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Accuracy of the semiclassical approximation for the time-dependent propagator

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Abstract. For chaotic systems the semiclassical approximation to the time-dependent propagator consists of a large number of terms, some of which may involve classical trajectories near focal points (caustics). Despite this the approximation has been found to remain accurate for relatively long times. In this article, that accuracy and potential reasons for its breakdown are studied. The principal tool is the Jacobi–Morse equation, the eigenvalue equation associated with the second variational derivative of the classical action. Our explanation for the accuracy lies partly in the following considerations: (1) verification of the efficacy of phase space smearing, (2) given an explicit form of the near caustic propagator, it is seen that the arguments concerning loops in phase space may be less relevant than the determination of the amount of separation in *path*-space, (3) and finally, the caustics in the chaotic examples studied may not be placed for maximum mischief.

1. Introduction

A recent article [1] dealt with 'unexpected long time accuracy' for the semiclassical time-dependent propagator for a system whose classical mechanics exhibits hard chaos. Unexpected behaviour of this sort has characterized much work on the quantization of chaotic systems. An early and germane example is the success [2] of the sum over classical paths expansion, in energy-dependent form, at providing energy levels for classically chaotic systems. For further background, see [3].

In this article we bring to bear a number of analytic methods in an effort to understand the aforementioned long-time accuracy results of Heller and Tomsovic [1, 4]. The principal reasons one might find the accuracy surprising is the existence of an enormous number of classical paths satisfying the two-time boundary conditions and the presumed influence of caustics, which generally invalidate elementary semiclassical approximations. There are other ways of phrasing this, such as the formation of folds and small (on $\hbar$-related scales) loops in the Lagrange manifolds [5], and we will discuss aspects of this description as well.

A second goal of this article is to further develop analytic techniques based on what we here name the *Jacobi–Morse equation*. This method was used in the analysis of caustics many years ago [6] and elaborated in [7]. It can sometimes provide information not otherwise available, although in other cases it may require lengthy analysis to recover simple results. In at least one example below we will do an exercise of the latter sort; nevertheless, that same exercise provides information leading to conclusions that have not otherwise been obtained. By the Jacobi–Morse equation I mean the Schrödinger-like equation that arises from the second variation of the classical action [8]. Because this article is already rather long I will not provide background or review the interrelations of this operator-second-variation with the van Vleck determinant, the equation of geodesic deviation, etc. This can be found in [7].

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Our calculations show how the results of [1] can have come about. If there is a general principle operating it is that there is more room in path space than phase space, so that semiclassical stationary phase contributions from the path integral can be separated even though when represented in phase space they appear to be close. Another principle that plays a role—in a sense an extension of the correspondence principle—is an interplay of classical chaos and a kind of quantum ergodicity. 'Ergodicity' suggests that one should reach all accessible points of phase space with equal likelihood. In terms of the semiclassical propagator this demands destructive interference of many terms. We shall see (at least in coordinate space) that this cancellation takes place precisely because of the classical chaos. In the process of accounting for the results of [1] we also find that the stadium may not be the best laboratory for discovering whether this long-time accuracy will hold for more realistic chaotic systems. The caustics, which are the source of most of the potential mischief and which necessarily exist by virtue of path proliferation, may not be as dangerous for this system as for others. This is because we find that many of them are at the walls of the stadium. How common focussing is within the stadium we do not know.

This article is divided in two parts, classical mechanics and quantum mechanics. In section 2 we concentrate on classical arguments concerning the multiplicity of paths, their proliferation and the role of caustics. We define the Jacobi–Morse equation and use it first to establish the existence of a caustic at each reflection off a wall. By variations of this technique we establish the temporal duration for the passage of a trajectory through a caustic, even in the presence of chaos. We also discuss the fragmentation of caustics due to the curved-flat transition along the wall. In section 3 we work from the semiclassical approximation but use a form that is applicable *in the immediate neighbourhood* of the caustic. In this way we derive the explicit form of the phase space propagator and confirm the conclusions in [9]: on the effectiveness of phase space averaging for ameliorating the effects of the caustic. We also examine the problem of nearby stationary points (classical paths) and small loops in phase space. This is where the 'general principle' mentioned above may operate. As the last step in treating [1], we consider the random walk arguments involved in the chaos induced destructive interference necessary to recover the ergodic form of the propagator. In a small digression we also consider results that this formalism can provide for the theory of random potentials. Finally, in section 4, we discuss our conclusions and questions that they raise.

2. Classical mechanics

In this section we work within a classical context. We make extensive use of the *Jacobi–Morse equation*, namely the study of the spectrum and eigenfunctions of the operator corresponding to the second variational derivative of the classical action. Leading up to this, we first discuss the proliferation of paths and distinguish two ways in which such proliferation can occur. Then we relate the rate of proliferation to the Lyapunov exponents. To study caustics we use the Jacobi–Morse equation and establish the existence of a caustic with each passage of the classical path through a reflection. Such caustics are well known, but they tend to be overlooked when one considers the difficulties caustics can cause for the semiclassical approximation in quantum mechanics. I also remark that rather little seems to be known about the location of the *fixed time* caustics in the stadium, in contrast to the more easily computed fixed energy caustics. Finally we take up the question of how rapidly trajectories pass through caustics, both for the ordinary caustics not involved in reflections of the hard wall and for those involved in such reflection. One might have thought that there would be rapid passage of the path through the caustic for chaotic dynamics, but from study of the Jacobi–Morse equation this is found not to be the case.

Throughout, we are concerned with the *fixed time* classical boundary-value problem. That is, let the classical coordinate space be X (a manifold). Two endpoints, x_0 and x_T, and a fixed time T are given. We seek paths $x(t)$ that satisfy the equations of motion such that $x(0) = x_0$ and $x(T) = x_T$.

2.1. Proliferation of paths

By compactifying a space of constant negative curvature one can arrive at multiple solutions of the two-time boundary-value problem. The Jacobi field can never vanish on such a space [10] and there are no caustics. This is a clean way to generate multiple solutions to the two-time boundary-value problem and is used in some studies of quantum chaos (e.g., [2]). It is not the context for studying problems due to caustics. The solutions of the two-time boundary-value problem are intimately related to the non-trivial topology of the space.

For spaces for which the topology is trivial the proliferation of paths occurs in conjunction with caustics. To see how this proliferation occurs, first consider the situation where the endpoint x_T is a focal point for the initial condition x_0 (for the particular, fixed T). For that same T the boundary-value problem for points $x_T + \Delta x$ has zero, one or two solutions. Those Δx for which there is but one solution form a surface (generically a hypersurface of co-dimension 1) on one side of which there are two solutions to the boundary-value problem, on the other zero. In terms of the trajectory $x(t)$ (which is the one that focusses at T), the region of zero solutions lies on the side where $x(t)$ was located for $t < T$ and the two-solution region lies where $x(t)$ is located for later times†. One can also consider the sequence of boundary-value problems for solutions $\xi(s)$, with $\xi(0) = x(0)$, $\xi(t) = x(t)$ (with $x(t)$ the particular path we have been considering). As $x(t)$ passes through conjugate points, $\delta^2 S$ acquires additional negative eigenvalues, as is known from Morse theory. In going through each of these one goes from having a certain variation in path space (that in the direction of the Jacobi field) correspond to a minimum to having it be a local maximum. In terms of the expansions of (13) and (14) below, one goes from having a term λu^2 (with λ large and positive) dominate to having a polynomial $\lambda u^2 + pu^3$ which will have an additional classical path associated with its stationary point when λ is near zero. This is the proliferation mechanism associated with caustics.

Although both kinds of path proliferation can occur in the same system, for the stadium there is only caustic driven proliferation. Therefore caustics must appear along the many solutions of the boundary-value problem and from the success of the numerical semiclassical work [1, 4] one might conclude that the caustic problem had been neutralized. As we show below, many caustics are at the *edges* of the stadium so that the necessity of caustics as deduced from path proliferation does not by itself indicate that their effect on the semiclassical approximation has been eliminated.

Finally we remark that focussing by itself does not lead to the exponential (with time) proliferation of paths. An example of caustics without path proliferation is given in the appendix.

2.2. Path multiplicity for chaotic dynamics

Using general arguments we now show that the multiplicity of paths satisfying given boundary conditions grows like $\exp(\Lambda t)$, where Λ is the largest Lyapunov exponent.

† Not to be confused: on the zero solution side $x(t)$ is a classical solution solving a different boundary-value problem. It only runs for a time $T - \Delta T$ (with ΔT positive) and reaches, not $x(T)$, but $x(T - \Delta T)$.

Assume a system in d-dimensions is confined to a spatial region of size $V \equiv L^d$. We look at classical paths that begin in a small volume v_i, with $|v_i| = \ell^d = v$. We wish to know how many families of trajectories begin in v_i at time 0 and end in some (possibly other) volume v_f of the same size, a time T later. An upper limit of energy is also assumed.

Under classical dynamics the initial region v_i stretches and shrinks along various directions, these rates (described by Lyapunov exponents) being governed by the multidimensional Jacobi equation. When one dimension of the volume v_i stretches beyond the length L there must be folding, and for large ΛT there is folding and refolding. The number of families of trajectories satisfying the two-time boundary condition will be the number of stretched tendrils that pass through the final volume v_f. This can be estimated if one assumes that the stretched v_i is randomly distributed throughout V. The longest dimension of the stretched v_i is $\ell_f = \ell \times \exp(\Lambda T)$. For a random distribution this can be thought of as ℓ_f/L sticks of length L that have been tossed into V. The number of such sticks that intersect v_f is estimated as follows: the probability that a (thin) stick hits a volume ℓ^d is the probability that a stick thickened† by ℓ^{d-1} intersects any particular point in V. But this is the ratio of the volume of the thickened stick to the entire volume, V. This ratio is $L \times \ell^{d-1}/V$. Multiplying this by the number of sticks gives the total (probable) number of intersections, which is therefore

$$\left[\frac{\ell e^{\Lambda T}}{L}\right] \cdot \left[\frac{L\ell^{d-1}}{L^d}\right] = \frac{v}{V} \exp(\Lambda T) . \qquad (1)$$

If the initial and final volumes are different a slightly more complicated answer emerges.

In this argument we have implicitly assumed that only one Lyapunov exponent is large, where 'large' means that for a given Lyapunov exponent Λ_k the quantity $\exp(\Lambda_k T)$ is large compared to L/ℓ. In the case of more than one large Lyapunov exponent, you will get—instead of the elongated stick discussed above—a sheet or hypersurface of dimension equal to the number of large exponents. This reduces the number of dimensions by which this hypersurface is thickened (in analogy to the thickened stick argument above) so the factor v/V still results. What is different is that now the number of families of paths is given by that factor times $\exp(T \sum \Lambda_k)$, where the sum runs over 'large' Λ_ks.

2.3. *Caustics at a wall*

In this subsection we will show that whenever a trajectory bounces off a wall there is a point along it, near the wall, that is conjugate to the initial point on the trajectory; in other words there is a caustic.

There are two kinds of wall: hard and soft, namely infinite or finite slope at the turning point. In WKB these do not go over to one another smoothly (as the slope goes to infinity) although the classical mechanics is the same. The boundary conditions used in the numerical studies of [1] appear to be hard wall, but for the analysis of where the classical caustics lie this does not matter. To show that in bouncing off a wall a trajectory acquires a conjugate point, we will establish that one of the eigenvalues of $\delta^2 S$, the second variation of the classical action, goes through zero. Motion parallel to the wall does not play a role and we confine attention to one dimension.

† That is, thickened by ℓ in each transverse direction. Note that the argument does not require (or prohibit) shrinking of other dimensions of v_i, only that they not grow.

Consider therefore the Hamiltonian $H = p^2/2m + V(x)$, with $V(x)$ small for $x > 0$ and large for $x < 0$. Examples (in which Ω is a large parameter) are

$$V(x) = \begin{cases} \theta(-x)\Omega & \text{hard wall} \\ \theta(-x)\Omega|x| & \text{linear wall} \\ \theta(-x)\frac{1}{2}m\Omega^2x^2 & \text{harmonic wall} \\ \exp(-\Omega x) & \text{exponential wall.} \end{cases} \tag{2}$$

We begin with the harmonic case. Without loss of generality, set $m = 1$ and the time interval to be $[-T/2, T/2]$. Also, our point is not affected by simplifying to the case of equal initial and final position values. The particle therefore has boundary conditions $x(-T/2) = x(T/2) = a$. This classical two-time boundary condition has the solution

$$x(t) = \begin{cases} v(t - \frac{1}{2}\tau) & \frac{1}{2}\tau < t < \frac{1}{2}T \\ (v/\Omega)\sin(\Omega(t - \frac{1}{2}\tau)) & 0 < t < \frac{1}{2}\tau \\ x(-t) & t < 0 \end{cases} \tag{3}$$

where $\tau \equiv \pi/\Omega$ and $v = 2a/(T - \tau)$. As usual [7], we solve

$$\ddot{\phi}(t) + V''[x(t)]\phi(t) + \lambda\phi(t) = 0 \tag{4}$$

where ϕ satisfies the boundary conditions $\phi(-T/2) = \phi(T/2) = 0$. Those λs for which this boundary-value problem can be solved are the points of the spectrum of $\delta^2 S$. The vanishing of such a λ signifies a conjugate point of the motion (with respect to the initial condition $x(-T/2) = a$) and a solution of the Jacobi equation. Equation (4) is of the Sturm–Liouville type and I call it and its higher dimensional generalization the *Jacobi–Morse equation.* Despite its resemblance to the Schrödinger equation, its appearance here is entirely in the service of the classical mechanics. Equation (4) can be rewritten in the suggestive form

$$-\ddot{\phi} + U(t)\phi = \lambda\phi \tag{5}$$

and for the harmonic oscillator soft wall $U(t)$ is a step function

$$U(t) \equiv -\Omega^2\theta(\tfrac{1}{2}\tau - |t|) \equiv -\frac{\mu}{\tau}\theta(\tfrac{1}{2}\tau - |t|) \tag{6}$$

with $\mu \equiv \pi^2/\tau$. We are interested in $\Omega \to \infty$ or $\tau \to 0$, so that (5) and (6) give a delta function, well known to possess a single bound state, at least if the boundary conditions are ignored. Note though that the *strength* of the delta function is also going to infinity, so that additional bound states could in principle appear. In fact it will be seen that in this problem the strength will be so large that there is *almost* a second bound state. For even eigenfunctions and ignoring the $t = \pm T/2$ boundary conditions, the equation for the eigenvalue is $\tan\theta = \sqrt{\pi^2/4\theta^2 - 1}$ with $\theta = k\tau/2$ and $k = \sqrt{\lambda + \Omega^2}$. This has exactly one solution and there is therefore always one even eigenfunction with $\lambda < 0$. One finds that $\lambda \approx -0.6464 \times \Omega^2$, so that $\lambda \to -\infty$ as $\Omega \to \infty$. Since $|\lambda|$ is large, ignoring the $\pm T/2$ boundary condition is permissible. The lowest odd eigenfunction is more subtle. Ignoring the $\pm T/2$ boundary condition yields an eigenvalue zero, so merely arguing from the constricting effect of the boundary condition already implies that the value is pushed higher and no further negative eigenvalues exist. It turns out that the positive value of this eigenvalue goes like Ω (rather than Ω^2). What is interesting is that if there were not perfect matching between the strength of the potential and its width, the scaling of U of (5) could have led to additional negative λ states. This will be explained below.

We confirm from this that a trajectory that has bounced off a soft wall develops a single conjugate point. However, the passage of the eigenvalue (of δS^2) through zero occurs close to the wall. In fact, very close, since by the time the trajectory moves away from the wall that eigenvalue has sunk to negative values proportional to Ω^2. (Strictly, our $x(\pm T/2) = a$ boundary condition does not say where the conjugacy occurs; nevertheless a straightforward calculation establishes the foregoing assertions.)

For the other kinds of soft walls there is always one eigenvalue that is well into the negative regime and another that is just pushed positive by boundary conditions at $t = \pm T/2$. For example, the exponential wall $V(x) = \exp(-\Omega x)$ (with $m = 1$) gives $x(t) = x_0 + (2/\Omega)\log\cosh(\Omega kt/2)$ with k, x_0, a and T related by $k^2 = 2\exp(-\Omega x_0)$ and $k\exp(\Omega a/2) = \sqrt{2}\cosh(\Omega kT/2)$. The eigenvalue equation for $\delta^2 S$ turns out to involve a 'potential' of the form

$$U(t) \equiv \frac{-2\omega^2}{\cosh^2 \omega t} \qquad \text{with} \quad \omega = a\Omega/T\,. \tag{7}$$

This is a well known potential [11], having special properties for the strength $-2\omega^2$. Like the U of (6), this potential has one bound state whose value goes infinitely negative ($\propto \Omega^2$). And like the other potential, were it not for the $t = \pm T/2$ boundary condition it would have a point in the spectrum exactly at zero.

The solution for each of our stiff (i.e. $\Omega \to \infty$) 'soft' walls displays two features. (i) The potential—which tends to a delta function—has a coefficient that tends to infinity, allowing in principle more than one bound state for that potential. The binding energy of the ground state goes to infinity. (ii) Nevertheless, in all cases the second (potential) bound state just barely does *not* occur. Here is the explanation: pick a fixed solution of the classical equations of motion, $x(\cdot)$. Consider a sequence of boundary-value problems defined by $x(0)$ and $x(T)$, and consider the value of $\lambda(T)$ for each T. (This is a different perspective from that which we have been using. Now both the final point $x(T)$ and T vary.) Until $x(T)$ bounces off the wall, there is no negative eigenvalue for $\delta^2 S$. Just after the bounce, $\delta^2 S$ should have its first negative eigenvalue since for two close paths the one that was behind would now be ahead (this is essential to the focussing). But for $x(T)$ slightly past the reflection, the boundary condition for the function $\phi(T)$ is precisely that it vanish a little more than halfway through the full potential $U(t)$, that is, the potential equation (7) associated with T of our previous perspective, namely T such that $x(T) = x(0)$. Having a negative eigenvalue at the halfway point would be the same as having an odd bound eigenfunction of the full $U(t)$. Thus $U(t)$ must be such that its first odd eigenfunction have its eigenvalue just above zero.

2.4. Temporal duration of the passage through a caustic

In a chaotic system it will not be easy to focus at distant future times. There is at least one initial direction along which points quickly separate, so that focussing can only be achieved by assiduously avoiding the bad direction or directions. Does this mean that there is something strange about the conjugacy, when it does occur? For example, one might speculate that passage through the focal point is more rapid than for non-chaotic systems, making a randomly selected path-point on a trajectory unlikely to be near a focal point. As far as I can tell, the focal points are not different from their non-chaotic counterparts, at least with regard to the rate (in time) at which the eigenvalues of the Jacobi–Morse equation increase and decrease as $x(t)$ passes through the focus. Here is a perturbation theory calculation that estimates that rate.

In this calculation we consider a family of Jacobi–Morse equations. A particular classical path $x(t)$ is picked with $0 \leqslant t \leqslant T_{\max}$ and for each $T < T_{\max}$ we examine the two-time boundary-value problem $\xi(0) = a$, $\xi(T) = b$ with $a = x(0)$ and $b = x(T)$. For simplicity we work in one dimension (but see the remark at the end of this subsection). Our original path $x(t)$ is of course a solution to this classical boundary-value problem. Thus for each T there will be an associated Jacobi–Morse equation and in writing this we now emphasize the dependence of the 'potential' U and the eigenvalue λ on T. The equation takes the form

$$-\ddot{\phi}_T(t) + U_T(t)\phi_T(t) = \lambda(T)\phi_T(t) \tag{8}$$

with $U_T(t) \equiv -V''(x(t))$ for $0 \leqslant t \leqslant T$ and $\phi_T(0) = \phi_T(T) = 0$. As T varies, so do the boundary conditions for the differential equation. In addition, new portions of the function $x(t)$ play a role. Suppose then that for some T_0 there is a conjugate point, that is, $\lambda(T_0) = 0$. (There is also an index for λ indicating which eigenvalue of the equation is under discussion, but since we are concentrating on a particular eigenvalue near zero we suppress this index.) We estimate $\lambda(T_0 + \Delta T)$ using a perturbation method. For $T = T_0 + \Delta T$ we again have (8) with $T_0 + \Delta T$ replacing T_0 everywhere. Define a new time variable $s \equiv t/(1+\epsilon)$, where $\epsilon \equiv \Delta T/T_0$, and define $\psi(s) \equiv \phi_{T_0+\Delta T}(t)$. Thus ψ has the same boundary conditions as ϕ_{T_0}, namely $\psi(0) = \psi(T_0) = 0$. To lowest order in ϵ, the equation for ψ is

$$-\psi''(s) + U(s)\psi(s) - \epsilon[2U(s) + sU'(s)]\psi = (\Delta\lambda)\psi$$

where U is U_{T_0}, the prime on ψ is $\mathrm{d}/\mathrm{d}s$, the prime on U is the derivative with respect to its argument and $\Delta\lambda = \lambda(T_0 + \Delta T)$ (since $\lambda(T_0) = 0$). By ordinary perturbation theory, $\Delta\lambda$ is estimated to be $\Delta\lambda = \epsilon\int_0^{T_0} \mathrm{d}t\phi(t)^*[2U(t) + tU'(t)]\phi(t)$, with ϕ the eigenfunction for the $\lambda = 0$ solution at $T = T_0$. This implies

$$\frac{\partial\lambda}{\partial T} = \frac{1}{T_0}\int_0^{T_0} \mathrm{d}t\phi(t)^*[2U(t) + tU'(t)]\phi(t)\,. \tag{9}$$

With repeated integrations by parts, making use both of the equation of motion for ϕ and its boundary conditions, (9) leads to

$$\frac{\partial\lambda}{\partial T} = -\dot{\phi}^2(T_0) \tag{10}$$

a result that recalls the appearance of the same quantity in a corresponding estimate in Morse theory (cf [7, p 85]). The negative definiteness of $\partial\lambda/\partial T$ reflects the fact that the number of conjugate points only *increases* along a path†. For our purposes, (10) stands out because it is nothing special. That is, the fact that the dynamics are chaotic makes this expression neither particularly large nor small. In principle, it might still happen that $\dot{\phi}^2(T)$ is large, but we will show below that (except for the bounces off the wall) this does not happen, basing our arguments on the Jacobi–Morse equation. It follows that the duration

† As remarked in [7, p 146] one can look on our semiclassical calculations as a differential equations proof of Morse theory. As such, (10) constitutes a component of that demonstration.

of conjugate points, the likelihood of landing upon one at any particular stage of a path's development, is as large or small as it is for non-chaotic dynamics.

Equation (10) is also consistent with the picture developed earlier in which the caustic due to reflection is located close to the wall. In that case the right-hand side of (10) *is* large. We thus have a situation in which $x(T_0)$ (the focal point), is within the wall (i.e. for a soft wall, is negative) and, as usual, ϕ vanishes at T_0. As remarked earlier, ϕ will look like the odd eigenfunction for the deep delta function potential. Most of its weight is in the square-well (on its way to becoming a delta function) potential; nevertheless, it vanishes near the edge of this well. This can only happen if the derivative is large.

Remark. The above demonstration dealt with one dimension. In higher dimensions one can follow the same steps, but instead of starting from (8), one uses the multidimensional Jacobi–Morse equation, (11), below. The added indices, coming on top of the several integrations by parts, make the demonstration lengthier. The result is $\partial\lambda/\partial T = -\sum_\ell |\dot{\phi}_\ell(T_0)|^2$. The only potential subtlety concerns (non-generic) higher order caustics which would necessitate the use of degenerate perturbation theory.

2.5. *Ordinary caustics and their fragmentation*

In general a free particle or a particle bouncing off straight walls will not focus and will have no caustics. Moreover, from the standpoint of the Jacobi equation, the only thing that *can* cause focussing is a non-zero second-derivative of the potential term ($V''[x(t)]$ in (4)). Therefore it is of interest to see how the large potential at the wall can cause the remote and finite ordinary focussing that occurs due to the curved surface in the stadium (or any other curved, hard surface). 'Finite' focussing refers in particular to the finiteness of $\dot{\phi}(T_0)^2$, even as the hardness parameter (which we have called Ω) goes to infinity.

To study this phenomenon we must go to at least two dimensions. The Jacobi–Morse equation is now a bit more complicated

$$-\ddot{\phi}_\ell - \sum_k \frac{\partial^2 V[x(t)]}{\partial x_\ell \partial x_k}\phi_k = \lambda\phi_\ell\,. \tag{11}$$

This is a Schrödinger-like equation for a multicomponent 'wavefunction'. Conventional focussing occurs when the path bounces off a curved surface. One can soften the potential and take V of the form $V(x, y) = \frac{1}{2}\theta(r-1)\Omega^2(r-1)^2$ with $r = \sqrt{x^2+y^2}$. Without loss of generality, we assume the path bounces off the mirror at $x = 1$, $y = 0$, coming in at some angle. We will not go into the details of the calculation, which is only slightly more complicated than what was encountered previously (equation (3), etc). The second partial of V, $V_{\ell k}$ as in (11) above, has two principal constituents. First there is an $O(\Omega^2)$ part for V_{xx} which does exactly what we calculated earlier for any bounce situation. However, because of the second component, we have additional richness and this is what allows focussing in the middle of the stadium. In particular, both V_{xy} and V_{yy} have $O(\Omega)$ pieces. This will allow a bound state in the orthogonal direction (the Jacobi field at the mirror surface is parallel to the tangent to the mirror) which, because the width of the potential is still $O(1/\Omega)$, gives an 'energy' scale of order unity. This allows the eigenvalue (of $\delta^2 S$) to pass through zero well away from the wall, and in fact in such a way as to give conventional caustics.

This calculation also allows us to argue that the quantity $\dot{\phi}^2(T)$ is not large for focal points away from the walls of the stadium. (This issue was raised following (10).) The function $\phi(t)$, $0 \leqslant t \leqslant T$, is an eigenfunction of the Jacobi–Morse equation with eigenvalue zero (that is what is meant by focussing). In this case the Jacobi–Morse equation is the Schrödinger equation of a particle in a box with an interior potential that is mostly zero. It is only non-zero when the path $x(t)$ (the argument of V'') hits the wall, and then it looks roughly like an attractive delta function. Therefore in the interior of the stadium the function ϕ is basically a sine function vanishing at T and doing nothing interesting since $x(t)$s last encounter with a wall. This last encounter occurred an O(1) time earlier (related to the distance the observation point is from the wall) and therefore the wave number associated with this portion of ϕ is also order unity. This wave number is essentially $|\dot{\phi}(T)|$. Even when this might be larger because of relative proximity to the wall, its size certainly has nothing to do with the exponential growth associated with chaos. (As will be discussed in section 3.6, there may be reasons for $\phi(T)$, hence $\dot{\phi}(T)$ to be small, namely localization in a quasi random potential. There is as yet no evidence for this, perhaps because the times studied have not been large enough.)

In two dimensions, a curved surface will generically give rise to a line of caustics and the same is expected of the curved portion of the stadium wall. However, the stadium boundary has a discontinuity in the second derivative of its bounding curve and at four points goes from circular to flat. The caustic line associated with the curved portion will cease at this point, since a flat reflector does not focus. (I here refer to the focussing *away* from the walls. As shown earlier, in the direction orthogonal to the wall there is always a caustic at the wall.) An exercise (not done by the author) would be to trace the disappearance of the caustic for the softened wall, which should reach a bit into the flat region, as $\Omega \to \infty$.

This same phenomenon will also have dramatic consequences on the structure of Lagrangian manifolds [12]. For one dimension, the caustic (that we derived above) is easy to see in the language of Lagrange manifolds. Without a softening of the wall you would have a line coming in (say from the left—the coordinate is taken as the abscissa, the momentum the ordinate) and its reflection going out with reversed momentum. With slight softening, these would be connected by a nearly vertical curve and the point furthest to the right on that curve would correspond to the caustic. As noted, the two-dimensional focussing in the interior of the stadium is more subtle and the fold in the manifold only develops as the manifold progresses back to the interior of the stadium. It follows that the fold *only* develops for the part reflected off the curved portion of the stadium wall and not the flat part. The manifold will therefore show a terminating wrinkle. Much of the intuitive thinking about limits of the semiclassical approximation involves considering the long fingers of less than interior area $\hbar$ that develop in the Lagrange manifold (see, e.g. figure 5 in [3]). The breaks that we have just shown must exist in the folding make much of this reasoning inapplicable to the stadium. It also means that the numerical success for the semiclassical approximation in the stadium does not in itself contradict the foregoing intuition.

3. Quantum mechanics

The rich variational structure of classical mechanics finds its way into quantum theory through the semiclassical expression† for the propagator

$$G(b,t;a) = \sum_{\alpha} \sqrt{\det\left[\frac{\mathrm{i}}{2\pi\hbar}\frac{\partial S_\alpha(b,t;a)}{\partial b \partial a}\right]} \exp\left(\frac{\mathrm{i}}{\hbar} S_\alpha(b,t;a)\right) . \qquad (12)$$

† Since (12) breaks down at caustics it does not quite carry all that structure. Equation (13) below, and its generalizations, deal with focussing phenomena.

The usual context is assumed: Hamiltonian, H, Lagrangian, L, corresponding classical system with classical action S, with the latter symbol serving to designate both a function of all smooth paths ($\int L\mathrm{d}t$) and the solution of the Hamilton–Jacobi equation for particular solutions (labelled by α) of the classical equations with $x_\alpha(s)$ equal to a at $s = 0$ and to b at $s = t$. The quantities a, b, $x(t)$, etc. are points in d-dimensional coordinate space. The propagator is defined as the integral kernel of the operator $\exp(-\mathrm{i}Ht/\hbar)$ and (12) is its small $\hbar$ approximation. The application of this formula to systems with chaos was first proposed by Gutzwiller. Until recently this formula had been mostly used after Fourier transformation as a way to deduce energy levels. It is the phase space smearing of the time-dependent version above and its successes in [1] that occupy us here.

As stated in the introduction, much of our analysis is based on the Jacobi–Morse equation, that is, the spectrum and eigenvalues of $\delta^2 S$, the second variational derivative of the action. As is found for example in [7], the van Vleck determinant, which is the determinant of the second derivative of the action *as a function of the boundary conditions for the propagator*, is essentially the inverse of the product of the eigenvalues of $\delta^2 S$. There are many interesting subtleties surrounding this relation in addition to the correspondences that we exploit directly in this paper.

An example of the interweaving of classical spectral properties and quantum mechanics is the information one can deduce concerning the product of eigenvalues of the operator $\delta^2 S$. In section 2, we noted that on reflection at a wall one eigenvalue goes through zero. But we actually found more than that. As the stiffness of the wall (Ω) grew, the eigenvalue went to $-\infty$ like $-\mathrm{const}\cdot\Omega^2$. Nevertheless, after the reflection we do not expect anything untoward in the behaviour of the van Vleck determinant. (Of course there is a sign change, usually invested with mysterious properties, but here seen merely as a negative eigenvalue in the product†). Indeed, there *is* nothing untoward, and it continues to satisfy a simple differential equation (the Jacobi equation). What is happening is that while one eigenvalue grows in absolute value, the others—the many others—shrink, in such a way as to prevent divergence. I have only checked this assertion numerically, but it is an immediate consequence of the relation of the van Vleck determinant, the determinant of a $d \times d$ matrix, to the infinite determinant of the operator $\delta^2 S$.

From this same relation it is clear that the set of eigenvalues $\{\lambda\}$ carries information on the positive Lyapunov exponent. This connection can be checked analytically in a specific example. It is simple to calculate the spectrum of $\delta^2 S$ for the one-dimensional parabolic potential $V(x) = ax^2/2$. The eigenvalues (of $\delta^2 S$) have the same form whether $a > 0$ or $a < 0$. But in one case the (inverse of the) van Vleck determinant has a $\sin\sqrt{a}t$ dependence and in the other $\sinh\sqrt{|a|}t$, which grows exponentially (consistent, by the way, with our assertions below on the shrinkage of each contribution to G in chaos). In this case though one can check explicitly the relation between the infinite product and the van Vleck determinant (but I will not reproduce the calculation here). It is interesting that the exponential shrinkage in the van Vleck determinant does not arise from any single eigenvalue but from a cumulative effect of all of them.

In the introduction we noted that there were (at least) two potential problems in the use of (12) for chaotic systems. First there is the possibility that the endpoint of the motion is conjugate to the initial point for some of the paths, that is, there are caustics. And secondly there is the tremendous multiplicity of paths. In the next subsections we take up these questions.

† For truly vertical walls quantum mechanics requires an additional sign change inside the square root. This has no influence in classical caustic counting nor on the caustics within the stadium.

3.1. Smearing the caustic 'blowup' with phase space averaging

The prefactor in (12), the square root of the van Vleck determinant, diverges when the endpoint of the classical path is conjugate to the starting point, that is, when there is focussing. Alternative descriptions of this blowup are either noting that one (or more) of the eigenvalues of $\delta^2 S$ vanishes or that the van Vleck determinant can also be expressed as $1/[\partial x_{\text{final}}/\partial p_{\text{initial}}]$ and that focussing corresponds to having little change in final position as the initial momentum varies. Either way, at a caustic there is a breakdown in the semiclassical approximation.

Now the singularity associated with a caustic is a coordinate space phenomenon. In [1] and [4], what is calculated is the matrix element of the propagator in a coherent state, effectively a phase space smearing of the propagator. It has been argued [9] that the phase space boundary conditions would smooth the caustic. In this article I will provide an explicit calculation of the coherent state matrix elements of the propagators at a caustic and indeed we will see that the (apparent) divergence is neutralized.

The coordinate space neighbourhood of a caustic is [6, 7] $O(\hbar^{2/3})$, so that it is a relatively small part of a $\sqrt{\hbar}$ by $\sqrt{\hbar}$ neighbourhood of phase space. However, in a two-dimensional coordinate space the (lowest-order Airy-type) caustic forms a line, which in general will pass through the coordinate space neighbourhood in question. Locally in path space, with respect to the path undergoing the focussing, on one side of the caustic line the two-time boundary condition (with the same T) has two solutions, on the other side zero. There are thus two questions: does the well known blowup of the semiclassical approximation in the neighbourhood of a caustic preclude its use in this context? What kind of semiclassical approximation can one have when for part of the region in question there is *no* classical path?

In this article I will deal with these questions using the language developed in [6]. This allows us to retain a coordinate space description within the context of a time-independent, Lagrangian-based propagator. For simplicity, and because the essential problem is already present, we will deal with the one-dimensional case. For fixed T, consider the semiclassical approximation for the propagator $G(x, T; y)$. In general this is given by a sum over classical paths but we concentrate here on the contribution from paths near a particular classical path connecting the endpoints. Specifically, suppose that for a and b there is a classical path $x(t)$ with $x(0) = a$ and $x(T) = b$ and that a and b are conjugate. The quadratic form $\delta^2 S$ has a vanishing eigenvalue and the corresponding mode, the Jacobi field, represents the shape of deviations from $x(t)$ that to lowest order (at least) go through both a and b, providing a fan of focussing paths. Starting from an expansion of S in terms of eigenvalues of $\delta^2 S$, the propagator for points in a neighbourhood of a and b takes the form (after integration over modes for which $\lambda \neq 0$)

$$G(b + \Delta b, T; a + \Delta a) = \exp\left[\frac{\mathrm{i}}{\hbar}\left[S(b, T; a) + p(T)\Delta b - p(0)\Delta a\right]\right]$$
$$\times \text{`}\sqrt{\frac{\mathrm{i}\lambda_1}{2\pi\hbar}\frac{\partial^2 S}{\partial b \partial a}}\text{'} \int \mathrm{d}u \exp\left\{\frac{\mathrm{i}}{\hbar}\left[pu^3 + qu\Delta b + ru\Delta a\right]\right\} \tag{13}$$

where p, q and r are O(1) numbers and $p(T)$ and $p(0)$ are the classical momenta at the indicated times. The expression within quotation marks is a finite limit for $\lambda_1 \to 0$. From (13) familiar properties of quantum caustics can be deduced. For example, the form $u^3/\hbar$ in the exponent implies that the significant range of integration for u is $u \lesssim \hbar^{1/3}$. This in turn implies that the u integral is $O(\hbar^{1/3})$ in place of the $O(\hbar^{1/2})$ size it would have if a quadratic

λa^2 were present in the action. Thus the propagator is greater by a factor $\hbar^{1/6}$, which means that the 'blowup' suggested by the breakdown of the simplest WKB approximation at the caustic is actually the change in leading asymptotic order. Similarly, noting that $u\Delta b/\hbar \sim 1$ defines the scale of Δb such that one is within the caustic region, we deduce that $\Delta b \sim \hbar^{2/3}$ is the width of the caustic†. Now the smearing of [4] is over a coordinate range of order $\sqrt{\hbar}$ so that $\Delta b \sim \hbar^{2/3} \ll \hbar^{1/2}$, suggesting that the effect of the caustics may turn out to be small. We shall see that this is so.

Using (13) the smearing effect will be calculated explicitly. Without loss of generality we assume that $p(T) = p(0) = 0$. Following [1], we take matrix elements of G between coherent states centered about a pair of position and momentum points. The worst case is to have the positions be conjugate and the momenta equal to the momenta of the path. Let C be the matrix element between coherent states $|a, 0\rangle = |\,\text{central position} = a,\ \text{central momentum} = 0\rangle$ and $|b, 0\rangle$. Then

$$C = \langle b, 0|\mathrm{e}^{-\mathrm{i}HT/\hbar}|a, 0\rangle = \int \mathrm{d}\Delta b\,\mathrm{d}\Delta a \exp\left(-\frac{(\Delta b)^2 + (\Delta a)^2}{\sigma}\right)$$

$$\times\,[\text{tame factor}] \int \mathrm{d}u \exp\left\{\frac{\mathrm{i}}{\hbar}\left[pu^3 + u(q\Delta b + r\Delta a)\right]\right\}$$

where 'tame factor' collects terms that do not affect our present arguments (such as $\exp[\mathrm{i}S(b, T; a)/\hbar]$) and σ characterizes the coordinate spread of the coherent states, so that $\Delta b \sim \sqrt{\sigma}$. Now do the Δb and Δa integrations:

$$C = [\text{tame}] \int \mathrm{d}u \exp\left[\frac{\mathrm{i}pu^3}{\hbar}\right] \exp\frac{1}{4/\sigma}\left[\left(\frac{\mathrm{i}uq}{\hbar}\right)^2 + \left(\frac{\mathrm{i}ur}{\hbar}\right)^2\right]$$

$$= [\text{tame}] \int \mathrm{d}u \exp\left(-\frac{s\sigma u^2}{\hbar^2} + \frac{\mathrm{i}pu^3}{\hbar}\right).$$

The quantity s is order unity. Taking $\sigma = \hbar$, it is easily shown that the $\mathrm{i}u^3/\hbar$ term is unimportant in the face of the $-u^2/\hbar$ term. The integral, and thus the propagator, has no blowup. In particular, the integral gives the usual $\sqrt{\hbar}$, not $\hbar^{1/3}$. Higher order focal points (leading term fourth or higher power of u in the exponent) are no worse.

The calculation just performed provides not merely an abstract argument in favour of the validity of smearing but an expression for the smeared propagator. Bear in mind, however, that we have only been looking at a single term in the propagator; full justification of the sum over classical paths expression involves other considerations as well, for example sizes of individual terms, as discussed elsewhere in this article.

Remark. We earlier raised the question of how one could have a semiclassical approximation when there is no classical path, as is the case on the wrong side of the caustic. The answer is that the expression (13) still has elements of Feynman's sum over *all* paths. The integral over u has been carried over from the original sum over 'all' paths, re-expressed in the basis defined by the eigenfunctions of $\delta^2 S$.

† A typographical error in [6] inverts the 2 and the 3 in giving the range of the caustic.

3.2. *Shrinking of the van Vleck determinant along a chaotic path*

In this subsection we discuss the behaviour of the van Vleck determinant as time increases and one moves along the classical chaotic path. We will provide estimates of this time dependence in the case of positive Lyapunov exponent or exponents. First consider the situation when only one exponent is large. Recall that $\partial^2 S/\partial a \partial b$ is $-1/(\partial x_{\text{final}}/\partial p_{\text{initial}})$. However, $\partial x_{\text{final}}/\partial p_{\text{initial}}$ represents the divergence rate of nearby paths—a quantity that grows in proportion to $\exp(\Lambda t)$, with Λ the Lyapunov exponent. As in [13], it follows that the van Vleck determinant shrinks like $\exp(-\Lambda T)$. Implicit in this is the assumption that nothing else interesting is happening. That is, notwithstanding the tendency of paths to diverge, there could be focussing as well. In terms of the directions defined by the diagonalization of $M_{ij} \equiv \partial^2 S/\partial a_i \partial b_j$, this means that initial perturbations in some directions go far away while others stay close and ultimately come back together. Such an event will cause the van Vleck determinant to diverge. In general, in the stadium or other systems, both processes take place. As we discussed above, the spatial region in which the caustic occurs is small as a function of $\hbar$, so that we will use the foregoing exponential estimates for the chaos induced shrinking of the van Vleck determinant.

In the event of more than one large Lyapunov exponent, more than one direction, that is, more than one Jacobi field, will grow in time. The van Vleck determinant, which is the product of the eigenvalues of M, will then grow like the product of all the factors, namely, $\exp(T \sum \Lambda_k)$. We remark that unlike phase space volumes, coordinate space volumes need not be preserved under classical dynamics.

3.3. *Duration of the passage through a caustic: quantum aspects*

In section 2.4 we showed that the time it takes for the (relevant) eigenvalue of the Jacobi–Morse equation to pass through zero was about the same for chaotic dynamics as for non-chaotic dynamics. However, as noted in section 3.2, and implicitly in the inverted parabola allusion in the opening of section 3, the product of the other eigenvalues is growing rapidly; if one were to ask the slightly different question: 'What is the time for the entire product to go from some fixed positive number to some fixed negative number' (or the other way round), then that time would indeed be short. However, that would be the wrong question. The need to have λ (the eigenvalue of the Jacobi–Morse equation) away from zero enters at a significant stage in the derivation of (12) from the Feynman path integral (see [7]). The semiclassical expansion is expressed over the stationary points of the action (the classical paths) and about each one of them one expands the path in coordinates that refer to the eigenfunctions of the Jacobi–Morse equation. For each classical path α one has

$$G_\alpha(b,t;a) = [\text{Normalization}]_N \exp\left(\frac{\mathrm{i}}{\hbar} S_\alpha(b,t;a)\right) \int \mathrm{d}u_1 \ldots \mathrm{d}u_N \exp\left[\frac{\mathrm{i}}{\hbar} \sum_k \lambda_k u_k^2\right]. \tag{14}$$

(The limit $N \to \infty$ is implicit.) If all eigenvalues are different from zero (on the appropriate scale of $\hbar$) then one gets a denominator that is the square root of the product of the eigenvalues, leading in the usual way to the van Vleck determinant. (This expansion lies behind the expression (13) above, in which one of the eigenvalues is *not* away from zero.) What is seen from (14) is that the need to have a given eigenvalue large or small has little to do with what the other eigenvalues are doing. (There could conceivably be a relation to the next term in the expansion. That is, if the 'p' of (13) were exceptionally large one might need to change the range of u over which the truncation (14) is valid. We will argue below that chaos does not demand large 'p'.) It is true nevertheless that multiplication by the large product of the eigenvectors that are not passing through zero will speed the rate at which the overall product passes given numbers. However, this growth (of the product) is (inversely) part of the overall shrinking of the van Vleck determinant. Thus it has already been accounted for, in that all terms in the sum involve this small van Vleck factor.

3.4. The range of integration for equation (13): small loops in the Lagrange manifolds

One of the principal intuitions in trying to gauge the time over which semiclassical approximations should remain valid has been the idea [5] that as the Lagrange manifold folds and refolds (because of caustics) the area within loops will become smaller than $\hbar$ and destroy the separation between paths needed to make the asymptotic (stationary phase) approximation (to the path integral) valid. We would like to examine this argument from the perspective of the Jacobi–Morse equation formalism. In the latter approach, it is points in path space that must be separated. Path space is larger than phase space and we believe that this is why the semiclassical approximation has its surprisingly large range of validity. Thus two paths just having passed through a caustic are indeed close to each other—also in path space—but when folding occurs, even though it brings phase space regions back together, it does not imply proximity in path space.

However, rather than deal in generalities we will examine (13) and the equations following it, since it is this integral whose stationary phase approximation we require. For the use we made of this integral one should have a sufficient range of (the dummy variable) u to integrate over and have the coefficient p neither too large nor too small (on appropriate scales of $\hbar$ to various powers, as usual). Since u and p appear as pu^3, the questions are interrelated. According to (12.18) of [6] (or (15.12) of [7]),

$$p = -\tfrac{1}{2}\int_0^T V'''(x(t))[\phi(t)]^3 \mathrm{d}t$$

where the primes on V refer to derivatives with respect to its spatial argument and ϕ is the eigenfunction associated with the vanishing eigenvalue of the Jacobi–Morse equation. Recall that from our earlier discussion the second derivative, V'', is approximately a δ-function (with finite multiplying coefficient, unlike the reflection case) for the caustics in the interior of the stadium, This δ-function peaks at the time at which the classical path $x(t)$ hits the wall. Integrating with V''' will therefore give the derivative of ϕ evaluated at the reflection point. This is not difficult to estimate. (If one is troubled by the singular functions, it is possible to use deep square wells in place of the δ-functions, but in fact the singularity is not severe and one merely needs to average the slope on two sides of the singular point.) For a one dimensional attractive potential $W(x) = -\mu\delta(x)$ with asymmetric boundaries (at $-r$ and $+R$, say) this derivative is $\mathrm{O}(1) \times [\exp(-\mu R) - \exp(-\mu r)]$. The asymmetric boundaries in this case refer to the previous and subsequent hitting times at the wall and are in general unequal. Since R, r and μ are all of order unity, so, in general, is p. It follows that the coefficients in the integral in (13) do not reflect the fact that $x(t)$ represents an extended solution of chaotic dynamics. (Other coefficients in (13) are innocuous.)

The allowed range of integration in (13) does have limitations but they should not be severe or common. If p had turned out to be extremely small there would be limits (in that case large variation of u would have been required), but this would be another way of saying that one is dealing with a higher order caustic. With small coefficients of cubic or higher order terms one gets into the catastrophe theory framework of [6], in which the

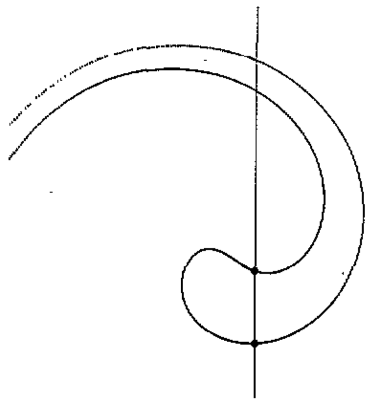

Figure 1. A loop in phase space, with coordinate space the horizontal axis. Where the curve is tangent to a vertical line there is a caustic. When $\Delta b \neq 0$, (see (13)) there are two (marked) points along the curve where the derivative of the polynomial in (13) vanishes, corresponding to paths solving the two point boundary-value problem (and yielding their momenta, which is the vertical axis in the figure). Continuing that vertical line away from those points yields other solutions. *However, since that line does not correspond to the range of integration of u*, these further intersections do not imply paths to be encountered in the further reaches of the u integration.

many paths are given by the unfolding of the catastrophe. But p is not in general small†. The other limitation on the range of u would come from the terminating wrinkles referred to above in connection with discontinuities in the second derivative of the boundary (for the stadium). These chop the caustics into shorter pieces. However, it does not seem to me that these should be common. Although there are many, many paths, *any given path* has not gone through many caustics, nor has it bounced off the walls many times. The large number of paths comes because one *exponentiates* the number of times a path goes through a caustic. Since for this chaotic system the Lyapunov number is essentially unity, the number of bounces of the wall and the number of caustics traversed by a given path are of the same order. For paths that did in fact approach the non-smooth portions of the wall there would be limitations on the integral, but for the times studied in [1] this is not so common an occurrence.

This brings up the question of order-$\hbar$ loops in phase space and the limitations they may place on the semiclassical approximation. In the language we are using here, this limitation is not evident, if it exists at all. In figure 1 we show a typical such situation. Where a vertical line is tangent to the loop there is a caustic. When one is away from the actual caustic the central point of the u integration does not lie in the phase plane. For $\Delta b \neq 0$, when the derivative of the polynomial in (13) vanishes one has two solutions of the classical boundary-value problem [6] and these define a vertical line (since by definition the final position is the same for both paths) that intersects the loop in two points near the caustic. The continuation of that line in phase space provides other solutions to the boundary-value problem. However, the continuation of u further away from its zero does not correspond to these solutions, but to a direction in path space that need have no further classical path solutions. (In general it will *not* correspond to such solutions since that would indicate a higher order caustic. This would mean that 'p' above would have to be small,

† The quantum localization phenomenon discussed in section 3.6 could reduce the eigenfunction near the endpoints, but there would be no reason for the coefficient p, defined as an integral over the entire time interval, to be small.

and we have just shown that it is not. Fourth or higher order caustics will involve more complex looping and folding, but as for the simpler caustic, only the singularities generated by the polynomial derived from the functional integral need be considered. Paths from later foldings are not in the range of 'u' integration.)

3.5. *Adding the many paths*

We return to the semiclassical expression for the propagator

$$G(b,t;a) = \sum_{\alpha} \sqrt{\det\left[\frac{\mathrm{i}}{2\pi\hbar}\frac{\partial S_\alpha(b,t;a)}{\partial b \partial a}\right]} \exp\left(\frac{\mathrm{i}}{\hbar} S_\alpha(b,t;a)\right) \tag{15}$$

with the sum running over classical paths $x_\alpha(t)$ that satisfy the boundary conditions. We assume that, as in [1], phase space averaging has been done and it is *families* of paths that satisfy the boundary conditions, i.e. collections of nearly identical paths that thread their way from one volume v_{i} to another v_{f} in a time that is long compared to the inverse of the Lyapunov exponent. We also assume that the momentum space restriction only reduces our path proliferation estimates by an overall (approximate) constant. Moreover, in this subsection we accept the proposition that the caustic problems have been ameliorated by the phase space averaging.

In trying to assess validity of (15), one is impressed by the enormous number of contributions to the sum, for even moderate times. In [1], as many as 30 000 paths enter the calculations. One wonders then if a subtle cancellation is needed in the sum (15) in order to get the correct result. We will see that there is a cancellation, that it is generic, and that it provides the classical–quantum correspondence.

The number of terms ($\equiv \mathcal{N}$) grows like $(v/V)\exp(T\Lambda)$ (or $\exp(T\sum\Lambda_k)$) while the contribution from each drops by $\exp(-T\Lambda/2)$ (or $\exp(-T\sum\Lambda_k/2)$). The phases of the terms are quite different from one another. After integration over the small phase space volume each term is of the form

$$[\text{van Vleck factor}]_\alpha \cdot \exp(\mathrm{i}S_\alpha/\hbar)\hat{\psi}(p_{\alpha f})^*\hat{\phi}(p_{\alpha i})$$

where ψ and ϕ are the wavefunctions within which G is sandwiched and (the Fourier transform of) each is evaluated at the gradient of S (i.e. the momentum) for that path. These momenta do not vary much (by assumption on ψ and ϕ) but the classical actions S_α do. For the stadium they are essentially the lengths of the paths. If we assume that the sum is a random walk in the complex plane then the norm of the propagator is the distance that walk is from the origin. For a random walk this will be of order $\sqrt{\mathcal{N}}$. It follows that G itself will be of order $\sqrt{v/V}$ ($\times$ appropriate wavefunctions), with the large numbers generated by the Lyapunov exponents dropping out. (That is, norm $= |G| \sim \sqrt{\mathcal{N}} \times$ step size $\approx \sqrt{(v/V)\exp(T\Lambda)} \times \sqrt{\exp(-T\Lambda)} = \sqrt{v/V}$.) The norm squared of the amplitude (the probability) is therefore precisely what one would expect for a particle that has been ergodically spread over the entire coordinate space.

Two points emerge from this calculation. First, despite the enormous number of contributions to the sum there is no reason to expect a breakdown of the semiclassical approximation. Secondly, the actual reduction of the propagator from a potentially disastrous $\sqrt{\mathcal{N}}$ ($= \mathcal{N} \times 1/\sqrt{\mathcal{N}} =$ *number of contributions times their size*) to order unity, is a 'random' cancellation of phases. You can (almost) always depend on the random walk to give the right size propagator, but how it gets that way will involve diverse contributions with no *a priori* relation to one another. The messiness of the chaotic dynamics is still present, but it does not invalidate the semiclassical propagator—on the contrary, it sets the propagator to a reasonable size. I find that the resulting structure, involving classical-chaos-induced 'random' behaviour, provides a satisfying extension on the correspondence principle.

3.6. Random potentials

There has already occurred a coincidence of technique for problems of quantum chaos and localization in a random potential [14]. The Jacobi–Morse equation provides a similar opportunity. Consider a path (for chaotic dynamics in a stadium) that has bounced off a wall many times and for which the van Vleck determinant is extremely small. Thinking of the Jacobi–Morse equation as a Schrödinger equation, this will look like a particle in a random potential. This assumes that the path is such that there is no regularity in its pattern of bounces off the wall. Without any further effort, we know that the product of the eigenvalues of this Schrödinger-like equation grows exponentially with the 'length' of the interval (in its original interpretation: time). This remark does not depend on the accuracy of the semiclassical propagator. Note though that the product involves an implicit truncation in that the upper eigenvalues will be influenced by the mesh used for the discretization.

Conversely, we can deduce from this correspondence that, as for random potentials in one dimension, the eigenfunctions of the Jacobi–Morse equation will be localized. That is, the eigenfunctions $\phi(t)$ used above will not generally extend over the entire interval $[0, T]$. In further analysis of the sort performed in this article, such a feature may prove significant.

4. Conclusions and prospects

There are two sorts of conclusions that I wish to draw from this article. One sort concerns the specific issue addressed: the remarkable long-time accuracy of the semiclassical time-dependent propagator for the stadium. The other concerns the technique employed, principally the Morse–Jacobi equation and the value of its eigenfunction expansion for tracking through path space.

The Morse–Jacobi equation is the eigenvalue equation that arises naturally from the path integral as a result of expanding about a variational extremal. For the purpose of learning about the classical mechanics, this method may at times be clumsy, for example in requiring lengthy analysis merely to establish that there is a focal point at a reflection. However, having established that, we were able to go on to obtain results about dynamical behaviour in the neighbourhood of the caustic. These results played a role in establishing important quantum properties. For example, our estimates for the coefficient of the cubic term for the Airy integral near the caustic implied that small area loops of the Lagrange manifold need not undermine the semiclassical expansion. This is closely related to the general principle proposed in the introduction, namely that a factor in justifying the semiclassical approximation in the presence of a large number of classical paths is the existence of a lot more room in path space than in phase space.

Another technical feature that provided a satisfying interweaving of classical and quantum properties—an extension of the correspondence principle, in effect—is the Brownian-motion-like phase cancellation that provides the right coordinate space density for the propagator, notwithstanding the large number of paths. Classical chaos guarantees pseudo-random phase contributions and this is just what is needed to make the sum of a large number of terms attain the correct value. (The phases in fact are not random and the correct quantum phase can also be obtained from the propagator. But for the classical result one does not need the phase information.)

With regard to the results of [1] we find several factors that play a role in their observed long-time accuracy. (i) Even though path proliferation implies a large number of caustics, they are not necessarily placed for greatest mischief. That is, we found that with every reflection there is a caustic, a caustic located right at the stadium wall. (And these are not dangerous for the semiclassical expansion.) Additional caustics are expected in the middle of the stadium, but as far as anyone knows they may be few. (ii) Even with caustics, an explicit expression for the phase space smeared propagator shows that the focussing related blowup is smoothed. (iii) Arguments related to small folds in the Lagrange manifold do not seem to apply for at least two reasons. First in using the path integral stationary phase approximation, the variables (in the Morse–Jacobi reduced integral) do not range over phase space, but over path space, where they do not encounter solutions of the two-time boundary problem corresponding to the other folds. Secondly, flat regions of the stadium boundary lead to termination of caustic lines for those caustics that may be in the stadium.

Although the matters discussed here reflect on the 'log $\hbar$' time barrier, there are other limitations on 'long' time accuracy whose existence was pointed out in [15]. These limitations appear to be on the scale of $1/\hbar$, which is quite a bit longer than that discussed in [1].

Our results suggest many further questions. One that should not be difficult is to find the (fixed time) caustics for the stadium. Another—which would be difficult—is to repeat the work of [1] for a more realistic potential, but one that exhibits chaos as complete as that of the stadium†. The present paper has certainly not exhausted the power of the Jacobi–Morse equation. For example, we nowhere used the fact that the 'wavefunctions' should be localized as a result of the quasi random potential. The approaches suggested by the Jacobi–Morse equation seem to be complementary to those now popular in the field of quantum chaos, and given the difficulty of making *any* analytic headway for chaotic systems, they should prove useful.

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Appendix. Two-time boundary conditions for motion in a disk

In this appendix we exhibit a system with caustics but without exponential path proliferation. The system is the stadium without its chaos-producing straight sides—simply a disk. In particular we show that the number of energy-bounded solutions of the two-time boundary-value problem grows linearly with time. This demonstrates that the caustics associated with reflection off the semicircular caps of the stadium do not of themselves entail path proliferation.

A particle moves in two dimensions, freely, within a circle. Use coordinates (r, θ) with $0 \leqslant r \leqslant 1$ and $0 \leqslant \theta < 2\pi$. Given $z_\alpha \equiv (r_\alpha, \theta_\alpha)$, $\alpha = \mathrm{i}$ (initial), f (final), and an elapsed time T, we seek paths, up to a maximum energy E, connecting these points.

Motion within the circle is described by successive angles at which the particle hits the circumference. If (ψ_1, ψ_2) is a pair of successive hitting angles, then the nth hit has angle

† [16] does discuss a softer potential, but in the example studied the enormous proliferation of paths does not match that of the stadium.

$\psi_n = \psi_2 + (n-2)(\psi_2 - \psi_1)$. For given (r, θ) let the direction of motion of the particle through that point be ϕ (measured counterclockwise from the radius passing through (r, θ)). It follows that ψ_1 and ψ_2 are given by the two solutions of $\psi = \theta + \phi - \sin^{-1}(r \sin\phi)$. The step size, $\Delta\psi \equiv \psi_2 - \psi_1$, is

$$\Delta\psi = \pi - 2\sin^{-1}(r\sin\phi)\,. \tag{A1}$$

Thus for any single $z = (r, \theta)$ and associated trajectory angle ϕ, one can compute the step size for trajectories passing through z. The step size is obviously independent of θ.

For the two-time boundary condition, z_i and z_f lie on a common trajectory so that the respective step sizes computed using (A.1) must be the same. Therefore if a putative initial direction ϕ is given, the final direction is given by $\sin^{-1}[(r_i/r_f)\sin\phi]$ (with two-fold ambiguity). This means that the ring impact point, Ψ, just before the trajectory passes through z_f, is also fixed.

For any particular z_i, putative ϕ, energy bound E and time T, there will be a finite collection of ring impact points whose cardinality N is bounded by $T\sqrt{E/2(1-r_i^2)}$. Note that this bound is independent of ϕ. (There is an O(1) correction that we ignore.) To have a solution of the two-time boundary condition, one of these ring impact points must coincide with Ψ, which also depends in a mild way on ϕ.

As ϕ varies (from 0 to 2π), the N associated impact points move around the circle, leading to N potential solutions of the two-time boundary condition. Order unity corrections to this argument can occur because of motion of Ψ and relatively small changes in N as ϕ varies. In addition the two-valued inverse sine-function may also induce a further factor two. Notwithstanding these effects, the number of solutions is bounded by N, which for fixed E (and provided $r_i r_f < 1$) grows linearly with T.

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