle &= \frac{\pi^{-\frac{1}{4}} b^{-\frac{1}{2}}}{\sqrt{m_{qq} + im_{qp}}} e^{\frac{i}{\hbar} \mathcal{I}_r} \exp \left[-\frac{1}{2} \frac{1-\gamma}{1+\gamma} \left(\frac{x - q_r}{b} \right)^2 \right. \\ & \left. + \frac{i}{\hbar} \left\{ p_r (x - q_r) + \frac{1}{2} p' q' + S_H \right\} \right]. \end{aligned} \quad (4.29)$$

This formula, and *not* the HK formula, is the logical consequence of transforming the semiclassical coherent state propagator to a mixed representation by applying the standard semiclassical approximations.

4.2. Some properties of the mixed propagator

According to equation (4.29) the mean position of the packet $\langle \hat{q} \rangle$ and its mean momentum $\langle \hat{p} \rangle$ are given by q_r and p_r , the real classical trajectory originating at q' , p' . Its squared width $\langle (\hat{q} - q_r)^2 \rangle$ comes out of the real part of the coefficient of the Gaussian, which should be and is negative. Since we have

$$\frac{1 - \gamma}{1 + \gamma} = \frac{m_{pp} - im_{pq}}{m_{qq} + im_{qp}} = \frac{1 - i(m_{pp}m_{qp} + m_{qq}m_{pq})}{m_{qq}^2 + m_{qp}^2} \quad (4.30)$$

we find

$$\langle (\hat{q} - q_r)^2 \rangle = \frac{b^2}{2} (m_{qq}^2 + m_{qp}^2) = \Delta q_{\text{class}}^2 \quad (4.31)$$

where $\Delta q_{\text{class}}^2$ is the classical spreading of a Gaussian initial ensemble corresponding to the initial phase space distribution $|\langle p, q | p', q' \rangle|^2$. In similar fashion we have

$$\langle (\hat{p} - p_r)^2 \rangle = \frac{b^2}{2} (m_{pq}^2 + m_{pp}^2) = \Delta p_{\text{class}}^2. \quad (4.32)$$

We see incidentally that the denominator of the prefactor in (4.29) can never vanish, and therefore the mixed propagator can never be singular, because the determinant of the tangent matrix must equal unity. This follows from symplecticity, which in one dimension is the same as Liouville's theorem.

Another straightforward calculation yields the normalization of the packet

$$\begin{aligned} N(t) &= \int dx |\langle x | K(t) | z' \rangle|^2 = \frac{1}{\sqrt{\pi}b} \sqrt{m_{qq}^2 + m_{qp}^2} \int dx \\ &\times \exp \left\{ -\frac{1}{2} \left[\frac{1 - \gamma}{1 + \gamma} + \frac{1 - \gamma^*}{1 + \gamma^*} \right] \frac{(x - q_r)^2}{b^2} \right\} = 1. \end{aligned} \quad (4.33)$$

Normalization is conserved and equal to unity at all times, which is as it should be.

It may not be superfluous to mention once again that the sign of the square root in equation (4.29) is to be determined by continuous displacement along the trajectory, given that this square root is unity at $t = 0$.

4.3. Comparison with Heller's IVR

Now we proceed to the comparison with Heller's approximation mentioned earlier. This approximation is also known as 'the thawed Gaussian approximation' or TGA. A different derivation of the TGA was given later by Kay [Kay94a] and used by him in numerical comparisons with other approximations [Kay94b]. Although Heller does not give a final formula, while Kay does, we shall stick to Heller's presentation, as we do not find Kay's arguments convincing: they seem to be based on convenience and (very limited) numerical agreement, rather than solid basic principles. Heller's paper assumes a Hamiltonian of the form $p^2/2m + V(q)$. Here we shall consider a general Hamiltonian $H(p, q)$ and we shall carry the derivation all the way to an explicit formula, which Heller does not do. The result will be that Heller's approximation leads to a formula identical to our equation (4.29) except for two differences: (1) the classical Hamiltonian that must be used to compute the trajectories, instead of being the smoothed \mathcal{H} or the Q -symbol defined in section 3, is the Weyl symbol H_W of the quantum mechanical operator; (2) the term $e^{\frac{i}{\hbar}T_r}$ is absent. Hence the discussion of section 3 returns to the fore: there exist indeed different approximations, all legitimately derived, and the question becomes one of deciding under what circumstances one or the other can be expected to be better. We already saw in section 3 that, in the extreme semiclassical

limit, when \hbar becomes very small, Heller's approximation is expected to be best [Kur89]. At low energy, on the other hand, we expect (4.29) to be best. We gave a qualitative argument for this in section 3, but we have also performed several numerical comparisons, which we reserve for a future publication, as this paper is probably too long already.

Heller's idea is to assume that the original wavepacket $\langle x|z' \rangle$ remains Gaussian as it propagates, but that the parameters of the Gaussian change with time thus:

$$\langle x|K(t)|z' \rangle = \exp \frac{i}{\hbar} [\alpha(t)(x - q(t))^2 + p(t)(x - q(t)) + \beta(t)]. \quad (4.34)$$

He further assumes that $q(t)$ and $p(t)$, which are the expectation values of the operators \hat{q} and \hat{p} , follow a real classical trajectory for some classical Hamiltonian $H(q, p)$. On the other hand he takes $\alpha(t)$ and $\beta(t)$ to be complex, so that there are six undetermined real functions in the formula. The problem is to determine them. The exact quantum mechanical packet obeys the Schrödinger equation with a certain quantum Hamiltonian operator $\hat{H}(\hat{q}, \hat{p})$. What should be the connection between H and \hat{H} ? The most straightforward assumption, and the one that works for the simple problems of elementary quantum mechanics, is to say that they are Weyl related, i.e. \hat{H} is the Weyl operator associated with H , and H is the Weyl symbol associated with \hat{H} . But we do not want to make this assumption explicitly: it should come out of the calculation, and it will.

Heller argues that, since the wavepacket is small, the only part of the quantum Hamiltonian that matters is the part which, in phase space, refers to the vicinity of the classical trajectory, i.e. the region where the wavepacket is appreciably different from 0. In that small region it is permissible to expand the quantum Hamiltonian up to second order in the variables $\hat{q} - q$ and $\hat{p} - p$. This 'local quadratic expansion' is the embodiment in this case of the semiclassical approximation, quite similar to the stationary-exponent approximation in section 2 and to the second-order expansion in equation (4.10). Hence we expand the Hamiltonian operator as follows:

$$\begin{aligned} \hat{H}(\hat{q}, \hat{p}) = & H(q, p) + H_q(\hat{q} - q) + H_p(\hat{p} - p) + \frac{1}{2} \{ H_{qq}(\hat{q} - q)^2 + H_{pp}(\hat{p} - p)^2 \\ & + H_{qp}[(\hat{q} - q)(\hat{p} - p) + (\hat{p} - p)(\hat{q} - q)] \} \end{aligned} \quad (4.35)$$

where \hat{q} is the operator 'multiplication by x ', \hat{p} is $-i\hbar\partial/\partial x$ and $H_q, H_p, H_{qq}, H_{pp}, H_{qp}$ are the first and second derivatives of $H(q, p)$, which are functions of q and p and do not contain any operators. The crucial point to note here is that, if formula (4.35) is true, the Weyl symbol of the operator $\hat{H}(\hat{q}, \hat{p})$ is simply $H(q, p)$, without any additional terms. This comes out from repeated applications of the Wigner transformation (3.17), where one does the integrals by using the standard properties of the Dirac delta-function and its derivatives. Denoting the Weyl symbol with the subscript W, one finds

$$\begin{aligned} (\hat{q})_W = q & & (\hat{p})_W = p \\ (\hat{q}^2)_W = q^2 & & (\hat{p}^2)_W = p^2 \\ (\hat{q}\hat{p})_W = qp + \frac{1}{2}i\hbar & & (\hat{p}\hat{q})_W = pq - \frac{1}{2}i\hbar \end{aligned} \quad (4.36)$$

etc.

Note that the Q -symbol of the right-hand side of (4.35) would be very different. For instance, while the Weyl symbol of $(\hat{q} - q)^2$ vanishes, its Q -symbol is the squared width of the packet. Thus we have chosen $H(q, p)$ to be the Weyl symbol of \hat{H} , and this is not a trivial choice. It is however a purely arbitrary choice for now. The crucial moment will come when we prove that $q(t)$ and $p(t)$ obey Hamilton's equations for this particular classical $H(q, p)$. This moment is close at hand. Meanwhile, we note that the last bracket $[\dots]$ of (4.35) can be written

$$2(\hat{q} - q)(\hat{p} - p) - i\hbar.$$

Now we try to satisfy the Schrödinger equation $i\hbar\partial\psi/\partial t = \hat{H}\psi$. For $\psi(t)$ we substitute the wavepacket (4.34) and for \hat{H} we substitute (4.35). We find

$$\begin{aligned} \frac{1}{\psi}i\hbar\frac{\partial\psi}{\partial t} &\equiv -\dot{\alpha}(x-q)^2 + 2\alpha\dot{q}(x-q) - \dot{p}(x-q) + p\dot{q} - \dot{\beta} \\ \frac{1}{\psi}\hat{H}\psi &\equiv H(q, p) + H_q(x-q) + \frac{1}{2}H_{qq}(x-q)^2 + 2H_p\alpha(x-q) \\ &\quad + H_{pp}[2\alpha^2(x-q)^2 - i\hbar\alpha] + H_{qp}[2\alpha(x-q)^2 - \frac{1}{2}i\hbar]. \end{aligned} \quad (4.37)$$

Matching powers of $(x-q)$, we get the following three complex equations to determine the six unknown real functions:

$$\dot{\alpha} = -2\alpha^2 H_{pp} - 2\alpha H_{qp} - \frac{1}{2}H_{qq} \quad (4.38)$$

$$2\alpha\dot{q} - \dot{p} = 2\alpha H_p + H_q \quad (4.39)$$

$$\dot{\beta} = p\dot{q} - H(q, p) + i\hbar\alpha H_{pp} + \frac{1}{2}i\hbar H_{qp}. \quad (4.40)$$

We start with the imaginary part of (4.39), which gives

$$\dot{q} = H_p. \quad (4.41)$$

Then the real part of the same equation says

$$\dot{p} = -H_q. \quad (4.42)$$

Hence $q(t)$ and $p(t)$ follow a classical trajectory of H , provided that the latter is the Weyl symbol of \hat{H} . Two equations remain, (4.38) and (4.40).

To solve (4.38) we notice that this equation becomes identical to that for $X(t)$, equation (2.47), if we identify v with q , u with p and $\frac{1}{\hbar}\mathcal{H}$ with H . Following the calculation that leads to equation (2.50), we find immediately

$$\alpha = \frac{1}{2} \frac{\delta p}{\delta q} \quad (4.43)$$

where δq and δp are deviations from the classical trajectory, which satisfy

$$\delta\dot{q} = H_{qp}\delta q + H_{pp}\delta p \quad (4.44)$$

$$\delta\dot{p} = -H_{qq}\delta q - H_{pq}\delta p. \quad (4.45)$$

Using the tangent matrix equation (2.73) we get

$$\alpha = \frac{1}{2} \frac{\frac{c}{b}m_{pq}\delta q' + m_{pp}\delta p'}{m_{qq}\delta q' + \frac{b}{c}m_{qp}\delta p'} = \frac{1}{2} \frac{\frac{c}{b}m_{pq} + 2m_{pp}\alpha'}{m_{qq} + 2\frac{b}{c}m_{qp}\alpha'} \quad (4.46)$$

where

$$\alpha' = \frac{1}{2} \frac{\delta p'}{\delta q'} = \frac{i\hbar}{2b^2} = \frac{ic}{2b}. \quad (4.47)$$

Therefore

$$\begin{aligned} \alpha &= \frac{c}{2b} \frac{m_{pq} + im_{pp}}{m_{qq} + im_{qp}} = \frac{ic}{2b} \frac{m_{pp} - im_{pq}}{m_{qq} + im_{qp}} \\ &= \frac{ic}{2b} \frac{1 - \gamma}{1 + \gamma}. \end{aligned} \quad (4.48)$$

Equation (4.40) can now be integrated. It can be written

$$\begin{aligned}
 \dot{\beta} &= p\dot{q} - H(q, p) + \frac{i\hbar}{2} \frac{\delta p}{\delta q} H_{pp} + \frac{i\hbar}{2} H_{qp} \\
 &= L + \frac{i\hbar}{2\delta q} (\delta p H_{pp} + \delta q H_{qp}) \\
 &= L + \frac{i\hbar}{2\delta q} \delta \dot{q} \\
 &= L + \frac{i\hbar}{2} \frac{d}{dt} (\log \delta q)
 \end{aligned} \tag{4.49}$$

where L is the Lagrangian. Integrating both sides gives

$$\beta = S_H + \frac{i\hbar}{2} \log \delta q \tag{4.50}$$

up to an additive constant, S_H being Hamilton's action (for the Weyl Hamiltonian), and with

$$\delta q = m_{qq} \delta q' + \frac{b}{c} m_{qp} \delta p' = \delta q' \left(m_{qq} + \frac{2b}{c} m_{qp} \alpha' \right). \tag{4.51}$$

The initial value $\delta q'$ is determined by $\beta(0) = q' p' / 2 = i\hbar / 2 \log \delta q'$, which gives

$$\delta q' = e^{-iq' p' / \hbar}. \tag{4.52}$$

Substituting equations (4.51), (4.52), and (4.47) into (4.50) gives

$$\begin{aligned}
 \beta &= S_H + \frac{i\hbar}{2} \log \left[\delta q' \left(m_{qq} + \frac{2b}{c} \alpha' m_{qp} \right) \right] \\
 &= S_H + \frac{i\hbar}{2} \log \left[e^{-iq' p' / \hbar} (m_{qq} + i m_{qp}) \right] \\
 &= S_H + \frac{p' q'}{2} + \frac{i\hbar}{2} \log (m_{qq} + i m_{qp})
 \end{aligned} \tag{4.53}$$

or

$$e^{\frac{i}{\hbar} \beta} = \frac{1}{\sqrt{m_{qq} + i m_{qp}}} e^{\frac{i}{\hbar} (S_H + p' q' / 2)} \tag{4.54}$$

up to a multiplicative constant.

With these expressions for α and β , one sees immediately that the Heller wavepacket (4.34) is identical to ours (4.29), except for the different Hamiltonian (Weyl's) and the absence of the \mathcal{I}_r exponential. Equation (4.33) shows that the normalization of the Heller packet is conserved at all times.

4.4. Recovering Van Vleck's formula from the IVR

The semiclassical limit of the evolution operator in the coordinate representation is given by the well known Van Vleck formula [Van28]. It is desirable, therefore, that other semiclassical representations of this operator reduce to Van Vleck's when transformed back to coordinates. In this subsection we shall calculate

$$K(x'', t; x', 0) := \langle x'' | K(t) | x' \rangle = \int \langle x'' | K(t) | z' \rangle \frac{d^2 z'}{\pi} \langle z' | x' \rangle \tag{4.55}$$

for both mixed propagators, Heller's and ours. The integration over q' and p' will be performed by the stationary-exponent approximation. We shall see that Heller's approximation recovers Van Vleck's formula exactly. Our semiclassical approximation recovers it only in the limit of

small \hbar (see discussion in section 3), but this is also the only limit in which the Van Vleck approximation can be justified.

We start by inserting the Heller propagator in equation (4.55). Using expression (2.4) for $\langle x|z\rangle$ we get

$$\begin{aligned} K_{\text{Heller}}(x'', t; x', 0) &= \int \frac{dq' dp'}{2\pi\hbar} \frac{\pi^{-\frac{1}{2}} b^{-1}}{\sqrt{(m_{qq} + im_{qp})}} \\ &\times \exp \left[-\frac{1}{2} \left(\frac{1-\gamma}{1+\gamma} \right) \left(\frac{x'' - q_r}{b} \right)^2 + \frac{i}{\hbar} \left\{ p_r (x'' - q_r) + \frac{1}{2} p' q' + S_H \right\} \right] \\ &\times \exp \left[-\frac{(x' - q')^2}{2b^2} - \frac{i}{\hbar} p' (x' - q'/2) \right]. \end{aligned} \quad (4.56)$$

We call $\xi = \xi(q', p')$ the exponent in the second and third lines of (4.56). The stationary conditions are $\partial\xi/\partial q' = 0$ and $\partial\xi/\partial p' = 0$. We write ξ explicitly first:

$$\xi = -\frac{1}{2b^2} \left[\left(\frac{1-\gamma}{1+\gamma} \right) (x'' - q_r)^2 + (x' - q')^2 \right] + \frac{i}{\hbar} [p_r (x'' - q_r) + p' (q' - x') + S_H]. \quad (4.57)$$

The derivatives are

$$\begin{aligned} \frac{\partial\xi}{\partial q'} &= \frac{1}{b^2} \left[\left(\frac{1-\gamma}{1+\gamma} \right) (x'' - q_r) \frac{\partial q_r}{\partial q'} + (x' - q') \right] \\ &\quad + \frac{i}{\hbar} \left[\frac{\partial p_r}{\partial q'} (x'' - q_r) - p_r \frac{\partial q_r}{\partial q'} + p' + \frac{\partial S_H}{\partial q'} + \frac{\partial S_H}{\partial q_r} \frac{\partial q_r}{\partial q'} \right] \\ &= \frac{1}{b^2} \left[(x'' - q_r) \left(\left(\frac{1-\gamma}{1+\gamma} \right) m_{qq} + im_{pq} \right) + (x' - q') \right] \\ &= \frac{1}{b^2} \left[\left(\frac{1}{m_{qq} + im_{qp}} \right) (x'' - q_r) + (x' - q') \right] \end{aligned} \quad (4.58)$$

where we have used $\frac{\partial S_H}{\partial q'} = -p'$, $\frac{\partial S_H}{\partial q_r} = p_r$ and equations (2.73). Similarly we find

$$\frac{\partial\xi}{\partial p'} = \frac{i}{\hbar} \left[\left(\frac{1}{m_{qq} + im_{qp}} \right) (x'' - q_r) - (x' - q') \right]. \quad (4.59)$$

The stationary conditions are satisfied if $q' = x'$ and $q_r(q', p', t) = x''$. This last equation defines p' implicitly, so that the contributing trajectory is the one that leaves x' at time zero and reaches x'' at time t . The value of ξ computed at the stationary trajectory is simply iS_H/\hbar . In order to perform the integrals we need the second-order derivatives of ξ . The algebra is straightforward and the results are

$$\xi_{qq} = -\frac{1}{b^2} \frac{2m_{qq} + im_{qp}}{m_{qq} + im_{qp}} \quad (4.60)$$

$$\xi_{qp} = \xi_{pq} = -\frac{1}{\hbar} \frac{m_{qp}}{m_{qq} + im_{qp}} \quad (4.61)$$

$$\xi_{pp} = -\frac{i}{c^2} \frac{m_{qp}}{m_{qq} + im_{qp}}. \quad (4.62)$$

Notice that all derivatives of ξ were calculated keeping the elements of the monodromy matrix fixed. Their variations would involve the computation of third- or higher-order derivatives of S .

Inserting all these expressions into equation (4.56), we find that the coordinate propagator becomes

$$\begin{aligned}
 K_{\text{Heller}}(x'', t; x', 0) &= \pi^{-\frac{1}{2}} b^{-1} \frac{1}{\sqrt{m_{qq} + im_{qp}}} e^{iS_H/\hbar} \\
 &\quad \times \int \frac{dQ dP}{2\pi\hbar} \exp \left[\frac{1}{2} (\xi_{qq} Q^2 + 2\xi_{qp} QP + \xi_{pp} P^2) \right] \\
 &= \pi^{-\frac{1}{2}} b^{-1} \frac{1}{\sqrt{m_{qq} + im_{qp}}} \frac{e^{iS_H/\hbar}}{\hbar \sqrt{\xi_{qq}\xi_{pp} - \xi_{qp}^2}}
 \end{aligned} \tag{4.63}$$

where Q and P are the variations of q' and p' from the stationary point. The quantity under the second square root in the last line is the determinant of the quadratic form in the second line. By equations (4.60)–(4.62) it is equal to

$$\xi_{qq}\xi_{pp} - \xi_{qp}^2 = \frac{2im_{qp}}{\hbar^2(m_{qq} + im_{qp})} \tag{4.64}$$

and the final result is

$$K_{\text{Heller}}(x'', t; x', 0) = \frac{1}{b\sqrt{2\pi im_{qp}}} e^{iS_H/\hbar} \tag{4.65}$$

which is Van Vleck's famous expression.

Given the close similarity between Heller's wavepacket and ours, a calculation identical to ours will obviously give the result

$$K(x'', t; x', 0) = \frac{1}{b\sqrt{2\pi im_{qp}}} e^{i(S_H+I)/\hbar} \tag{4.66}$$

all classical quantities being calculated with the smoothed Hamiltonian \mathcal{H} instead of the Weyl H . This reduces to the Van Vleck formula for small \hbar , and it might well be better for larger \hbar , but we have no evidence for this at the moment.

5. Comparison with the Herman–Kluk propagator

In addition to Heller's thawed Gaussian approximation, there is in the literature a different IVR formula for the mixed propagator $\langle x|K(t)|z \rangle$. This is the HK formula [Her84], derived by convoluting the Van Vleck propagator with coherent states and performing the resulting integrals by the method of stationary phase. This formula has been used many times in the last few years.

We have already pointed out in section 4.1 the mistake of Grossmann and Xavier [Gro98a] in their tentative derivation of the HK formula from the semiclassical coherent-state propagator (2.63). In fact, in their original paper [Her84], Herman and Kluk make a similar mistake in their evaluation of the stationary phase integrals. When performing these integrals they find (as we found in section 4.1) that the stationary trajectory is complex and given by mixed boundary conditions (equations (16) and (17) of [Her84]). However, instead of expanding the exponent of the integrand for this complex trajectory about a nearby real trajectory, they make a change of variables to initial position and momentum and assume these new variables to be real. Therefore, from the point of view of semiclassical analysis, the HK formula is incorrect. In section 5.2 we shall discuss why, in spite of that, it may still work.

Here is the HK formula, for the mixed representation introduced in (4.3), taken from [Klu86] with some adjustment of notations:

$$\langle x|K(t)|z'\rangle_{\text{HK}} = \pi^{-\frac{1}{4}} b^{-\frac{1}{2}} \sqrt{\frac{1}{2}(m_{pp} + m_{qq} - im_{qp} + im_{pq})} \\ \times \exp \left[-\frac{1}{2} \left(\frac{x - q_r}{b} \right)^2 + \frac{i}{\hbar} \left\{ p_r (x - q_r) + \frac{1}{2} p' q' + S_H \right\} \right]. \quad (5.1)$$

Once again, the \mathcal{I}_r term is absent and the classical Hamiltonian used by HK is the Weyl Hamiltonian. Besides these, there are two other differences between equation (4.29) and equation (5.1), both of them quite important at first sight. One is in the coefficient of the Gaussian exponent, the other is in the prefactor. The coefficient $(1 - \gamma)/(1 + \gamma)$ of the Gaussian in (4.29) was essential for obtaining the right semiclassical widths (4.31) and (4.32), but it is absent in HK! The difference in the prefactors is also astonishing. One formula has the square root occurring in the denominator and the other in the numerator. But actually the two prefactors are related by

$$\sqrt{\frac{1}{2}(m_{pp} + m_{qq} - im_{qp} + im_{pq})} = \frac{1}{\sqrt{m_{qq} + im_{qp}}} \sqrt{\frac{1 + \gamma}{1 - |\gamma|^2}} \quad (5.2)$$

which shows that both differences between the two formulae imply that HK set γ equal to 0. This is quite generally incorrect, except for the plain harmonic oscillator, for which both formulae give identical results.

There is another major difference between formulae (4.29) and (5.1), the normalization, which is for (5.1)

$$N_{\text{HK}}(t) = \frac{1}{2\sqrt{\pi}b} \sqrt{(m_{qq} + m_{pp})^2 + (m_{pq} - m_{qp})^2} \int dx \exp \left\{ -\frac{(x - q_r)^2}{b^2} \right\} \\ = \frac{1}{\sqrt{1 - |\gamma(t)|^2}}. \quad (5.3)$$

This normalization is not conserved since γ is usually time dependent. This is a grave flaw which shows up in almost every example. For the free particle, for instance, (4.29) is exact, while (5.1) fails completely in describing the spreading of the wavepacket.

It may be argued with some validity that, since the $|z'\rangle$ form an overcomplete set, the fact that the propagation of each $|z'\rangle$ according to HK is wrong does not necessarily mean that a wrong result will always occur when a $|z'\rangle$ -integral is performed, as in equation (4.3). This is in fact a crucial point concerning the applicability of the HK formula, and we shall discuss it in detail in section 5.2.

5.1. A numerical example

We show here a detailed numerical illustration of the differences between HK and our semiclassical IVR formula. We consider the scattering of a particle with initial wavefunction $\langle x|z'\rangle$ by a potential barrier. We choose the following Hamiltonian to test our results:

$$H = \frac{p^2}{2} + V_0 [e^{\alpha(x-A)} + e^{-\alpha(x+A)}] \\ = \frac{p^2}{2} + 2 V_0 e^{-\alpha A} \cosh \alpha x \quad (5.4)$$

where V_0 , α and A are parameters. The first term in the potential function represents an exponential wall located at $x = +A$. The second exponential *closes* the system at the left end with a second wall at $x = -A$.

The wavepacket will be launched from $x = 0$ with positive momentum. If A is large compared with the coherent-state width b , the packet will not see this left wall in its way towards the first collision. However, the fact that the motion is bound simplifies the quantum mechanical treatment, avoiding the complications of the continuous spectrum. We have set $A = 5$ and $\alpha = V_0 = 1$ for the potential and $q' = 0$, $p' = 1$ and $b = 0.3$ for the initial coherent state $|z'\rangle$. Planck's constant was set to $\hbar = 0.05$, which gives $c = \hbar/b \approx 0.167$.

For short times the particle experiences almost no force, being well described by the free particle propagation. In this approximation the classical trajectory is just

$$\begin{aligned} q &= q' + p't \\ p &= p'. \end{aligned} \quad (5.5)$$

All the quantities entering the semiclassical formulae can be computed immediately and the result is

$$\begin{aligned} m_{qq} &= m_{pp} = 1 & m_{pq} &= 0 & m_{qp} &= ct/b \\ S_H &= p'^2 t/2 - c^2 t/4 & \mathcal{I}_r &= c^2 t/4 \\ \gamma &= itc/(itc + 2b). \end{aligned} \quad (5.6)$$

Substituting these expressions in (4.29) gives

$$\begin{aligned} \langle x|K(t)|z'\rangle &= \frac{\pi^{-\frac{1}{4}} b^{-\frac{1}{2}}}{\sqrt{1 + itc/b}} \exp \left[-\frac{1}{2} \frac{1}{1 + itc/b} \left(\frac{x - q' - p't}{b} \right)^2 \right. \\ &\quad \left. + \frac{i}{\hbar} \left\{ p'(x - q' - p't) + \frac{1}{2} p'q' + \frac{1}{2} p'^2 t \right\} \right] \end{aligned} \quad (5.7)$$

which coincides with the exact quantum mechanical result. The HK formula, on the other hand, gives

$$\begin{aligned} \langle x|K(t)|z'\rangle_{\text{HK}} &= \pi^{-\frac{1}{4}} b^{-\frac{1}{2}} \sqrt{1 - itc/2b} \exp \left[-\frac{1}{2} \left(\frac{x - q' - p't}{b} \right)^2 \right. \\ &\quad \left. + \frac{i}{\hbar} \left\{ p'(x - q' - p't) + \frac{1}{2} p'q' + \frac{1}{2} p'^2 t \right\} \right]. \end{aligned} \quad (5.8)$$

This shows that HK not only describes poorly the width of the evolved packet but it also produces a non-physical increase in the total probability.

For times of the order of A/p' the free-particle approximation is no longer valid and we have to solve the problem numerically. The exact quantum mechanical solution of $H|\Psi_n\rangle = E_n|\Psi_n\rangle$ for the Hamiltonian (5.4) was performed by diagonalizing H using as basis states $\langle x|\phi_n\rangle = \frac{1}{\sqrt{L}} \sin(n\pi x/2L + n\pi/2)$ where the width L is chosen such that $V(L) = E_{\text{max}}$. This is in fact the most accurate method (when you can use it). E_{max} is an upper limit to the eigenenergies to be calculated and it is related to the number N of basis states used in the diagonalization by $E_{\text{max}} = N^2\pi^2\hbar^2/(8L^2)$. This guarantees that the basis states span the energy interval from 0 to E_{max} and that the part of the potential with $-L \leq x \leq L$ has $V(x) < E_{\text{max}}$. We have used $N = 400$ in our computations, which gives $E_{\text{max}} \approx 9.4$ and $L \approx 7.2$. With this choice the first 260 energy levels converge with at least five digits (as compared with a larger diagonalization), spanning an energy interval from 0 to 5.5. The initial wavepacket $\langle x|z'\rangle$ can be easily expressed in terms of the $|\phi_n\rangle$ basis and, therefore, in the basis $|\Psi_n\rangle$ of eigenstates of H .

The semiclassical calculation of both HK and our semiclassical formula needs only one single trajectory starting from (q', p') and its tangent matrix to compute the whole function

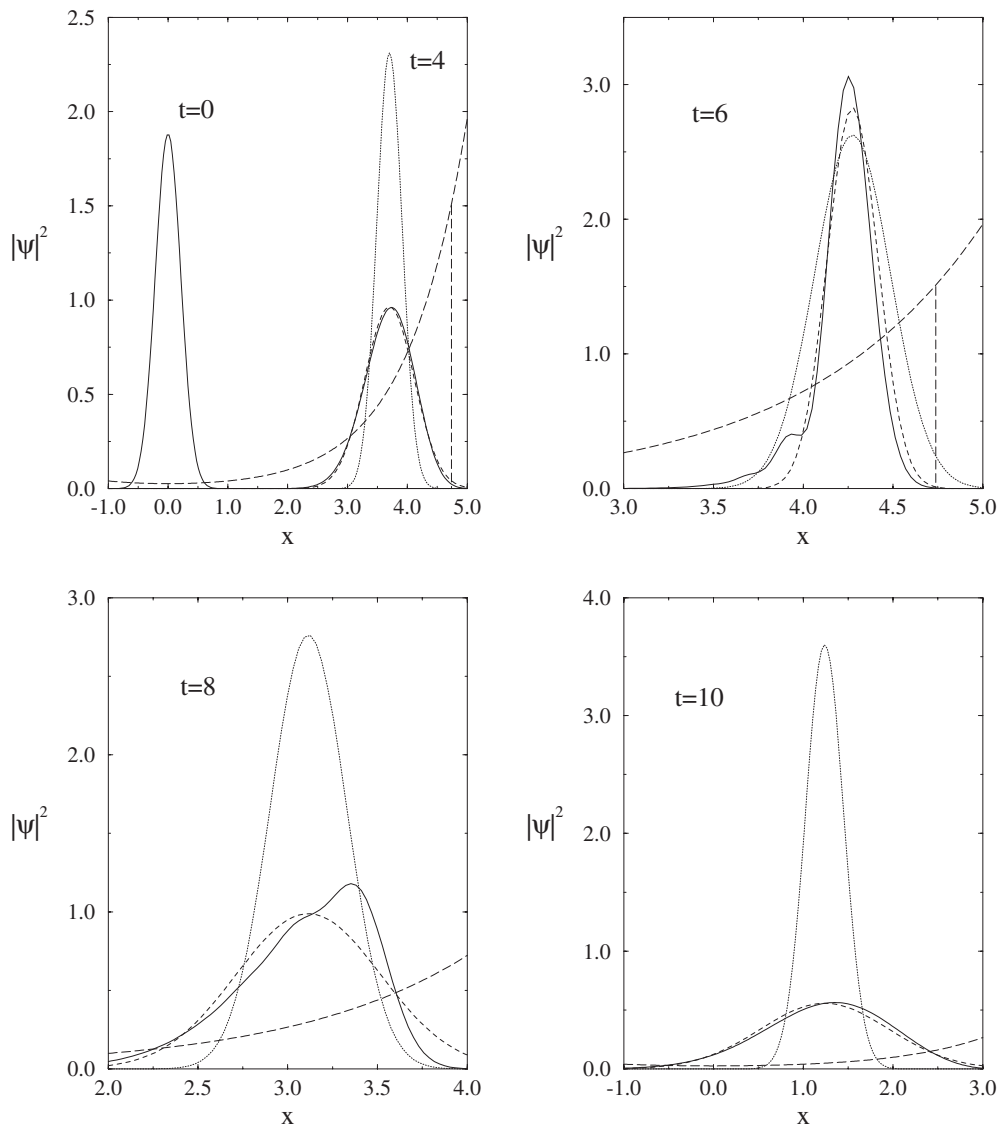


Figure 1. Square modulus of the time-evolved coherent state launched from $q' = 0$ and $p' = 1$ for the initial wavepacket at $t = 0$ and exact and semiclassical calculations at $t = 4, 6, 8$ and 10 . The long-dashed curve shows the potential function and the dashed bar shows the location of the classical turning point. The solid curve shows the exact propagation, the short-dashed curve shows our semiclassical formula and the dotted curve shows the HK approximation.

$\langle x|K(t)|z' \rangle$. In our formula this trajectory is a solution of Hamilton's equations for the smoothed Hamiltonian $\langle v|\hat{H}|u \rangle$, which is given by

$$\mathcal{H} = \frac{p^2}{2} + 2 V_1 e^{-\alpha A} \cosh \alpha x + \hbar^2 b^2 / 4 \tag{5.9}$$

where $V_1 = V_0 \exp(b^2 \alpha^2 / 4)$. The results are shown in figure 1 showing the square modulus of the wavefunction for the times $t = 0, 4, 6, 8$ and 10 . The Gaussian at $t = 0$ represents the initial coherent state. The long-dashed curve shows the (properly scaled) potential function

and the dashed vertical bar shows the location of the classical turning point. The lines at $t = 4$ show the time-evolved wavefunction according to the exact calculation (solid), our formula (short-dashed) and the HK approximation (dotted). Notice the increase in the height of the HK Gaussian, in opposition to the exact evolution, which spreads and decreases. Our semiclassical formula is in very good agreement with the exact calculation. For $t = 6$, one has the impression that HK is not so bad, since the wavepacket height increases again. That is, however, only a fortuitous occurrence, as demonstrated in for $t = 8$ and for $t = 10$. For longer times the peak of the HK Gaussian increases more and more, whereas the exact wavepacket height decreases to compensate for the spreading. At times of the order of 25 (not shown) the exact propagator (and our semiclassical formula) has a peak of height around 0.2 while HK's peak is around 8. At this time the width in HK is also completely wrong.

5.2. Van Vleck's formula and the HK propagator

We saw in the previous subsection that the propagation of Gaussian states via HK is very imperfect. It works only for harmonic potentials or for very short propagation times. In spite of this, the HK formula became rather popular in the last 5 years, and was applied to several problems in chemical physics. Among those we cite the photodissociation of CO₂ [Wal95], the collinear scattering of H₂ by H [Gar96], and the non-adiabatic dynamics in pyrazine molecules [Tho00]. Several theoretical articles were also published, testing the HK formula in model systems [Kay94b, Mai00] or proposing modifications in the formula for increasing its accuracy [Her97, Tho00]. All these applications deal, not with the plain mixed propagator $\langle x|K(t)|z' \rangle$, but with integrals over the phase space variables q' and p' , such as in equation (4.3).

The question is then how a poor time evolution of Gaussian wavepackets, as in HK, may produce acceptable results after integration over q' and p' . In this subsection we shall clarify this point and, at the same time, show why HK is so expensive computationally [Wal95] and sometimes just does not work [McC00]. First of all we shall calculate the coordinate propagator (4.55) using the semiclassical formula of HK for $\langle x''|K(t)|z' \rangle$. Once again the integration over q' and p' will be performed by the stationary-exponent approximation, just as we did in section 4.4. We shall see that HK does recover Van Vleck's formula [Van28] exactly! And that is the reason why sometimes it works. At the end of this subsection we shall comment on this result and discuss why HK does not lead to long-time convergence when the integrals over q' and p' are performed numerically. We shall also point out why the HK prefactor diverges for chaotic trajectories when the correct prefactor should, instead, go to zero.

We use the same notation as in section 4.4 and follow the same steps. The coordinate propagator for HK can be written

$$K_{\text{HK}}(x'', t; x', 0) = \int \frac{dq' dp'}{2\pi\hbar} \pi^{-\frac{1}{2}} b^{-1} \sqrt{\frac{1}{2}(m_{pp} + m_{qq} - im_{qp} + im_{pq})} e^{\xi(q', p')} \quad (5.10)$$

where the exponent $\xi(q', p')$ and its derivatives are

$$\xi = -\frac{1}{2b^2}[(x'' - q_r)^2 + (x' - q')^2] + \frac{i}{\hbar}[p_r(x'' - q_r) + p'(q' - x') + S_{\text{H}}] \quad (5.11)$$

$$\frac{\partial \xi}{\partial q'} = \frac{1}{b^2}[(x'' - q_r)(m_{qq} + im_{pq}) + (x' - q')] \quad (5.12)$$

$$\frac{\partial \xi}{\partial p'} = \frac{i}{\hbar}[(x'' - q_r)(m_{pp} - im_{qp}) - (x' - q')]. \quad (5.13)$$

The stationary conditions are satisfied if $q' = x'$ and $q_r(q', p', t) = x''$ and the value of ξ

computed at this trajectory is iS_H/\hbar . The second-order derivatives are

$$\xi_{qq} = -\frac{1}{b^2} [1 + m_{qq}(m_{qq} + im_{pq})] \quad (5.14)$$

$$\xi_{qp} = \xi_{pq} = -\frac{i}{\hbar} [1 - m_{qq}(m_{pp} - im_{qp})] = -\frac{1}{\hbar} m_{qp}(m_{qq} + im_{pq}) \quad (5.15)$$

$$\xi_{pp} = -\frac{ib}{c\hbar} m_{qp}(m_{pp} - im_{qp}). \quad (5.16)$$

Inserting all these expressions into equation (5.10), we find that the coordinate propagator becomes

$$\begin{aligned} K_{\text{HK}}(x'', t; x', 0) &= \pi^{-\frac{1}{2}} b^{-1} \sqrt{\frac{1}{2}(m_{pp} + m_{qq} - im_{qp} + im_{pq})} e^{iS_H/\hbar} \\ &\times \int \frac{dQ dP}{2\pi\hbar} \exp \left[\frac{1}{2} (\xi_{qq} Q^2 + 2\xi_{qp} QP + \xi_{pp} P^2) \right] \\ &= \pi^{-\frac{1}{2}} b^{-1} \sqrt{\frac{1}{2}(m_{pp} + m_{qq} - im_{qp} + im_{pq})} \times \frac{e^{iS_H/\hbar}}{\hbar \sqrt{\xi_{qq}\xi_{pp} - \xi_{qp}^2}}. \end{aligned} \quad (5.17)$$

Once again the quantity under the square root in the denominator is the determinant of the quadratic form in the second line, which is

$$\xi_{qq}\xi_{pp} - \xi_{qp}^2 = \frac{i}{\hbar^2} m_{qp}(m_{pp} + m_{qq} - im_{qp} + im_{pq}). \quad (5.18)$$

The final result is

$$K_{\text{HK}}(x'', t; x', 0) = \frac{1}{b\sqrt{2\pi im_{qp}}} e^{iS_H/\hbar} \quad (5.19)$$

and it coincides with the Van Vleck formula (4.65).

We can now understand why HK may sometimes work, even if it is not a correct semiclassical formula, and we can also understand the origin of its main drawbacks. The latter include the very slow convergence of the integrals over q' and p' when done numerically [Wan00, Mcc00], the lack of normalization [Her84] and the blow-up of the prefactor for chaotic trajectories [Mai00]. In fact, numerical convergence of the integrals over q' and p' is often achieved only after resorting to smoothings [Her97, Mcc00, Tho00, Sun00], and the results have not always been satisfactory.

The reason why HK does sometimes give good results is precisely that it is able to recover Van Vleck. In fact, Kay [Kay94a] derived the HK formula by making an ansatz for the propagator and demanding that this ansatz satisfy the basic condition of agreeing with Van Vleck. In words, if one insists on keeping the width of the propagated wavepacket constant, then one *must* arrive at the HK pre-factor if one wants to get Van Vleck when integrating over q' and p' . The price paid for doing so is non-conservation of the norm, a high price to say the least. Therefore, if HK is to be used at all, it has to be under an integral. However, even when integrated, HK leads to very slow convergence and oscillatory behaviour, especially at long times. To see why this happens, we note that the square root of the determinant of the quadratic form in the stationary integral (5.17) is a measure of the phase-space area $\Delta q' \Delta p'$ that matters in the integration. We have

$$(\Delta q' \Delta p')_{\text{HK}} \approx \frac{1}{\sqrt{|\xi_{qq}\xi_{pp} - \xi_{qp}^2|}} = \frac{\hbar}{\sqrt{|m_{qp}|}} \frac{1}{\sqrt{|m_{pp} + m_{qq} - im_{qp} + im_{pq}|}}. \quad (5.20)$$

As we saw in section 5.1, $\sqrt{|m_{pp} + m_{qq} - im_{qp} + im_{pq}|}$ increases with time, for our numerical example as well as for the free particle. This means that the relevant phase-space zone of

initial trajectories that one needs to sample gets smaller with time. The physical interpretation of this is very simple: any initial swarm of trajectories spreads as time passes. However, only those trajectories in the neighbourhood of the one connecting x' to x'' contribute significantly. The size of this neighbourhood is determined by the size of the propagated wavepacket. In the case of HK the propagated packet keeps its width fixed at $\Delta q \Delta p = bc = \hbar$. For long times the initial spread of trajectories that *end* inside this small region shrinks very fast. This is why the numerical integration of equation (5.10) by sampling initial trajectories is bound not to converge for long times, since very few trajectories are going to be picked up in the relevant region.

Compare this with the relevant phase-space spread for the integration with our formula

$$(\Delta q' \Delta p') \approx \frac{1}{\sqrt{|\xi_{qq} \xi_{pp} - \xi_{qp}^2|}} = \frac{\hbar}{\sqrt{2m_{qp}}} \sqrt{|m_{qq} + im_{qp}|}. \quad (5.21)$$

We know that $\sqrt{|m_{qq} + im_{qp}|}$ increases with time, since the wavepacket spreads, and so does the phase space region of contributing trajectories, ensuring an integration which must be more efficient.

We also mention that the application of semiclassical formulae to chaotic systems is known to be difficult due to the exponential proliferation of contributing trajectories from x' to x'' for long times. This is compensated in part by the exponentially small contribution of each individual orbit to the propagator. The HK prefactor, however, assigns an already divergent contribution to each of these trajectories, leaving no hope for accurate results [Mai00].

As a final comment we note that the smoothing technique introduced by Herman [Her97] has the role of cutting off the contributions from trajectories whose action have a large first-order variation. In our semiclassical formula this cutoff is performed automatically by the prefactor. This is in fact exactly what one expects from a *stationary phase* integral.

6. The energy representation

In the special case of time-independent systems, the Fourier transform in time of the coherent-state propagator, which we shall refer to as the (coherent-state) Green function, has poles at the quantized energy levels. For its diagonal elements ($z' = z''$) the residues are the so-called Husimi distributions, i.e. the absolute squares of the eigenfunctions in the coherent-state representation, which are also called the Bargmann wavefunctions. In this section we shall derive the semiclassical expressions for the poles and residues of the Green function. We shall obtain from them the semiclassical quantization rule for the energy levels and the semiclassical Husimi distributions.

6.1. The monodromy matrix in one dimension

When the trajectory is a periodic orbit, with the initial point returning to itself after the *period* T , the tangent matrix M of section 2.6 is called the monodromy matrix. In the next subsections it will be necessary to know the element M_{vv} for a real periodic orbit traversed n times, i.e. for $t = nT$. We shall calculate it here. First we shall review a general formula for arbitrary canonical variables, then we shall switch back to the (u, v) variables.

Let Q and P be canonical variables and $H(Q, P)$ the Hamiltonian. We want to find the monodromy matrix M for periodic orbits in the (Q, P) representation. M has four elements, which we shall determine from four linear equations. For the first two equations we apply M to (\dot{Q}, \dot{P}) , the velocity vector in phase space. This should yield this vector again, because a

small displacement along the trajectory maps onto itself. Thus

$$M \begin{pmatrix} \dot{Q} \\ \dot{P} \end{pmatrix} = \begin{pmatrix} \dot{Q} \\ \dot{P} \end{pmatrix}. \quad (6.1)$$

For the other two equations we consider a small displacement $(\delta Q, \delta P)$ non-collinear with (\dot{Q}, \dot{P}) , and we assume for now that the Hamiltonian is not harmonic, so that the period T of a periodic orbit depends on its energy. Then $(\delta Q, \delta P)$ points to another periodic orbit, with a different period $T + \delta T$ and a different energy $E + \delta E$. When we apply the M matrix to $(\delta Q, \delta P)$, since the propagation time is only T , the result falls short of the original displacement by $\delta T \times (\text{velocity})$, hence

$$M \begin{pmatrix} \delta Q \\ \delta P \end{pmatrix} = \begin{pmatrix} \delta Q \\ \delta P \end{pmatrix} - \delta T \begin{pmatrix} \dot{Q} \\ \dot{P} \end{pmatrix}. \quad (6.2)$$

Obviously, given the four equations (6.1) and (6.2), M must have the form

$$M = \mathbf{1} + N \quad (6.3)$$

where N must obey the four equations

$$N \begin{pmatrix} \dot{Q} \\ \dot{P} \end{pmatrix} = 0 \quad (6.4)$$

$$N \begin{pmatrix} \delta Q \\ \delta P \end{pmatrix} = -\delta T \begin{pmatrix} \dot{Q} \\ \dot{P} \end{pmatrix}. \quad (6.5)$$

From equations (6.4) one sees that N must have the form

$$N = \begin{pmatrix} \dot{P}a & -\dot{Q}a \\ \dot{P}b & -\dot{Q}b \end{pmatrix} \quad (6.6)$$

with a and b still unknown. From equations (6.5) one calculates a and b as

$$a = \frac{\delta T}{\delta E} \dot{Q} \quad b = \frac{\delta T}{\delta E} \dot{P} \quad (6.7)$$

where δE , the energy difference, actually appears as $\dot{Q}\delta P - \dot{P}\delta Q$, which is δE by Hamilton's equations. The final form of the monodromy matrix in the (Q, P) representation is therefore

$$M = \mathbf{1} + \frac{dT}{dE} \begin{pmatrix} \dot{Q}\dot{P} & -\dot{Q}^2 \\ \dot{P}^2 & -\dot{Q}\dot{P} \end{pmatrix} \quad (6.8)$$

where dT/dE is the derivative of $T(E)$, the period of the orbit as a function of its energy. Although we restricted ourselves to the anharmonic case, it is obvious that this formula holds for the harmonic case also, for which dT/dE vanishes.

We shall now apply this to the variables u and v . But the latter are not quite true canonical variables because of the factor $i\hbar$ in the equations of motion (2.36). To avoid this source of confusion we define temporary canonical variables $U = \sqrt{i\hbar}u$ and $V = \sqrt{i\hbar}v$. Then the general result (6.8) certainly applies to U and V . When we reintroduce u and v , we find for the monodromy matrix in the (u, v) representation

$$M(u, v, T) = \mathbf{1} + i\hbar \frac{dT}{dE} \Gamma \quad (6.9)$$

where Γ is given by

$$\Gamma = \begin{pmatrix} \dot{u}\dot{v} & -\dot{u}^2 \\ \dot{v}^2 & -\dot{u}\dot{v} \end{pmatrix}. \quad (6.10)$$

It is easy to check that, because $\Gamma^2 = 0$, the monodromy matrix for n traversals of the orbit is just

$$M(u, v, nT) = M(u, v, T)^n = \mathbf{1} + ni\hbar \frac{dT}{dE} \Gamma. \quad (6.11)$$

In the next subsections we need only one matrix element, which we denote by

$$(M^n)_{vv} = 1 - ni\hbar \frac{dT}{dE} \dot{u} \dot{v}. \quad (6.12)$$

6.2. Prologue: the Green function for the harmonic oscillator

The Feynman-type propagator $K_F(z'', t; z', 0)$ in the coherent-state representation, like other such propagators in quantum mechanics, is discontinuous at $t = 0$. One distinguishes between the ‘forward propagator’, which is defined by equation (2.5) for $t > 0$ but vanishes for $t < 0$, and the ‘backward propagator’, which vanishes for $t > 0$. The Green function is the Fourier transform of the forward propagator, hence it is obtained by integrating the time only in the interval $t \in [0, \infty]$. We are interested in its diagonal elements, which we denote by

$$G(z, E + i\gamma) := \frac{1}{i\hbar} \int_0^\infty dt K(z, t; z, 0) e^{i(E+i\gamma)t/\hbar}. \quad (6.13)$$

The small positive quantity γ is introduced for convergence; at the end it will be set equal to 0. When we insert the semiclassical propagator (2.72), G becomes

$$G(z, E + i\gamma) = \frac{1}{i\hbar} \sum_v \int_0^\infty dt \frac{1}{\sqrt{(M_v)_{vv}}} \exp[\phi_v(t)] \quad (6.14)$$

with

$$\phi_v(t) = \frac{i}{\hbar} \left[S_v(v'', u', t) + \mathcal{I}_v(v'', u', t) + \frac{i\hbar}{2} (|z''|^2 + |z'|^2) + (E + i\gamma)t \right]. \quad (6.15)$$

Instead of the variables v'' and u' , we could also have written equation (6.15) in terms of the single variable z , since $u' = z$ and $v'' = z^*$. But this does not mean that the trajectory going from z to z in some arbitrary time t is periodic. As we have already discussed (see before equation (2.38)), the trajectory is usually complex and neither u nor v match at the end points. However, for the case of interest here, namely one-dimensional bound systems, there exists for each phase-space point z a (minimal) time $T = T(z)$ for which the orbit through z is periodic and real. Then the end points do match and T is the period. Obviously this particular time $t = T$ will play a special role in the integration of equation (6.13), and so will its multiples $t = nT$, which correspond to repeated traversals of the periodic orbit. Therefore, after evaluating the integral (6.13) by the stationary exponent method, we shall expand the stationary time $t_0 = t_0(z, E)$ about the classical period $nT(z)$. The resulting Green function will be a good approximation to the actual Green function $G(z, E)$ only for arguments z and E satisfying $t_0(z, E) \approx nT(z)$.

Before we carry out the calculation of $G(z, E)$ for a general Hamiltonian, it is instructive to find out the result of these approximations, stationary exponent plus expansion about $t_0 = nT$, for the harmonic oscillator. This will help us understand the nature of the approximations.

We consider an oscillator of unit mass and frequency ω , and we take the parameter b of equation (2.3) to be $\sqrt{\hbar/\omega}$. Then the semiclassical propagator is easily shown to be

$$K(z, t) = e^{-i\omega t/2} \exp[|z|^2 (e^{-i\omega t} - 1)] \quad (6.16)$$

which is also the exact result. The first exponential is the prefactor $M_{vv}^{-1/2}$. This K is now carried into equation (6.13), which becomes

$$G(z, E + i\gamma) = \frac{1}{i\hbar} \int_0^\infty dt e^{-i\omega t/2} \exp\left(\frac{i}{\hbar}(E + i\gamma)t + |z|^2(e^{-i\omega t} - 1)\right). \quad (6.17)$$

The whole of the second exponent is proportional to $1/\hbar$, when $|z|^2$ is written in terms of q and p . But there is no \hbar in the prefactor. Hence we are exactly in the situation mentioned at the end of section 3.3. We look for the time t_0 at which the second exponent is stationary. We find that t_0 is given by the condition

$$E + i\gamma = \hbar\omega e^{-i\omega t_0} |z|^2. \quad (6.18)$$

The solutions of this equation can be written $t_0 = T_0 + nT$, where n is an integer, $T = 2\pi/\omega$, and $T_0 = T_0(z, E)$ is pure imaginary (in the limit $\gamma \rightarrow 0$). Thus there is an infinite number of times at which the second exponent is stationary. For each t_0 we expand this exponent to second order in the vicinity and we perform the Gaussian integral. Then we add all these results together to obtain the following G :

$$\begin{aligned} G(z, E + i\gamma) &= \frac{1}{i\hbar} \sum_{n=1}^{\infty} e^{-\frac{1}{2}i\omega(nT+T_0)} \exp\left(\frac{i}{\hbar}(E + i\gamma)(nT + T_0) + |z|^2(e^{-i\omega T_0} - 1)\right) \\ &\quad \times \int_0^\infty dt \exp\left(-\frac{1}{2}\omega^2|z|^2(t - t_0)^2 e^{-i\omega T_0}\right) \\ &= \frac{1}{i\hbar|z|} \sqrt{\frac{2\pi}{\omega^2 e^{-i\omega T_0}}} \sum_{n=1}^{\infty} \exp\left[\frac{2\pi i n}{\hbar\omega} \left(E + i\gamma - \frac{\hbar\omega}{2}\right)\right] \\ &\quad \times \exp\left[|z|^2(e^{-i\omega T_0} - 1) + i\left(E + i\gamma - \frac{1}{2}\hbar\omega\right) \frac{T_0}{\hbar}\right] \\ &= \frac{1}{i\hbar|z|} \sqrt{\frac{2\pi}{\omega^2 e^{-i\omega T_0}}} \frac{\exp\left[\frac{2\pi i}{\hbar\omega} \left(E + i\gamma - \frac{1}{2}\hbar\omega\right)\right]}{1 - \exp\left[\frac{2\pi i}{\hbar\omega} \left(E + i\gamma - \frac{1}{2}\hbar\omega\right)\right]} \\ &\quad \times \exp\left[|z|^2(e^{-i\omega T_0} - 1) + i\left(E + i\gamma - \frac{1}{2}\hbar\omega\right) \frac{T_0}{\hbar}\right]. \end{aligned} \quad (6.19)$$

In the above we started the sum over n at $n = 1$. Why not $n = 0$? The answer is that it does not make any difference, as long as we use this theory only to calculate the energies of the stationary states and their Husimi distributions. This is discussed in the paragraph following equation (6.34) in the next section.

The poles of (6.19) can now be found in the limit $\gamma \rightarrow 0$. They are given by the condition $E =: E_m = \hbar\omega(m + 1/2)$ with integer m . The residue for $E = E_m$, which is the Husimi distribution, is

$$\rho_{\text{Husimi}}(z) = \frac{1}{\sqrt{2\pi}|z|^2 e^{-i\omega T_0}} \exp\left[|z|^2(e^{-i\omega T_0} - 1) + im\omega T_0\right]. \quad (6.20)$$

Using (6.18) for T_0 with $E = E_m$ and $\gamma = 0$, we obtain $e^{-i\omega T_0}|z|^2 = m + 1/2$ and (6.20) becomes

$$\rho_{\text{Husimi}}(z) = \frac{1}{\sqrt{2\pi}(m + 1/2)} e^{m+1/2-|z|^2} \left(\frac{|z|^2}{m + 1/2}\right)^m. \quad (6.21)$$

This result should be compared with the exact Husimi distribution

$$\rho_{\text{Husimi}}^{\text{exact}}(z) = \frac{1}{m!} e^{-|z|^2} |z|^{2m} \quad (6.22)$$

which is an annulus with its maximum at $|z|^2 = m$. The mean value of $|z|^2$ is $m + 1$ and the logarithmic second derivative at the maximum is $-1/m$, giving a width of order \sqrt{m} . Both formulas, exact and semiclassical, have the same z -dependence, namely, $|z|^{2m} e^{-|z|^2}$. They differ only in the coefficient. Obviously (6.22) is correctly normalized and (6.21) is not. The difference is small, however. Using Stirling's approximation for $m!$, we can write (6.21) as

$$\rho_{\text{Husimi}}(z) = \frac{1}{m!} e^{-|z|^2} |z|^{2m} \left(1 + \frac{1}{2m+1}\right)^{m+1/2} e^{-1/2}. \quad (6.23)$$

For large m the quantity to the left of $e^{-1/2}$ becomes $e^{+1/2}$. Thus the semiclassical Husimi becomes exact in the limit of large quantum numbers, and it is a valid approximation for all phase-space points z .

For general Hamiltonians we shall not be able to do such a complete calculation. As we shall see, the stationary time t_0 is given by an implicit equation that cannot be generally solved. The best thing to do to get an explicit result will be to expand t_0 about the classical period nT . Now we can check this additional approximation explicitly for the harmonic oscillator. Let us pretend that equation (6.18) cannot be solved exactly for $t_0(E, z)$ and, instead, let us solve it by expanding t_0 about nT . So we write $t_0 = nT + T_0$ and consider only small values of T_0 . Taking $\gamma = 0$ in equation (6.18) and expanding for small T_0 , we find

$$T_0 \approx \frac{\hbar\omega|z|^2 - E}{i\hbar\omega^2|z|^2}. \quad (6.24)$$

Since T_0 is independent of n we may go through the same steps as in equation (6.19). The position of the poles does not depend on T_0 and it is not affected by this approximation. The Husimi distribution, however, does depend on T_0 explicitly. For $E = E_m$ we get

$$T_0 \approx \frac{|z|^2 - m - 1/2}{i\omega|z|^2}. \quad (6.25)$$

T_0 is small whenever $|z|^2$ is close to $m + 1/2$, which is the classical orbit with quantized energy E_m . Therefore, for each eigenstate, there is a phase-space region centred on this classical orbit where the approximation is justified. This region should encompass most of the distribution when m is sufficiently large. Expanding equation (6.20) to second order in T_0 and using (6.25) we obtain

$$\rho_{\text{Husimi}}(z) \approx \frac{1}{\sqrt{2\pi}|z|} \exp\left[-\frac{(|z|^2 - m - 1/2)^2}{2|z|^2}\right]. \quad (6.26)$$

The maximum of this annulus comes at $|z|^2 = m + 1/8m + \dots$, which agrees with the exact maximum for the first two orders of $1/m$. The logarithmic second derivative also agrees for the leading order. Therefore, the result of expanding the stationary time about the classical period is to restrict the region of validity of the Husimi distribution to not too small quantum numbers.

6.3. The Green function for general Hamiltonians

We now return to our general calculation, equation (6.13). In what follows we shall omit the subscript v . It will be replaced shortly by the multiple traversals around periodic trajectories. The stationary exponent condition is given by $\phi'(t_0) = 0$, with $\phi(t)$ given by (6.15). It is

$$\phi'(t_0) = \frac{i}{\hbar} \left(\left. \frac{\partial S}{\partial t} \right|_{t_0} + \left. \frac{\partial \mathcal{I}}{\partial t} \right|_{t_0} + E + i\gamma \right) \equiv 0. \quad (6.27)$$

The third equation (2.60) gives

$$\partial S/\partial t|_{t=t_0} = -\mathcal{E}(z, t_0). \quad (6.28)$$

This script \mathcal{E} is the energy of the classical trajectory, not to be confused with E , which is the energy variable in the Green function. For the first time derivative of \mathcal{I} , defined in equation (2.65), we have

$$\partial \mathcal{I}/\partial t|_{t=t_0} = \frac{1}{2} \frac{\partial^2 \mathcal{H}}{\partial u \partial v} \Big|_{t=t_0} + \frac{1}{2} \int_0^{t_0} \left[\frac{\partial^3 \mathcal{H}}{\partial^2 z \partial z^*} \frac{\partial z}{\partial t} \Big|_{t=t_0} + \frac{\partial^3 \mathcal{H}}{\partial z \partial^2 z^*} \frac{\partial z^*}{\partial t} \Big|_{t=t_0} \right] dt'. \quad (6.29)$$

The terms under the integral involve third derivatives of \mathcal{H} with respect to the phase-space variables. We have consistently neglected such terms up to now and we must do so here again. Hence we use only the first term, to which we give a simpler name

$$\partial \mathcal{I}/\partial t|_{t=t_0} \approx \frac{1}{2} \frac{\partial^2 \mathcal{H}}{\partial z \partial z^*} =: \epsilon(z, t_0). \quad (6.30)$$

The stationary condition is then written

$$E + i\gamma - \mathcal{E}(z, t_0) + \epsilon(z, t_0) = 0. \quad (6.31)$$

Besides the contributions from the stationary points $t = t_0$, there is also a contribution to G coming from the vicinity of $t = 0$. As we shall see later, this contribution is not needed in the calculation of the energy levels and the Husimi distributions, hence we shall ignore it. We have also discarded it in the previous calculation for the harmonic oscillator.

In order to perform the time integral, we need to expand $\phi(t)$ around t_0 to second order. The first derivative at t_0 is zero by definition. The second derivative is

$$\phi''(t_0) = \frac{i}{\hbar} \left(\frac{\partial^2 S}{\partial t^2} \Big|_{t_0} + \frac{\partial^2 \mathcal{I}}{\partial t^2} \Big|_{t_0} \right). \quad (6.32)$$

For the second derivative of S we introduce the notation

$$\alpha(z, t_0) := \partial^2 S/\partial t^2|_{t=t_0}. \quad (6.33)$$

From (6.29) we see that $\partial^2 \mathcal{I}/\partial t^2$ involves only third- or higher-order derivatives of \mathcal{H} and therefore we can discard it completely.

We can now calculate $G(z, E + i\gamma)$. The effect of our expansion is that we have applied once again the Gaussian approximation to the integral in equation (6.13), which is then straightforward:

$$\begin{aligned} G(z, E + i\gamma) &= \frac{1}{i\hbar} \frac{1}{\sqrt{M_{vv}(t_0)}} \exp \left\{ \frac{i}{\hbar} [S(z, t_0) + \mathcal{I}(z, t_0) + i\hbar|z|^2 + (E + i\gamma)t_0] \right\} \\ &\quad \times \int_0^\infty \exp \left(\frac{i\alpha(z, t_0)}{2\hbar} (t - t_0)^2 \right) dt \\ &= \frac{1}{i\hbar} \sqrt{\frac{2\pi i\hbar}{M_{vv}(t_0)\alpha(z, t_0)}} \exp \left\{ \frac{i}{\hbar} [S(z, t_0) + \mathcal{I}(z, t_0) + i\hbar|z|^2 + (E + i\gamma)t_0] \right\}. \end{aligned} \quad (6.34)$$

Actually this integral is a sum of Gaussians, because there are many solutions to equation (6.31), as we have seen with the harmonic oscillator. As we mention later, α has a positive imaginary part for $t_0 \approx nT$; this follows from equation (6.53), plus the fact that S is real. It means that the integral is strongly convergent for very large times, both positive and negative. However, the integral in equation (6.13) does not extend over the interval $-\infty < t < +\infty$, but over

$0 < t < +\infty$: is there a problem at $t = 0$? Yes, there might very well be a problem, both for $t = 0$ and for $t_0 \approx nT$ and small n . There is no problem for large n , since nT becomes arbitrarily large. We intend to use this Green function only for the semiclassical calculation of the energy levels and the Husimi distributions. These are determined by the poles of the Green function and by their residues, respectively, and the poles and residues are determined solely by the behaviour of the integrand of (6.13) at very large times. Hence we are safe in ignoring possible mistakes at small t . In particular, the contributions from trajectories with $t \approx 0$ give rise to the Thomas–Fermi approximation, which we shall not consider here. Therefore it is alright for our purpose to calculate the integral as if it extended from $-\infty$ to $+\infty$.

We shall now transform the prefactor by finding a convenient way of expressing $\alpha(z, t_0)$. In the many differentiations which follow, it is important to remember that the independent variables in S are u' , v'' and t . One should do the differentiations first, and only afterwards may one compute the functions for the stationary orbit by replacing t by t_0 , u' by z and v'' by z^* . First we write two different ways of expressing $\partial S/\partial t$

$$\partial S/\partial t = -\mathcal{H}[u', v'(u', v'', t)] \quad \partial S/\partial t = -\mathcal{H}[u''(u', v'', t), v'']. \quad (6.35)$$

This leads to two different ways of writing α

$$\alpha(z, t_0) = \left. \frac{\partial^2 S}{\partial t^2} \right|_{t=t_0} = - \left. \frac{\partial \mathcal{H}}{\partial v'} \frac{\partial v'}{\partial t} \right|_{t=t_0} \quad (6.36)$$

$$\alpha(z, t_0) = \left. \frac{\partial^2 S}{\partial t^2} \right|_{t=t_0} = - \left. \frac{\partial \mathcal{H}}{\partial u''} \frac{\partial u''}{\partial t} \right|_{t=t_0}. \quad (6.37)$$

In equation (6.36) we use Hamilton's equations (2.36) to express $\partial H/\partial v'$ and the second equation (2.60) to express $\partial v'/\partial t$. In equation (6.37) we do similar transformations with the other variables. This gives the two forms

$$\alpha(z, t_0) = -i\hbar \dot{u}' \frac{i}{\hbar} \left. \frac{\partial^2 S}{\partial u' \partial t} \right|_{t=t_0} = i\hbar \dot{v}'' \frac{i}{\hbar} \left. \frac{\partial^2 S}{\partial v'' \partial t} \right|_{t=t_0}. \quad (6.38)$$

Referring now to equation (6.35), using Hamilton's equations once again, and using the first and second equations (2.60) once again, we transform the second derivatives of S as follows:

$$\frac{\partial^2 S}{\partial u' \partial t} = - \frac{\partial \mathcal{H}(u'', v'')}{\partial u''} \frac{\partial u''}{\partial u'} = i\hbar \dot{v}'' \frac{i}{\hbar} \frac{\partial^2 S}{\partial u' \partial v''} \quad (6.39)$$

$$\frac{\partial^2 S}{\partial v'' \partial t} = - \frac{\partial \mathcal{H}(u', v')}{\partial v'} \frac{\partial v'}{\partial v''} = -i\hbar \dot{u}' \frac{i}{\hbar} \frac{\partial^2 S}{\partial u' \partial v''}. \quad (6.40)$$

After cancellation of the \hbar , both forms of the equations give the same result for α , namely

$$\alpha(z, t_0) = - \dot{u}' \dot{v}'' \left. \frac{\partial^2 S}{\partial u' \partial v''} \right|_{t=t_0} = - \dot{u}' \dot{v}'' A_{uv} \Big|_{t=t_0} = i\hbar \dot{u}' \dot{v}'' / M_{vv}(z, t_0). \quad (6.41)$$

Amazingly, the denominator under the square root in equation (6.34) has become simply $i\hbar \dot{u}' \dot{v}''$, where the velocities are computed at the complex trajectory with $t = t_0$. One should, however, be careful about the phase of the M_{vv} under the square root, as already mentioned in sections 2 and 4. We shall discuss it in a moment.

In spite of this great simplification it is still hard to find the poles of $G(z, E)$ by looking at equation (6.34). This is because the stationary time t_0 is given implicitly by equation (6.31) and it refers to complex trajectories. According to our discussion following equation (6.15), large contributions to $G(z, E + i\gamma)$ are expected for t_0 close to nT , where T is the period of the real orbit through z . Therefore, as we did for the harmonic oscillator, we proceed to expand

equation (6.34) about $t_0 = nT$, summing over n . We write $t_0 = nT + T_0$, substitute it into equation (6.31), and expand the terms to find T_0 :

$$E + i\gamma - \mathcal{E}(z, nT) + \epsilon(z, nT) - \partial\mathcal{E}(z, t)/\partial t|_{t=nT} T_0 + \partial\epsilon(z, t)/\partial t|_{t=nT} T_0 \approx 0. \quad (6.42)$$

Equation (6.30) shows again that $\partial\epsilon(z, t)/\partial t$ involves only third or higher derivatives of \mathcal{H} and therefore we discard it. For real periodic orbits, the functions \mathcal{E} and ϵ depend only on z and we have

$$\partial\mathcal{E}(z, t)/\partial t|_{t=nT} = -\partial^2 S/\partial t^2|_{t=nT} = -\alpha(z, nT) =: -\alpha^{(n)}(z). \quad (6.43)$$

Equation (6.42) can then be written

$$(E + i\gamma - \mathcal{E}(z, nT) + \epsilon(z, nT)) + \alpha^{(n)}(z)T_0 \approx 0. \quad (6.44)$$

Our basic assumption is that $T_0 \ll nT$ for each solution t_0 labelled by n . Hence the sum of the terms inside the parenthesis above should be small. Solving equation (6.44) for T_0 gives

$$T_0 = -\frac{E + i\gamma - \mathcal{E}(z) + \epsilon(z)}{\alpha^{(n)}(z)}. \quad (6.45)$$

In the limit $\gamma \rightarrow 0$, the points z satisfying $\mathcal{E}(z) - \epsilon(z) = E$ have $t_0(z, E) = nT(z)$. When we expand the Green function about $t_0 = nT$, we are restricting the validity to the neighbourhood of these points. Notice that, in contrast to the case of the harmonic oscillator, T_0 does depend on n and the sum over multiple traversals has to be performed after the expansion about $t_0 = nT$.

We are now in a position to discuss the pre-factor which, according to equation (6.41), is given (up to its phase) by the square root of $\dot{u}'(t_0) \dot{v}''(t_0)$. Its main contribution comes from periodic orbits and, once again, we have to expand each of these velocities for t_0 close to nT . Using Hamilton's equation for $\dot{u}'(t_0)$ we get

$$\begin{aligned} \dot{u}'(t_0) &= -\frac{i}{\hbar} \frac{\partial \mathcal{H}}{\partial v'} \Big|_{t=t_0} \approx \dot{u}'(nT) - \frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial v'^2} \frac{\partial v'}{\partial t} \Big|_{t=nT} T_0 \\ &= \dot{z} - \frac{i}{\hbar} \frac{\partial^2 \mathcal{H}}{\partial v'^2} \left(\frac{i}{\hbar} \frac{\partial^2 S}{\partial t \partial u'} \Big|_{t=nT} \right) T_0 \\ &= \dot{z} + \frac{i}{\hbar} \mathcal{H}_{vv} \dot{z}^* T_0 / M_{vv}^n \\ &= \dot{z} + \frac{1}{\hbar^2 \dot{z}} \mathcal{H}_{vv} T_0 \alpha^{(n)} \end{aligned} \quad (6.46)$$

where we have used equations (2.60), (6.39), (2.71) and (6.41). Doing a similar calculation for $\dot{v}''(t_0)$ we find

$$\dot{u}'(t_0) \dot{v}''(t_0) \approx |\dot{z}|^2 (1 + \mathcal{O}(\alpha^{(n)} T_0)). \quad (6.47)$$

Now we want to argue that the terms of order $\alpha^{(n)} T_0$ are small and that, in fact, the prefactor can be simply calculated at the periodic orbit itself, so that (6.47) is just $|\dot{z}|^2$. We gave a similar argument in section 3.3, where the neglected terms were of order \hbar compared to the terms kept. Here, however, their order is $\sqrt{\hbar}$, not as small, but still small! We shall verify this *a posteriori* once we have calculated the Husimi distribution. We shall find later that the Husimi attains significant magnitudes only when $E - \mathcal{E}(z) + \epsilon(z)$, which is the same as $\alpha^{(n)} T_0$ by (6.45), is of order $\sqrt{\hbar}$.

To calculate the phase of the prefactor, or the tangent matrix, for a real periodic orbit, one must follow it when moving around the orbit. The harmonic oscillator provides again a simple illustration of what happens: in this case the solution of Hamilton's equations (2.36) with initial conditions $u(0) = u'$, $v(0) = v'$ is simply $u(t') = u' e^{-i\omega t'}$ and $v(t') = v' e^{i\omega t'}$. The tangent matrix is diagonal and $M_{vv} = e^{i\omega t'}$. The pre-factor of the time-dependent propagator

is, therefore, $e^{-i\omega t/2}$ (see equation (6.16)). When this is calculated at a periodic orbit, we see that after one period, for $t = T = 2\pi/\omega$, M_{vv} has rotated by 2π and the phase of the pre-factor is $e^{-i\pi} = -1$. The phase for $t = 2n\pi/\omega$ is just $e^{-in\pi}$.

This phase of $-n\pi$ is not particular to the harmonic potential; it is a consequence of the fact that the motion is periodic in two-dimensional phase space. To see this, consider a periodic orbit of energy \mathcal{E} and period T in a generic system. The tangent matrix propagates small displacements about this orbit. Any such small displacement is going to point to a nearby periodic orbit with energy $\mathcal{E} + \delta\mathcal{E}$ and period $T + \delta T$. As we move once around the orbit the displacement vector stays hooked to these two reference orbits and, therefore, has to rotate once as well. The total rotation is not exactly 2π , since the period of the nearby orbit is slightly different from T . The angle of rotation is actually $2\pi + \theta$, where the θ piece follows from equation (6.12) for M_{vv} . When M_{vv} is raised to the $-1/2$ power in the prefactor, this 2π contributes a phase of $-\pi$ to the propagator, just as in the harmonic oscillator. Then there is the angle θ , which is a function of n and which remains in the prefactor. Equation (6.12) shows that θ never gets very large; for all n it is bounded either by 0 and $\pi/2$, or by $-\pi/2$ and 0, depending on the signs. However, by virtue of equation (6.41) the phase θ disappears completely from the calculation and the only relevant phase from the square root is $-n\pi$. From now on we shall take this phase out of the prefactor and include it explicitly in the exponential. Replacing $\dot{u}'v''$ in equation (6.41) by $|\dot{z}|^2$ we get

$$G(z, E + i\gamma) = \frac{\sqrt{2\pi}}{i\hbar|\dot{z}|} \exp \left\{ \frac{i}{\hbar} \left[S(z, t_0) + \mathcal{I}(z, t_0) + i\hbar|z|^2 + (E + i\gamma)t_0 - n\pi\hbar \right] \right\}. \quad (6.48)$$

Next we expand S and \mathcal{I} around $t_0 = nT$. Since the zero-order orbit is the real periodic one, we may write, using equation (2.54)

$$S(z^*, z, nT) = n\mathcal{S}(\mathcal{E}(z)) - n\mathcal{E}(z)T - i\hbar|z|^2. \quad (6.49)$$

Here $\mathcal{E}(z)$ is the energy of the real periodic orbit going through z . It should not be confused with E , the quantal energy variable. $\mathcal{S}(\mathcal{E}(z))$ is the 'reduced action'

$$\mathcal{S}(\mathcal{E}(z)) = \frac{i\hbar}{2} \int_0^T (\dot{u}v - \dot{v}u) dt' \quad (6.50)$$

which, for the real periodic orbit, is a function only of \mathcal{E} , or of the period T , themselves functions of z . The third equation (2.60) gives

$$\partial S/\partial t|_{t=nT} = \partial S/\partial t|_{t=T} = -\mathcal{E}(z). \quad (6.51)$$

Either \mathcal{E} or T can be used as the independent variable for the periodic trajectory. The second derivative of S becomes (see equations (6.33) and (6.41))

$$\partial^2 S/\partial t^2|_{t=nT} = \alpha^{(n)}(z) = i\hbar|\dot{z}|^2/M_{vv}^{(n)}. \quad (6.52)$$

Using equation (6.12) and $dS/d\mathcal{E} = T$, we find

$$\frac{1}{\alpha^{(n)}} = \frac{M_{vv}^{(n)}}{i\hbar|\dot{z}|^2} = \frac{1}{i\hbar|\dot{z}|^2} - \frac{n}{|\dot{z}|^2} \frac{dT}{d\mathcal{E}} \dot{u}'v'' = \frac{1}{i\hbar|\dot{z}|^2} - n \frac{d^2\mathcal{S}}{d\mathcal{E}^2}. \quad (6.53)$$

From the definition (2.65), we have $\mathcal{I}(z^*, z, nT) = n\mathcal{I}(z^*, z, T)$. Once again, for the periodic orbit, \mathcal{I} depends only on the classical energy or on the period and we can call it $\mathcal{I}(\mathcal{E}(z))$. For the first time derivative we have by (6.30)

$$\partial \mathcal{I}/\partial t|_{t=nT} \approx \frac{1}{2} \frac{\partial^2 \mathcal{H}}{\partial z \partial z^*} = \epsilon(z). \quad (6.54)$$

Calling $\psi(E, z)$ the exponent in equation (6.48) and using equations (6.49)–(6.54) we get, up to second order in T_0 ,

$$\begin{aligned} \psi(E, z) \approx & \frac{i}{\hbar} n \left[S(\mathcal{E}(z)) + \mathcal{I}(\mathcal{E}(z)) - \pi\hbar + \frac{dS}{d\mathcal{E}}(E - \mathcal{E}(z) + i\gamma) \right] \\ & + \frac{i}{\hbar} \left[(E - \mathcal{E}(z) + \epsilon(z) + i\gamma)T_0 + \frac{\alpha^{(n)}}{2}T_0^2 \right]. \end{aligned} \quad (6.55)$$

Next we add and subtract $\epsilon \, dS/d\mathcal{E}$ inside the brackets on the first line and use equation (6.45) for T_0 in the second line. The term in T_0^2 becomes minus one half of the term in T_0 . When we add these two terms we get

$$\begin{aligned} \psi(E, z) = & \frac{i}{\hbar} n \left[S(\mathcal{E}(z)) + \mathcal{I}(\mathcal{E}(z)) - \pi\hbar + \frac{dS}{d\mathcal{E}}(E - \mathcal{E}(z) + \epsilon(z) + i\gamma) - \epsilon(z) \frac{dS}{d\mathcal{E}} \right] \\ & - \frac{i}{2\hbar\alpha^{(n)}} (E - \mathcal{E}(z) + \epsilon(z) + i\gamma)^2. \end{aligned} \quad (6.56)$$

Finally we use equation (6.53) for $\alpha^{(n)}$:

$$\begin{aligned} \psi(E, z) = & \frac{i}{\hbar} n \left[S(\mathcal{E}(z)) + \mathcal{I}(\mathcal{E}(z)) - \pi\hbar + \frac{dS}{d\mathcal{E}}(E - \mathcal{E}(z) + \epsilon(z) + i\gamma) - \epsilon(z) \frac{dS}{d\mathcal{E}} \right. \\ & \left. + \frac{1}{2} \frac{d^2S}{d\mathcal{E}^2} (E - \mathcal{E}(z) + \epsilon(z) + i\gamma)^2 \right] - \frac{1}{2\hbar^2|\dot{z}|^2} (E - \mathcal{E}(z) + \epsilon(z) + i\gamma)^2. \end{aligned} \quad (6.57)$$

The first, fourth and sixth terms in (6.57) are the Taylor expansion of the function $S(E + i\gamma + \epsilon(z))$ to second order around \mathcal{E} . This is an acceptable approximation as long as $E - \mathcal{E}(z) + \epsilon(z) + i\gamma$, i.e. $T_0\alpha^{(n)}$, is small. Since ϵ is of order \hbar we can further write $S(E + i\gamma + \epsilon(z)) \approx S(E + i\gamma) + T(E + i\gamma)\epsilon(z)$, neglecting terms of order \hbar^2 . Then equation (6.57) can be written

$$\begin{aligned} \psi(E, z) \approx & \frac{i}{\hbar} n \{ S(E + i\gamma) + \mathcal{I}(\mathcal{E}) + \epsilon(z)[T(E + i\gamma) - T(\mathcal{E})] - \pi\hbar \} \\ & - \frac{1}{2\hbar^2|\dot{z}|^2} (E - \mathcal{E}(z) + \epsilon(z) + i\gamma)^2. \end{aligned} \quad (6.58)$$

Since \mathcal{I} and ϵ are themselves of order \hbar , we may also replace \mathcal{E} by $E + i\gamma$ in the argument of both $\mathcal{I}(\mathcal{E})$ and $T(\mathcal{E})$, the error in doing so being of order $T_0\alpha^{(n)}\hbar$. This simplifies $\psi(E, z)$ even more and we get just

$$\psi(E, z) \approx \frac{i}{\hbar} n \{ S(E + i\gamma) + \mathcal{I}(E + i\gamma) - \pi\hbar \} - \frac{1}{2\hbar^2|\dot{z}|^2} (E - \mathcal{E}(z) + \epsilon(z) + i\gamma)^2. \quad (6.59)$$

Inserting this as the exponent in equation (6.48) and summing over n we obtain

$$\begin{aligned} G(z, E + i\gamma) = & -\frac{i}{\hbar} \frac{\sqrt{2\pi}}{|\dot{z}|} \sum_{n=1}^{\infty} \exp \left\{ \frac{i}{\hbar} n [S(E + i\gamma) + \mathcal{I}(E + i\gamma) - \pi\hbar] \right. \\ & \left. - \frac{(E - \mathcal{E}(z) + \epsilon(z) + i\gamma)^2}{2\hbar^2|\dot{z}|^2} \right\}. \end{aligned} \quad (6.60)$$

We may now perform the sum over all multiple traversals. The result is

$$G(z, E + i\gamma) = -\frac{i}{\hbar} \frac{\sqrt{2\pi}}{|\dot{z}|} \frac{e^{i(S+\mathcal{I}-\pi\hbar)/\hbar}}{1 - e^{i(S+\mathcal{I}-\pi\hbar)/\hbar}} \exp \left\{ -\frac{(E - \mathcal{E}(z) + \epsilon(z) + i\gamma)^2}{2\hbar^2|\dot{z}|^2} \right\} \quad (6.61)$$

where S and \mathcal{I} are taken at $E + i\gamma$.

6.4. Semiclassical energy levels and Husimi functions

Since the poles of the exact G are the stationary state energies, and their residues are the corresponding Husimi distributions, we are now in a position to calculate semiclassical approximations to these quantities. We let $\gamma \rightarrow 0$. If $\gamma \neq 0$ the poles are displaced by $i\gamma$. Poles occur whenever $(S + \mathcal{I} - \pi\hbar)/\hbar = 2m\pi$. This is the quantization rule, which can be rewritten

$$(S + \mathcal{I})(E_m) = (m + 1/2)h. \quad (6.62)$$

This is what replaces the usual WKB formula, which can be obtained from the coordinate Green function. One should not forget that S here is not the same as the S in the WKB formula, and that the latter does not contain any \mathcal{I} , of course. One should also realize that the $+1/2$ is obtained in very different ways in the two cases. In the usual WKB, the semiclassical approximation diverges at the turning points, and one must use some delicate arguments around this problem to derive a connection formula. Here, on the other hand, there is no divergence and we derived the $+1/2$ with a simple continuity argument.

The residue of

$$-\frac{i}{\hbar} \frac{e^{i(S+\mathcal{I}-\pi\hbar)/\hbar}}{1 - e^{i(S+\mathcal{I}-\pi\hbar)/\hbar}} \quad (6.63)$$

at $E = E_m$ is

$$\frac{1}{d(S + \mathcal{I})/d\mathcal{E}} = \frac{1}{T(E_m) + (d\mathcal{I}/d\mathcal{E})|_{E_m}}. \quad (6.64)$$

Hence the residue of G , which is the Husimi distribution for the level E_m , is

$$\rho_{\text{Husimi}}(z) = \frac{\sqrt{2\pi}}{|\dot{z}| [T(E_m) + (d\mathcal{I}/d\mathcal{E})|_{E_m}]} \exp \left\{ \frac{-(E_m - \mathcal{E}(z) + \epsilon(z))^2}{2\hbar^2 |\dot{z}|^2} \right\}. \quad (6.65)$$

It is centred close to the classical trajectory with the quantized energy. Both its amplitude and its width are modulated by the phase-space velocity $|\dot{z}|$. The width is given by the Gaussian factor. In terms of either variable \mathcal{E} or z , it is of order $\sqrt{\hbar}$. This follows from the fact that $\hbar|\dot{z}|^2$ is of order unity (see equations (2.2) and (2.3)). Therefore, our decision not to expand the pre-factor (see equation (6.47)), and the approximation after equation (6.58), amount to discarding corrections proportional to $\sqrt{\hbar}$ in the Green function. These are not as small as the other corrections to the semiclassical approximation, which were of order \hbar (see section 3.3), but they are still small and vanish in the semiclassical limit.

For the second type of path integral discussed in section 3, the quantization rule can be obtained by changing \mathcal{I} to $-\mathcal{I}$ in the time-dependent propagator and carrying this change all the way through the Green function treatment. The quantization rule and Husimi functions become then

$$(S - \mathcal{I})(E_m) = (m + 1/2)h \quad (6.66)$$

and

$$\rho_{\text{Husimi}}^{(2)}(z) = \frac{\sqrt{2\pi}}{|\dot{z}| [T(E_m) - (d\mathcal{I}/d\mathcal{E})|_{E_m}]} \exp \left\{ \frac{-(E_m - \mathcal{E}(z) - \epsilon(z))^2}{2\hbar^2 |\dot{z}|^2} \right\} \quad (6.67)$$

where all quantities are computed with H_2 , instead of $H_1 \equiv \mathcal{H}$.

According to our discussion in section 3, one could also use the Weyl Hamiltonian and drop \mathcal{I} . In this case there would be no $\epsilon(z)$ coming from $\partial\mathcal{I}/\partial t$. The quantization rule in this case becomes

$$S(E_m) = (m + 1/2)h \quad (6.68)$$

which is exactly the WKB rule, and the Husimi functions are

$$\rho_{\text{Husimi}}^{\text{Weyl}}(z) = \frac{\sqrt{2\pi}}{|z| T(E_m)} \exp \left\{ -\frac{(E_m - E(z))^2}{2\hbar^2 |z|^2} \right\}. \quad (6.69)$$

This expression is similar to a formula suggested previously by Kurchan *et al* (see equations (5.21) and (5.22) in [Kur89]; see also [Car92] for a numerical application).

The semiclassical energy levels will be slightly different for the three prescriptions, equations (6.62), (6.66) and (6.68). In fact it can be shown, using arguments similar to those in appendix C, that they all coincide up to first order in \hbar . This is in accordance with the fact that corrections to the WKB energies are of order \hbar^2 [Vor77]. Our quantization rule (6.62) does include some corrections of order \hbar^2 , but not all of them. These corrections might improve the calculation of the energy levels with respect to WKB, especially for low-lying energy levels. Numerical work is currently being done to explore the possibilities. In this we still have one big freedom, the choice of b , the width of the coherent state, *for each energy level*. For the ground state, the variational principle tells us that \mathcal{H} is always larger than or equal to the true energy. Therefore we must choose b so as to minimize the energy. For the other states, however, no such direct rule exists and other prescriptions leading to an optimal b have to be devised.

For the harmonic oscillator, all three formulae give the exact result $E_m = (m + 1/2)\hbar\omega$ and the same Husimi distributions, independent of what b is chosen for the coherent state width. For the case of $b = \sqrt{\hbar/\omega}$ all three semiclassical formulae give

$$\rho_m(z) = \frac{1}{\sqrt{2\pi}|z|} \exp \left[-\frac{(|z|^2 - m - 1/2)^2}{2|z|^2} \right] \quad (6.70)$$

which is the result we obtained in section 6.2.

7. Conclusion

One inescapable conclusion is that there is more than one semiclassical approximation to quantum mechanics in phase space, even when one restricts oneself to the coherent state representation. It has often been said that all semiclassical approximations are identical in the end, that they always consist in expanding some exponent to second order in the vicinity of the classical trajectory and then doing a collection of Gaussian integrals, that all such expansions should be the same except for the choice of independent variables and therefore that the Gaussian integrals should always produce the same result. This argument is wrong, the basic reason being that the classical trajectory about which the expansion takes place differs from method to method, because the classical Hamiltonian differs from method to method. The confusion in the literature is in part due to this, but not entirely. People have ignored terms that looked small or unfamiliar, even when these were clearly part of the approximation they were using. They have done complex integrals as if these were real. They have ignored phases. They have been inconsistent with the Hamiltonian they used, often changing it in midstream.

Although the number of different, equally valid approximations is actually infinite, it is convenient to focus on only three of them, which have been discussed at some length in section 3. They correspond to three different choices for the classical Hamiltonian associated with a given quantal Hamiltonian. They are the Weyl Hamiltonian H_W , the smoothed Hamiltonian $H_1 \equiv \mathcal{H}$ and the antismoothed Hamiltonian H_2 . It is essential to realize that, in all semiclassical approximations, the smoothed Hamiltonian is always associated with an exponential term containing a special correction to the action which we have called \mathcal{I} . The temptation to omit this unfamiliar term is great, but it should be resisted, as without it one cannot get a correct quantization rule, for instance. Similarly, the antismoothed Hamiltonian

is always associated with $-\mathcal{I}$. The Weyl Hamiltonian does not come with such a correction term, which in a way makes it the simplest of the three. On the other hand, there is no simple approximation involving coherent states which yields the Weyl Hamiltonian. It occurs in some of the other methods, for instance the Wigner–Weyl method mentioned in section 1, and also the Heller method of section 4.3. The advantage of the smoothed Hamiltonian is that, since it is smoothed, approximations based on power series expansions are especially good for it. This is the Hamiltonian that we have used in most of our work. The antismoothed Hamiltonian, lacking both of the characteristics that make the other two desirable, does not seem to have been used in practice by anyone.

The first test cases for a semiclassical approximation should be the free particle and the harmonic oscillator. All three of the above approximations become exact then. Once again, this is so only when the \mathcal{I} term is appropriately included. Without \mathcal{I} , both H_1 and H_2 are wrong; only H_W remains. Beyond these two systems, the question of which of the three approximations gives better results has no single answer; it depends very much on the specific quantity calculated. We are planning to address this point in another paper. It is true that the three versions differ from each other only by terms of order \hbar , but a difference of this order can be essential in the quantization rule, and it may also be significant for the long-time behaviour.

We shall now summarize our other results. They can be grouped in three categories: coherent-state propagator, IVR and energy Green function. We gave in section 2 a very complete derivation of the semiclassical coherent-state propagator in one dimension, smoothed Hamiltonian version. This is equation (2.63) or (2.72). Then in section 3 we compared it with several other semiclassical approximations. In particular, we obtained an explicit expression for the antismoothed Hamiltonian version. We believe both of these results to be new.

In an attempt to provide a rigorous derivation of the well known HK formula, we derived in section 4 our own new IVR. Like HK, we set out to calculate semiclassically the mixed propagator $\langle x|K(t)|z'\rangle$ in terms of real trajectories starting from $q(0) = q'$, $p(0) = p'$. Our result, equation (4.29), is very different from HK's. Also in section 4, we considered Heller's old idea for an IVR, which is not based on the coherent state formalism, and we derived an explicit expression for it, valid for any smooth Hamiltonian function of q and p . We found that Heller's IVR and ours are very similar, the difference being that Heller's has the Weyl Hamiltonian and no \mathcal{I} term. We returned to the HK IVR in section 5 and pointed out mistakes made in its derivation. The nonconservation of the HK norm is a fatal flaw, we think. The HK expression does not follow from the semiclassical limit of the coherent-state propagator, but it can be derived from an ansatz where one assumes a fixed width for the propagated wavepacket and one demands that the resulting propagator recover that of Van Vleck when transformed to the representation $\langle x|K(t)|x'\rangle$. We show, however, that the applicability of such a formula is very limited and should fail for long times and/or for chaotic systems.

Finally, in section 6 we derived the corresponding semiclassical approximations for the energy Green function in the coherent-state representation. For each of the approximations, we used this Green function to find a quantization rule, which yields the energy levels in terms of classical quantities. We also used it to get a semiclassical approximation to the Husimi distribution for each level.

There are at least two ways that one might go farther in this field. One needs to carry out numerical comparisons between the various semiclassical approximations and determine the conditions under which one or the other might be preferable. We have made a small start in this direction, but we leave the results for a future publication. One needs also to extend this work to two dimensions, which will allow applications to more interesting problems, in particular problems with partially chaotic classical mechanics. There too we have made a significant start; it promises to be a rather complicated field and we shall say no more about it here.

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Appendix A. Calculating the prefactor by the determinantal method

In this appendix we present an alternative way of performing the multiple Gaussian integral which occurs in the calculation of the semiclassical propagator. In section 2.3, we started by doing the integrals one by one, and then we derived a recursion relation between successive integrals. Here we start with the determinant of the quadratic form, and we derive recursion relations between determinants of successively higher orders. This method is very general and can be applied for any number of dimensions. We use it here again for an integral in section 3.1 concerning the semiclassical approximation of a different kind of coherent-state propagator.

We start with equation (2.23), where we had to perform a $2(N-1)$ -dimensional Gaussian integral of the form

$$\int \exp \left\{ -\frac{x^T M x}{2} \right\} d^L x = \frac{(2\pi)^{L/2}}{\sqrt{\det M}} \quad (\text{A.1})$$

where M is a complex, positive definite $L \times L$ matrix. All the work comes in calculating the ‘prefactor’, or the square root of the determinant. We rewrite equation (2.23) as

$$K_1(z'', t; z', 0) = e^{f(z^*, z)} \int \left\{ \prod_{j=1}^{N-1} \frac{d\eta_j^* d\eta_j}{2\pi i} \right\} e^{\zeta}. \quad (\text{A.2})$$

The boundary conditions (2.19) ensure that j varies only from 1 to $N-1$. We have already written ζ in equation (3.12). Here we define the abbreviations

$$A_j = \frac{i}{\hbar} \frac{\partial^2 H_1(z_{j+1}^*, z_j)}{\partial z_j^2} \quad B_j = \frac{i}{\hbar} \frac{\partial^2 H_1(z_j^*, z_{j-1})}{\partial z_j^{*2}} \quad C_j = \frac{i}{\hbar} \frac{\partial^2 H_1(z_{j+1}^*, z_j)}{\partial z_{j+1}^* \partial z_j} \quad (\text{A.3})$$

and we write

$$-2\zeta = 2 \sum_{j=1}^{N-1} \eta_j \eta_j^* + \sum_{j=1}^{N-1} \tau A_j \eta_j^2 + 2 \sum_{j=1}^{N-2} (\tau C_j - 1) \eta_{j+1}^* \eta_j + \sum_{j=1}^{N-1} \tau B_j \eta_j^{*2}. \quad (\text{A.4})$$

The subscript 1 in equations (A.2) and (A.3) is the notation of section 3 and means that the first form of path integral is being used. We shall calculate $K_2(z'', t; z', 0)$ as well later in this appendix. We use η (without subscript!) to denote a double-sized vector containing all the η_j as well as their complex conjugates in the order $\eta_{N-1}, \eta_{N-1}^*, \eta_{N-2}, \eta_{N-2}^*, \dots, \eta_1, \eta_1^*$. Then equation (A.4) can be rewritten

$$\zeta = -\frac{\eta^T G^{(N-1)} \eta}{2} \quad (\text{A.5})$$

where

$$G^{(N-1)} := \begin{pmatrix} \tau A_{N-1} & 1 & 0 & 0 & 0 & 0 & \cdots \\ 1 & \tau B_{N-1} & \tau C_{N-2} - 1 & 0 & 0 & 0 & \cdots \\ 0 & \tau C_{N-2} - 1 & \tau A_{N-2} & 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & \tau B_{N-2} & \tau C_{N-3} - 1 & 0 & \cdots \\ 0 & 0 & 0 & \tau C_{N-3} - 1 & \tau A_{N-3} & 1 & \cdots \\ 0 & 0 & 0 & 0 & 1 & \tau B_{N-3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (\text{A.6})$$

is a tridiagonal band matrix whose dimensionality is twice the value of its superscript.

The integration formula (A.1) *cannot* be applied directly to (A.2), because in the latter the variables and the paths are complex. However, this is a problem that we have already considered and solved at the beginning of section 2.3. If we compare carefully equation (2.25) with (2.24), we find in the complex case that, for each pair of variables, we must introduce an additional minus sign in front of the determinant in the square root. It is also clear that the 2π will cancel out. Hence the correct formula is

$$K_1(z'', t; z', 0) = e^{f(z^*, z)} \frac{1}{\sqrt{(-1)^{N-1} \det G^{(N-1)}}}. \quad (\text{A.7})$$

Then the calculation of the determinant proceeds in the following way. First, the determinant is expanded with respect to its first column

$$\det G^{(N-1)} = \tau A_{N-1} \times \begin{vmatrix} \tau B_{N-1} & \tau C_{N-2} - 1 & 0 & 0 & 0 & \cdots \\ \tau C_{N-2} - 1 & \tau A_{N-2} & 1 & 0 & 0 & \cdots \\ 0 & 1 & \tau B_{N-2} & \tau C_{N-3} - 1 & 0 & \cdots \\ 0 & 0 & \tau C_{N-3} - 1 & \tau A_{N-3} & 1 & \cdots \\ 0 & 0 & 0 & 1 & \tau B_{N-3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix} - \begin{vmatrix} 1 & 0 & 0 & 0 & 0 & \cdots \\ \tau C_{N-2} - 1 & \tau A_{N-2} & 1 & 0 & 0 & \cdots \\ 0 & 1 & \tau B_{N-2} & \tau C_{N-3} - 1 & 0 & \cdots \\ 0 & 0 & \tau C_{N-3} - 1 & \tau A_{N-3} & 1 & \cdots \\ 0 & 0 & 0 & 1 & \tau B_{N-3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix}. \quad (\text{A.8})$$

The second determinant can easily be expanded with respect to its first line: it is simply $\det G^{(N-2)}$. The first determinant, on the other hand, is that of a different quadratic form which we call $F^{(N-1)}$. Thus we have the recursion relation

$$\det G^{(N-1)} = \tau A_{N-1} \det F^{(N-1)} - \det G^{(N-2)}. \quad (\text{A.9})$$

Now we can expand $\det F^{(N-1)}$ analogously, which leads to a second recursion relation

$$\begin{aligned} \det F^{(N-1)} &= \tau B_{N-1} \det G^{(N-2)} - (\tau C_{N-2} - 1)^2 \det F^{(N-2)} \\ &= \tau B_{N-1} \det G^{(N-2)} + 2\tau C_{N-2} \det F^{(N-2)} - \det F^{(N-2)} + O(\tau^2). \end{aligned} \quad (\text{A.10})$$

Since eventually we shall go to the limit $\tau \rightarrow 0$, $N \rightarrow \infty$, we may drop the terms of order τ^2 . We can get rid of many minus signs by making the definitions

$$g_{N-1} = (-)^{N-1} \det G^{(N-1)} \quad f_{N-1} = (-)^{N-1} \det F^{(N-1)}. \quad (\text{A.11})$$

Equations (A.9) and (A.10) can now be rewritten as

$$\begin{aligned} g_{N-1} &= g_{N-2} + \tau A_{N-1} f_{N-1} \\ f_{N-1} &= f_{N-2} - \tau B_{N-1} g_{N-2} - 2\tau C_{N-2} f_{N-2}. \end{aligned} \quad (\text{A.12})$$

In the continuous-time limit, these recursion relations turn into two first-order differential equations

$$\dot{g} = Af \quad \dot{f} = -Bg - 2Cf. \quad (\text{A.13})$$

By letting τ go to 0 in the determinants themselves, one sees easily that the initial conditions are

$$g(0) = 1 \quad f(0) = 0. \quad (\text{A.14})$$

One way to solve the differential equations is to introduce the functions

$$\tilde{g} = g \exp \left[\int_0^t C(t') dt' \right] \quad \tilde{f} = f \exp \left[\int_0^t C(t') dt' \right]. \quad (\text{A.15})$$

Equations (A.13) become now

$$\dot{\tilde{g}} = A\tilde{f} + C\tilde{g} \quad \dot{\tilde{f}} = -B\tilde{g} - C\tilde{f} \quad (\text{A.16})$$

with initial conditions $\tilde{g} = 1$ and $\tilde{f} = 0$. Replacing the abbreviations A, B, C by their definitions in equation (A.3), we see that (A.16) is formally identical to the differential equations (2.49) if we let \tilde{g} be δv and \tilde{f} be δu . The initial values are $\delta u(0) \equiv \delta u' = 0$ and $\delta v(0) \equiv \delta v' = 1$.

We need to know $g(t)$, which is the quantity under the square root in (A.7); we do not need $f(t)$. Since $\tilde{g}(t) = \delta v''$, we can use equation (2.62) with $\delta v' = 1$ to write

$$g(t) = \delta v'' \exp \left(- \int_0^t C(t') dt' \right) = \left(\frac{i}{\hbar} \frac{\partial^2 S}{\partial u' \partial v''} \right)^{-1} \exp \left(- \int_0^t C(t') dt' \right). \quad (\text{A.17})$$

Substituting back into equation (A.7) and replacing C by its definition gives

$$K_1(z'', t; z', 0) = e^{f(z^*, z)} \sqrt{\frac{i}{\hbar} \frac{\partial^2 S}{\partial u' \partial v''}} \exp \left\{ \frac{i}{2\hbar} \int_0^t dt' \frac{\partial^2 H_1}{\partial u \partial v} \right\}. \quad (\text{A.18})$$

Finally, by calculating $\exp\{f(z^*, z)\}$ in the same way as in section 2 (see equation (2.43) and section 2.5), we obtain a result identical to equation (2.63):

$$\begin{aligned} K_1(z'', t; z', 0) &= \sqrt{\frac{i}{\hbar} \frac{\partial^2 S}{\partial u' \partial v''}} \exp \left\{ \frac{i}{2\hbar} \int_0^t dt' \frac{\partial^2 H_1}{\partial u \partial v} \right\} \\ &\times \exp \left\{ \frac{i}{\hbar} S(v'', u', t) - \frac{1}{2} (|v''|^2 + |u'|^2) \right\}. \end{aligned} \quad (\text{A.19})$$

Let us now repeat this calculation for Klauder and Skagerstam's 'second form of the path integral' discussed in section 3.1. We follow very closely what we just did for K_1 , with small but important differences. According to equation (3.11), the quadratic form for K_2 is

$$-2\zeta = 2 \sum_{j=1}^{N-1} \eta_j^* \eta_j - 2 \sum_{j=1}^{N-2} \eta_{j+1}^* \eta_j + \sum_{j=1}^{N-1} \tau A_j \eta_j^2 + \sum_{j=1}^{N-1} \tau B_j \eta_j^{*2} + 2 \sum_{j=1}^{N-1} \tau C_j \eta_j^* \eta_j \quad (\text{A.20})$$

with the (different) definitions

$$A_j = \frac{i}{\hbar} \frac{\partial^2 H_2(z_j^*, z_j)}{\partial z_j^2} \quad B_j = \frac{i}{\hbar} \frac{\partial^2 H_2(z_j^*, z_j)}{\partial z_j^{*2}} \quad C_j = \frac{i}{\hbar} \frac{\partial^2 H_2(z_j^*, z_j)}{\partial z_j^* \partial z_j}. \quad (\text{A.21})$$

The matrix G^{N-1} becomes

$$G^{(N-1)} := \begin{pmatrix} \tau A_{N-1} & 1 + \tau C_{N-1} & 0 & 0 & 0 & 0 & \cdots \\ 1 + \tau C_{N-1} & \tau B_{N-1} & -1 & 0 & 0 & 0 & \cdots \\ 0 & -1 & \tau A_{N-2} & 1 + \tau C_{N-2} & 0 & 0 & \cdots \\ 0 & 0 & 1 + \tau C_{N-2} & \tau B_{N-2} & -1 & 0 & \cdots \\ 0 & 0 & 0 & -1 & \tau A_{N-3} & 1 + \tau C_{N-3} & \cdots \\ 0 & 0 & 0 & 0 & 1 + \tau C_{N-3} & \tau B_{N-3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (\text{A.22})$$

Calling the matrix obtained by removing the first column and the first row of G^{N-1} F^{N-1} , and expanding both G^{N-1} and F^{N-1} with respect to their first lines, we get

$$\begin{aligned} \det G^{(N-1)} &= \tau A_{N-1} \det F^{(N-1)} - (1 + \tau C_{N-1})^2 \det G^{(N-2)} \\ \det F^{(N-1)} &= \tau B_{N-1} \det G^{(N-2)} - \det F^{(N-2)}. \end{aligned} \quad (\text{A.23})$$

Once again we get rid of signs with the help of definitions (A.11) and we take the limit $\tau \rightarrow 0$, $N \rightarrow \infty$ to get

$$\dot{g} = Af + 2Cg \quad \dot{f} = -Bg. \quad (\text{A.24})$$

Finally we define

$$\tilde{g} = g \exp \left[- \int_0^t C(t') dt' \right] \quad \tilde{f} = f \exp \left[- \int_0^t C(t') dt' \right]. \quad (\text{A.25})$$

Note that, compared with the analogous definitions (A.15), the present ones have a minus sign! We obtain again

$$\dot{\tilde{g}} = A\tilde{f} + C\tilde{g} \quad \dot{\tilde{f}} = -B\tilde{g} - C\tilde{f} \quad (\text{A.26})$$

which are the same equations as (A.16). Therefore the propagator K_2 is given again by (A.18) except that, this time, there is a minus sign in front of the \mathcal{I} term!

Appendix B. Proof of equation (3.27)

We start by rewriting equation (3.24) as

$$A = \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar} \phi(x)} dx \quad (\text{B.1})$$

where $\phi(x) := f(x) - i\hbar \log g(x)$. To calculate A beyond the SPA we expand ϕ about its stationary point X to fourth order:

$$\phi(x) = \phi(X) + \frac{1}{2!} \phi^{(2)} \delta x^2 + \frac{1}{3!} \phi^{(3)} \delta x^3 + \frac{1}{4!} \phi^{(4)} \delta x^4 + \cdots \quad (\text{B.2})$$

where $\delta x = x - X$ and $\phi^{(n)} = d^n \phi / dx^n (X)$. Next we change the integration variable to

$$y = \sqrt{\frac{|\phi^{(2)}|}{2\hbar}} e^{i\alpha/2 - i\pi/4} \delta x \quad (\text{B.3})$$

where α is the phase of $\phi^{(2)}$. Substituting (B.2) and (B.3) into (B.1) we get

$$\begin{aligned} A &\approx \sqrt{\frac{2\hbar}{|\phi^{(2)}|}} e^{i\pi/4 - i\alpha/2} e^{\frac{i}{\hbar} \phi(X)} \\ &\times \int_{-\infty}^{+\infty} \exp \left[-y^2 + i \frac{\phi^{(3)}}{6\hbar} \left(\frac{2\hbar}{|\phi^{(2)}|} \right)^{3/2} e^{3i\pi/4 - 3i\alpha/2} y^3 + \frac{i\hbar \phi^{(4)}}{6|\phi^{(2)}|^2} e^{i\pi - 2i\alpha} y^4 \right] dy \end{aligned}$$

$$\begin{aligned}
&\approx \sqrt{\frac{2\hbar}{|\phi^{(2)}|}} e^{i\pi/4 - i\alpha/2} e^{\frac{i}{\hbar}\phi(X)} \\
&\quad \times \int_{-\infty}^{+\infty} e^{-y^2} \left[1 + \frac{i\hbar\phi^{(4)}}{6|\phi^{(2)}|^2} e^{i\pi - 2i\alpha} y^4 - \frac{\hbar(\phi^{(3)})^2}{9|\phi^{(2)}|^3} e^{3i\pi/2 - 3i\alpha} y^6 \right] dy \\
&= \sqrt{\frac{2\pi\hbar}{|\phi^{(2)}|}} e^{i\pi/4 - i\alpha/2} e^{\frac{i}{\hbar}\phi(X)} \left[1 - \frac{i\hbar\phi^{(4)}}{8|\phi^{(2)}|^2} e^{-2i\alpha} + \frac{5i\hbar(\phi^{(3)})^2}{24|\phi^{(2)}|^3} e^{-3i\alpha} \right] \\
&\approx \sqrt{\frac{2\pi\hbar}{|\phi^{(2)}|}} e^{i\pi/4 - i\alpha/2} \\
&\quad \times \exp \left\{ \frac{i}{\hbar} \left[\phi(X) + \frac{\hbar^2}{24|\phi^{(2)}|^3} (5e^{-3i\alpha}(\phi^{(3)})^2 - 3e^{-2i\alpha}|\phi^{(2)}|\phi^{(4)}) \right] \right\}. \quad (\text{B.4})
\end{aligned}$$

We now proceed to expand the various terms above in powers of \hbar so as to compare this result with SPA. The stationary point X of ϕ can be written in terms of the stationary point x_0 of f as

$$X = x_0 + i\hbar \frac{g^{(1)}}{f^{(2)}g^{(0)}} + \mathcal{O}(\hbar^2) =: x_0 + i\hbar x_1 + \mathcal{O}(\hbar^2). \quad (\text{B.5})$$

Also

$$\phi(X) = f(x_0) - i\hbar \log g(x_0) + \hbar^2 \left[\frac{x_1 g^{(1)}}{g^{(0)}} - \frac{f^{(2)} x_1^2}{2} \right] + \mathcal{O}(\hbar^3) \quad (\text{B.6})$$

$$\phi^{(2)} = f^{(2)} + i\hbar f^{(3)} x_1 - i\hbar \frac{g^{(2)}g^{(0)} - g^{(1)2}}{g^{(0)2}} + \mathcal{O}(\hbar^2) \quad (\text{B.7})$$

where $g^{(n)} = d^n g/dx^n(x_0)$ and $f^{(n)} = d^n f/dx^n(x_0)$. From the last expression we find

$$|\phi^{(2)}|^{-1/2} = |f^{(2)}|^{-1/2} (1 + \mathcal{O}(\hbar^2)) \quad (\text{B.8})$$

and

$$\alpha = \frac{\pi}{2}(s-1) + \frac{\hbar f^{(3)} x_1}{f^{(2)}} - \hbar \frac{g^{(2)}g^{(0)} - g^{(1)2}}{g^{(0)2} f^{(2)}} + \mathcal{O}(\hbar^2). \quad (\text{B.9})$$

Substituting these equations into (B.4) we obtain, after some simplifications, the desired result, equation (3.27), with

$$R(x_0) = \frac{f^{(2)}g^{(2)} - f^{(3)}g^{(1)}}{2f^{(2)2}g^{(0)}} + \frac{5(f^{(3)})^2 - 3f^{(2)}f^{(4)}}{24(f^{(2)})^3}. \quad (\text{B.10})$$

Appendix C. Cancellation of first-order terms in $S + \mathcal{I}$

Our goal here is to show that the quantity $(S + \mathcal{I})$ appearing in the phase of the propagator, equation (2.72), can be written as $S_W + \mathcal{O}(\hbar^2)$, where S_W is the action computed with the classical Hamiltonian H_C , which we assume to be the same as the Weyl symbol H_W . In order to do that we must relate \mathcal{H} to H_W and write the classical trajectories governed by \mathcal{H} in terms of those governed by H_W .

The relation between H_W and $\mathcal{H} \equiv H_1$ is given by the second of equations (3.23). Expanding the exponential operator we obtain

$$H_W(u, v) = \mathcal{H}(u, v) - \frac{1}{2} \frac{\partial^2 \mathcal{H}}{\partial u \partial v}(u, v) + \dots \quad (\text{C.1})$$

The second term on the right is what we have called $\epsilon(u, v)$ in section 6 (see equation (6.30)). We assume that H_W does not depend explicitly on \hbar , and that \mathcal{H} may be written as a power series in \hbar , starting at \hbar^0 . The same holds for $\epsilon(u, v)$, with the series starting at \hbar^1 . Since the next term in the expansion (C.1) is of order \hbar^2 , equation (C.1) can be rewritten as

$$H_W(u, v) = \mathcal{H}(u, v) - \epsilon(u, v) + \mathcal{O}(\hbar^2). \quad (\text{C.2})$$

The inverse equation, where \mathcal{H} is written in terms of H_W , is

$$\mathcal{H}(u, v) = H_W(u, v) + \epsilon_W(u, v) + \mathcal{O}(\hbar^2) \quad (\text{C.3})$$

where $\epsilon_W(u, v)$ is defined by equation (6.30) with H_W replacing \mathcal{H} .

Let $u = u(v'', u', t')$ and $v = v(v'', u', t')$ be the solutions of Hamilton's equations (2.36) with boundary conditions $u(v'', u', 0) = u'$, $v(v'', u', t) = v''$. Let also $u_0 = u_0(v'', u', t')$ and $v_0 = v_0(v'', u', t')$ be the solutions of the same Hamilton equations but with \mathcal{H} replaced by the classical Hamiltonian H_W and the same boundary conditions, $u_0(v'', u', 0) = u'$, $v_0(v'', u', t) = v''$. Since the difference between the functions \mathcal{H} and H_W is of order \hbar we write

$$\begin{aligned} u(v'', u', t') &= u_0(v'', u', t') + \hbar u_1(v'', u', t') + \mathcal{O}(\hbar^2) \\ v(v'', u', t') &= v_0(v'', u', t') + \hbar v_1(v'', u', t') + \mathcal{O}(\hbar^2). \end{aligned} \quad (\text{C.4})$$

Notice that t is the total propagation time, whereas t' is used for intermediate instants, $0 < t' < t$. Due to the boundary conditions we have

$$\begin{aligned} u_1(v'', u', 0) &= 0 \\ v_1(v'', u', t) &= 0. \end{aligned} \quad (\text{C.5})$$

For the sake of clarity we rewrite formula (2.54) for the action:

$$S(v'', u', t) := \int_0^t dt' \left[\frac{i\hbar}{2} (\dot{u}v - \dot{v}u) - \mathcal{H}(u, v, t') \right] - \frac{i\hbar}{2} (u''v'' + u'v'). \quad (\text{C.6})$$

We shall now expand the various terms in $S(v'', u', t)$ in powers of \hbar . We start with $\mathcal{H}(u, v)$ calculated along its own trajectory:

$$\begin{aligned} \mathcal{H}(u, v) &= H_W(u_0 + \hbar u_1, v_0 + \hbar v_1) + \epsilon_W(u_0, v_0) + \mathcal{O}(\hbar^2) \\ &= H_W(u_0, v_0) + \frac{\partial H_W}{\partial u}(u_0, v_0)\hbar u_1 + \frac{\partial H_W}{\partial v}(u_0, v_0)\hbar v_1 + \epsilon(u_0, v_0) + \mathcal{O}(\hbar^2) \\ &= H_W(u_0, v_0) - i\hbar^2 \dot{v}_0 u_1 + i\hbar^2 \dot{u}_0 v_1 + \epsilon(u_0, v_0) + \mathcal{O}(\hbar^2) \end{aligned} \quad (\text{C.7})$$

where the dot means d/dt' . Using equations (C.4) we also find

$$\begin{aligned} \frac{i\hbar}{2} (\dot{u}v - \dot{v}u) &= \frac{i\hbar}{2} (\dot{u}_0 v_0 - \dot{v}_0 u_0) + \frac{i\hbar^2}{2} (\dot{u}_1 v_0 + \dot{u}_0 v_1 - \dot{v}_0 u_1 - \dot{v}_1 u_0) + \mathcal{O}(\hbar^2) \\ &= \frac{i\hbar}{2} (\dot{u}_0 v_0 - \dot{v}_0 u_0) - i\hbar^2 (\dot{v}_0 u_1 - \dot{u}_0 v_1) + \frac{i\hbar^2}{2} \frac{d}{dt'} (v_0 u_1 - v_1 u_0) + \mathcal{O}(\hbar^2). \end{aligned} \quad (\text{C.8})$$

Finally, using equations (C.5), we have

$$\begin{aligned} \frac{i\hbar}{2} (u''v'' + u'v') &= \frac{i\hbar}{2} (u''_0 + \hbar u''_1)v'' + \frac{i\hbar}{2} u'(v'_0 + \hbar v'_1) + \mathcal{O}(\hbar^2) \\ &= \frac{i\hbar}{2} (u''_0 v'' + u'v'_0) + \frac{i\hbar^2}{2} (u''_1 v'' + u'v'_1) + \mathcal{O}(\hbar^2). \end{aligned} \quad (\text{C.9})$$

Substituting equations (C.7)–(C.9) in (C.6) we see that the second and third terms in equation (C.7) cancel the terms in the second parenthesis of (C.8). We get

$$\begin{aligned} S(v'', u', t) &= S_W(v'', u', t) + \int_0^t dt' \left[\frac{i\hbar^2}{2} \frac{d}{dt'} (v_0 u_1 - v_1 u_0) - \epsilon(u, v) \right] \\ &\quad - \frac{i\hbar^2}{2} (u''_1 v'' + u'v'_1) + \mathcal{O}(\hbar^2). \end{aligned} \quad (\text{C.10})$$

Using equation (C.5) once again, we cancel the first two terms on the second line against those under the total derivative sign. Recalling the definition (2.65) of \mathcal{I} , we finally get

$$S(v'', u', t) + \mathcal{I}(v'', u', t) = S_W(v'', u', t) + \mathcal{O}(\hbar^2). \quad (\text{C.11})$$

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