

# Quantum Chaos and Semiclassical Mechanics<sup>1</sup>

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As is well known there has been an explosion of interest in classical dynamics resulting from the relatively recent "discovery" that classical deterministic systems can be chaotic or in some sense random. Actually, their complexity had already been well appreciated by Poincaré in 1892 (MacKay, R. S. and Meiss, J. D. (1987), p. 7). Much interesting work is currently being done on classical chaos in both physics and philosophy. However, in the last fifteen years or so, the interest of some physicists has turned to the possibility that chaos, or chaotic behavior can be found in quantum mechanics as well. Unfortunately, things are much less clear cut in the quantum case than in the classical. In fact, there is very little agreement about whether chaos in quantum mechanics even exists. In part this is because there is apparently no generally accepted definition of what chaos in quantum mechanics could be. Despite this, the number of conferences and proceedings devoted to the topic of quantum chaos appears to be increasing at a rapid rate. In this paper I present some of the problems that have led to this rather strange situation. In particular, I will discuss one fairly influential proposal about how to define quantum chaos. I will focus on a particularly nasty and rather old problem in the foundations of physics; namely, that of understanding the connections between quantum and classical mechanics. Paradoxically, it appears that what gets studied under the rubric "quantum chaos" is parasitic upon classical dynamics. I want to suggest some ways of understanding this.

The paper is structured as follows. In the first section, I discuss briefly the nature and importance of chaos in classical physics. Section 2 outlines why it is so difficult to find chaos in quantum mechanics and presents a proposal for defining quantum chaos that explicitly recognizes this difficulty. The remaining 3 sections are an attempt to understand and elucidate the main features of this definition. In section 3 I begin to discuss to nature of the semiclassical systems referred to in the definition. This involves a discussion of the Correspondence Principle and the relations between the so-called "old quantum theory" and both classical mechanics and modern quantum mechanics. In section 4 I try to elucidate the crucial notion of "the classical counterpart" to a quantum system. Finally, I conclude in section 5 with a brief assessment of the status of semiclassical mechanics as a discipline distinct, in some important sense, from both classical and quantum mechanics.

## 1. Classical Chaos

Before turning to the discussion of quantum chaos, let me very briefly discuss classical chaos. I will be concerned here primarily with conservative Hamiltonian systems, ignoring for the most part chaos in so-called dissipative systems. There are, of course, conservative Hamiltonian systems that exhibit the most regular behavior imaginable. For example, an ideal harmonic oscillator such as a one-dimensional pendulum has a trajectory in its two dimensional phase space which for each particular energy is a simple circle in the  $(x, p)$  plane. At the same time, there are also Hamiltonian systems that can exhibit observational behavior that is apparently random. Here we can think of an (ideal) hard sphere gas in a box. By "observational" behavior here too, I mean the behavior of the trajectories that represent the system's evolution over time according to Hamilton's equations of motion in a  $2N$ -dimensional phase space (where  $N$  is the number of degrees of freedom of the system). At the "regular" end of this "dynamical spectrum" where the pendulum is found there are the integrable systems. These systems have their trajectories confined (at least) to  $N$ -dimensional doughnuts or tori in the larger  $2N$ -dimensional phase space. Furthermore, if one has two possible initial states that are nearby in phase space, then the trajectories starting from those points will diverge from one another at most linearly in time—that is, relatively slowly. Since the trajectory is confined to a torus, the evolution of the system will be either periodic or multiply periodic in time. At the other end of the spectrum are the chaotic systems. The trajectories for these systems can wander throughout the entire  $2N-1$ -dimensional surface of constant energy in the phase space. Furthermore, they exhibit extreme sensitive dependence on initial conditions: Trajectories from nearby initial states diverge exponentially from one another in time. This exponential divergence of trajectories is responsible for the observed randomness in the system's behavior. There is really an entire range of dynamical systems (again, even within the restriction to conservative Hamiltonian systems) in between the integrable and the chaotic; these are the so-called KAM systems, named after Kolmogorov, Arnold, and Moser. For the conceptual purposes of this paper, however, I will concentrate primarily on the two extremes.

To sum up this section, let me note the following. Classical chaos, I take it, is a property of the *dynamics* of systems. In particular, at least a necessary condition for a system to be chaotic is that its evolution exhibit an exponentially sensitive dependence on initial conditions. Integrable systems show no such behavior, and it is this fact that is primarily responsible for the relative ease with which their equations of motion can be solved.<sup>2</sup> One of the great benefits for physical theory coming from the discovery of chaotic dynamical behavior, has been that it provides (at least in certain ideal cases) a dynamical justification for attributing certain statistical/ergodic properties to deterministic systems. One can in effect prove that certain deterministic systems such as the hard sphere gas will behave in a way that is statistically indistinguishable from a roulette wheel. Demonstrations such as these take us a long way towards justifying various *a priori* statistical assumptions that are characteristic of classical statistical mechanics. One question for future research is whether quantum chaos (or at least what some people take to be quantum chaos) can play any sort of analogous role in grounding *quantum* statistical mechanics. Unfortunately, I do not have the time to consider this question here.

## 2. Quantum Chaos?

There are reasons why one might on the one hand expect and on the other, hope to find a quantum analog of classical chaotic time evolution. First there is the belief that in the limit classical mechanics should be recoverable from quantum mechanics. This, of course, is based on some appeal to and understanding of the Correspondence



Principle which was originally formulated by Bohr. The idea, roughly, is that because of this principle there *must* be chaos in those quantum systems whose classical analogs are chaotic. The main interpretive problems here are twofold. First, we must try to understand the exact nature of the limit referred to in the statement of the Correspondence Principle. Second, we must also try to understand what the phrase “classical analog of a quantum system” is supposed to mean. I will have considerably more to say about these problems below. At this point, however, I just want to note that there are relatively obvious grounds for expecting chaos to be present in quantum mechanics: Classical chaos is apparently a genuine *and* ubiquitous phenomenon. Given that quantum mechanics is supposed to be the more fundamental theory, it should be able to explain the observed *classical* behavior of dynamical systems, regardless of whether that behavior is chaotic or not.

As I mentioned, there is also a hope or desire to find a quantum analog of classically chaotic time evolution. This derives from the need, just as in the classical case, to ground certain *a priori* probabilistic or statistical assumptions of quantum statistical mechanics. Again, because of time constraints these issues will not be addressed here. Now there are compelling reasons to conclude that despite these hopes and expectations, quantum mechanics itself can exhibit *nothing* like the chaotic evolutions one witnesses in classical mechanics. In what follows I will consider finite, closed, isolated quantum systems—roughly the quantum equivalent to my earlier restriction to conservative classical Hamiltonian systems. The dynamical evolutions of quantum systems are governed by the Schrödinger equation. This is a partial differential equation and is of a completely different mathematical structure than the ordinary differential equations governing the evolution of classical systems. Let  $\hat{H}$  be the Hamiltonian operator for a finite, closed, isolated quantum system. The time dependent Schrödinger equation describes the evolution of the state vector  $|\psi(q,t)\rangle$  as follows:

$$(i) \quad i\hbar \frac{\partial}{\partial t} |\psi(q,t)\rangle = \hat{H} |\psi(q,t)\rangle$$

This equation has as its general solution the following:

$$(ii) \quad |\psi(q,t)\rangle = \sum_n c_n |\varphi_n\rangle e^{-\frac{i}{\hbar} E_n t}$$

where the  $|\varphi_n\rangle$  and  $E_n$  are the eigenstates and eigenvalues of  $\hat{H}$ . But,  $|\psi(q,t)\rangle$  is a multiply or conditionally periodic function in time. Given this then, the expectation value of any observable  $A$  is likewise multiply periodic.

$$(iii) \quad \langle A \rangle_t = \sum_{n,m} c_n^* c_m A_{nm} e^{-\frac{i}{\hbar} (E_n - E_m) t}$$

Recall that classically the integrable systems are those with dynamical trajectories confined to  $N$ -dimensional tori in phase space. Their evolutions are multiply periodic unlike chaotic systems which do not exhibit such regular behavior.

Therefore, despite the fact that there is a formal correspondence between the classical Hamiltonian and the quantum Hamiltonian operator (gotten by replacing the position variable  $q$  with the operator  $\hat{q}$ , and the momentum variable  $p$  with the operator

$$-i\hbar \frac{\partial}{\partial q} ),$$

*a finite and bound quantum system governed by the Schrödinger equation cannot exhibit the sort of sensitive dependence on its initial state characteristic of the classical chaotic systems.*

There is another reason to be sceptical about the possibility of finding chaos in quantum systems. This has to do with the fact that there really is no analog of a classical trajectory in the quantum theory. In a classically chaotic system the “typical” trajectory eventually (that is, in the limit  $t \rightarrow \infty$ ) explores the entire available phase space, becoming infinitely convoluted. There is complexity at all levels of description. But quantum mechanics involves Planck’s constant which has the units of phase space area, and through the uncertainty relations places a limit on the level at which such structure can be resolved. Regions of the phase space get “smoothed over” so that the concept of complexity at infinitely fine scales has no meaning in quantum mechanics. These considerations have led a number of investigators to give up completely the idea of a chaotic time evolution in quantum mechanics. Instead, they focus attention on other phenomena that appear to *correlate* with *classically* chaotic motion. An influential statement of this position is provided by Michael Berry:

Although we do not have chaotic quantum evolution, we do have here a *new quantum phenomenon* that emerges in the semiclassical limit in systems that classically *are* chaotic . . . (1987, p. 184.)

In fact Berry is led to formulate the following definition, not of quantum chaos, but rather, of the study of this new type of phenomena—what he calls “quantum chaology.”

*Definition.* Quantum chaology is the study of semiclassical, but nonclassical, phenomena characteristic of systems whose classical counterparts exhibit chaos. (1989, p. 335.)

There are a number of things going on in this definition, and the remainder of this paper will largely be an attempt to sort them out.

### 3. Classical/Quantum Correspondences

Berry’s definition of quantum chaology focuses on systems whose classical counterparts exhibit chaotic evolutions. It seems then that one of the most important issues requiring discussion is this notion of a “classical counterpart” of a system. I will take this up in detail in the next section. A second feature of the definition is that it refers to the semiclassical behavior of these systems with classically chaotic counterparts. This means that the systems are studied in the so-called semiclassical limit. This is the limit as Planck’s constant  $\hbar$  goes to zero. Of course, since Planck’s constant is not a dimensionless parameter, this is really the limit in which Planck’s constant can be considered to be negligible in comparison with other quantities having the same dimensions; namely, the classical actions. We will need to try to further understand the nature of this limit. For now let me simply note that it must be distinguished from what we can call the “classical limit” in which  $\hbar$  is identically *equal to zero*. This difference will be crucial to the argument later on.

Berry considers several examples of the kinds of phenomena that get discussed at Quantum Chaos conferences as a way of showing that his definition of quantum chaology captures what is being studied. Two such phenomena are the morphologies of wavefunctions and the statistical distributions of energy levels for bound systems. For example, it is apparently the case that probability distributions derived from wavefunctions of systems whose classical counterparts are chaotic are quite different in form than those whose classical counterparts are integrable. Likewise, energy levels are characterized by different statistical distributions depending on the nature of the “corresponding” classical dynamics. Berry argues that both sorts of phenomena are quantum theoretical as opposed to classical. In the case of wave-functions this is,



he claims, because in the classical limit (i.e., when  $\hbar = 0$ ) waves would oscillate infinitely fast and so wavefunctions simply won't exist. Likewise, the distribution of energy levels is quantum mechanical and not classical because the energy in bound classical systems is a continuous variable—there are no discrete energy eigenvalues. He concludes his paper with the following statement:

The spirit of the definition is not restrictive. Rather it is intended to reflect in a positive way what distinguishes quantum from classical chaology, namely seeking, discovering and explaining new phenomena which although semiclassically emergent are nevertheless *fully quantum mechanical*. (1989, p. 336. My emphasis.)

I disagree with this last claim. The phenomena being studied—the morphologies of wavefunctions and the statistical distributions of eigenvalues—are not classical. But this does not mean automatically that they are “fully quantum mechanical.” In fact, I will try to show that there are very good reasons to assert that the phenomena being observed in the semiclassical limit are neither classical nor fully quantum mechanical in nature. In other words, I think that we do not really observe new *quantum* phenomena in the semiclassical limit of systems whose classical counterparts are chaotic. Instead, we observe *semiclassical phenomena*. There is really a *third* theory involved here; and what is interesting and worthy of further philosophical investigation are the relations between it and both the classical and quantum theories. (An important question is whether this semiclassical “theory” is genuine or realistic, or whether it is some kind of artifact of the mathematical and philosophical problem of understanding the connection(s) between classical and quantum mechanics.)

Berry is correct in focusing on “the study of semiclassical . . . phenomena characteristic of systems whose classical counterparts exhibit chaos.” And, if we, with him want to call this “quantum chaology” that is perfectly fine. But, I think that the phenomena being studied, the semiclassical, but nonclassical properties and behavior, are not quantum mechanical phenomena either. They are properties of semiclassical systems. I hope that the following discussion of the nature of semiclassical mechanics can be seen as supporting this point of view.

To begin this discussion we need to get a better idea of the nature of semiclassical systems. In particular, what can be said about the type or types of correspondence that are said to obtain between these systems and their classical and quantum counterparts? It is helpful in answering these questions to consider the quantum theory as it was before 1925 when Heisenberg published his matrix mechanics paper. This “old quantum theory” resulted from attempts to explain observed nonclassical phenomena, such as the existence of discrete spectral lines, by appealing to an apparently *ad hoc* mixture of “quantum” postulates and classical principles. It is well known that some of the quantum postulates were completely at odds with the classical theory. For example, one of Bohr's boldest assumptions was that atomic systems could be found only in certain special states—the so-called stationary states characterized by a discrete set of allowed energies. The postulate of the existence of stationary states is in direct contradiction with the principles of classical electrodynamics. Despite these conflicts, the basic idea was to characterize the behavior of atomic systems to as great an extent as possible using the principles of classical dynamics.

This methodology proved remarkably successful in explaining the behavior of certain simple systems such as the hydrogen atom. Bohr, for instance, was able to derive a theoretical value for the Rydberg constant that was in remarkable agreement with the experimentally determined value. Nevertheless, it was soon noted that when ap-

plied to atoms that are only slightly more complicated (the helium atom for instance), the theory was quite unsuccessful.

It was recognized very early on that the problems were largely dynamical in nature. The old quantum theory appeared to give reasonable results for systems whose motions are periodic or multiply periodic—that is, for integrable systems. But it was a disaster when applied to nonintegrable systems. Thus the helium atom could not be effectively treated because it was modeled as a heavy nucleus with two orbiting electrons—that is, as a classical three-body problem, a nonintegrable system. Considerations such as these led Born to remark in 1924 that

. . . (T)he development of the quantum theory has shown that these [periodic and multiply periodic motions] probably exhaust the types of motions for which classical mechanics gives a valid description of the stationary states . . . (1967, p. 53.)

With the development of contemporary quantum mechanics following 1925, Bohr's old quantum theory was superseded and the dynamical problems just mentioned were completely set aside. However, what is today known as semiclassical mechanics should be seen as a natural extension of the old quantum theory—one quite consonant with the aim of treating the behavior of atomic systems using classical mechanics to as great an extent as possible. Nevertheless, semiclassical mechanics also clearly and crucially draws on what we now know about quantum mechanics.

It is clear from this brief discussion of the old quantum theory that its success depends somehow on an association or *correspondence* between certain features of the atomic system of interest and the dynamics of some classical system. Hans Radder has made a detailed and interesting study of the nature of the correspondence obtaining between the classical theory and the old quantum theory. He finds that there are three periods in the historical development of the old quantum theory which can be identified by different uses or interpretations of the Correspondence Principle. In the first phase, from about 1913-1915 Bohr speaks of correspondence in terms of a "numerical agreement of the values of some physical quantities in classical mechanics and electrodynamics and in Bohr's atomic theory." (Radder 1991, p. 203.) There was no claim during this period that any kind of conceptual continuity or correspondence between the two theories existed. However, the subsequent remarkable successes of the atomic theory in dealing with systems exhibiting multiply periodic motions led to the belief that there was more to the correspondence than simple numerical agreement in some restricted domain. In this second phase the correspondence was taken to be conceptual as well. For example, Kramers in 1919 (1956) argued for correspondence not just in the domain of large quantum numbers, but rather for *all* quantum numbers. Quantum frequencies were taken to be equivalent to certain averages over classical orbital frequencies. In Radder's words, "the same fundamental concepts [e.g. classical frequencies and harmonics, as well as classical Fourier coefficients] which govern the motion of electrons in their orbits, and the same function . . . determining transition probabilities are claimed to underlie both kinds of theory." (Radder 1991, p. 206.)

With the realization that Bohr's old quantum theory fails for all but the most simple atomic systems came the third phase in which the optimism that led to these claims of conceptual correspondence gave way to pessimism and ultimately to the complete abandonment of Bohr's conception of atomic systems. There remained a kind of numerical (and formal) correspondence in certain domains but the idea that the atomic theory, now well on its way to being reconstructed by Heisenberg and others, talked about the same sorts of entities and properties as did the classical theory was completely abandoned.



What I want to claim now is that with respect to modern semiclassical mechanics the situation is different. Radder is correct in identifying three separate theories as relevant for consideration: (1) classical mechanics and electrodynamics, (2) Bohr's atomic or "old" quantum theory, and (3) modern quantum mechanics. But what needs to be recognized is that just as in the historical discussion he offers, any modern discussion of the correspondence between classical and quantum mechanics also needs to consider relations of correspondence between three separate theories; between both the classical and semiclassical theories, and between the semiclassical and quantum theories. I would contend that in the latter case, a certain *conceptual* correspondence obtains even though the two theories must be understood as distinct. These, I believe, are all issues that are worthy of further investigations. Here I can only outline why I think this is so.

#### 4. The Classical Counterpart of a Quantum System

I would now like to discuss a plausible elucidation of the counterpart relation that appears in Berry's definition of quantum chaos. It will give us some insight into the nature of the systems studied in quantum chaos as well as some clues about why different types of classical motions (integrable or chaotic) can be said to correspond to different morphologies in wavefunctions and different statistical distributions of energy levels.

The idea of a classical counterpart depends crucially on geometric aspects of the classical phase space.<sup>3</sup> For the purposes of discussion we will consider a one degree of freedom bound system—an oscillator. (This is analogous to Bohr's early understanding and treatment of the hydrogen atom.) Let us consider this system at a particular constant energy. Then the phase space diagram for the system at that energy may look like the curve  $\Sigma$  in figure 1.

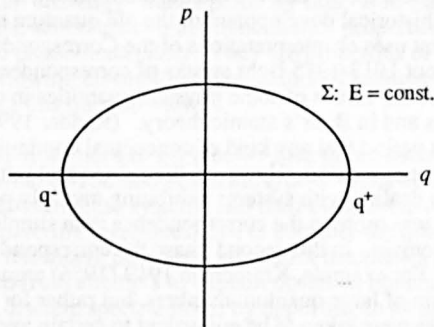


Figure 1. Level Curve  $\Sigma$  of a one dimensional oscillator.

The classical state of the system at a given time is specified by giving both the position  $q$  and the momentum  $p$ . The state of a quantum system at a given time will, we know, be specified by a wavefunction  $\Psi(q)$ . We would like to associate a wavefunction with the one dimensional surface or curve  $\Sigma$ .

The immediate problem is that quantum states makes reference only to the position coordinate  $q$ , apparently ignoring the other conjugate half,  $p$ , of the full set of coordinates  $(q,p)$ . We can treat the curve  $\Sigma$  as a function  $p(q)$  in analogy with the wavefunction  $\Psi(q)$ . However, it is quite apparent that such a "function" would generally have more than one value for a given value  $q$ . (See figure 2.)

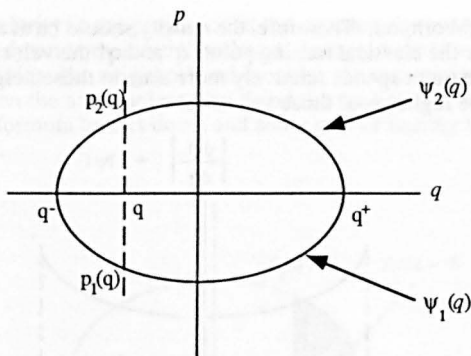


Figure 2.

We can get around this problem by splitting  $\Sigma$  into two branches, one upper where  $p(q) > 0$  and one lower where  $p(q) < 0$ . It now becomes possible to consider each branch as a single-valued function of the variable  $q$ :  $p_1(q)$  and  $p_2(q)$ . The idea is to construct a wave  $\psi_1(q)$  associated with  $p_1(q)$  and a second wave  $\psi_2(q)$  associated with  $p_2(q)$ . The superposition of these two waves will then give us the appropriate wavefunction associated with the entire surface  $\Sigma$ .

Two physical principles guide us in selecting the appropriate form for these wavefunctions. First note that the phase curve  $\Sigma$  represents a family of trajectories uniformly distributed around  $\Sigma$ , each point being an initial condition for a different trajectory. (Actually, in this one dimensional case each trajectory is equivalent to the curve  $\Sigma$ .) We would like the intensity of the wave to be proportional, in some sense, to the density of points or trajectories in the classical *coordinate* space  $q$ . If  $\Theta$  is a variable (an angle variable) that parameterizes the points along  $\Sigma$ , this density of classical points can be gotten by “projecting down”  $\left| \frac{d\Theta}{dq} \right|$  from  $\Sigma$  onto  $q$ . (See figure 3.)

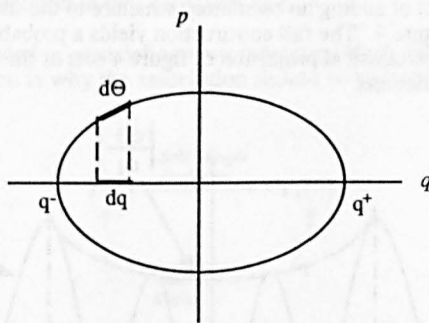


Figure 3.

The result of the projection looks something like figure 4. Note that this classical density curve has a minimum where the phase space curve in figure 3 is horizontal and rises asymptotically as the phase curve approaches the vertical. This is reasonable if one considers the amount of time the representative point travelling along the curve spends in these neighborhoods. When the point is in the neighborhood of  $q=0$ , it has maximum momentum  $p$ , hence maximum velocity and spends relatively little



time in that neighborhood. Therefore, the density should be at a minimum there. Conversely, near the classical turning points  $q^-$  and  $q^+$  the velocity is at a minimum and therefore the point spends relatively more time in those neighborhoods. So the density should be higher near those values for  $q$ .

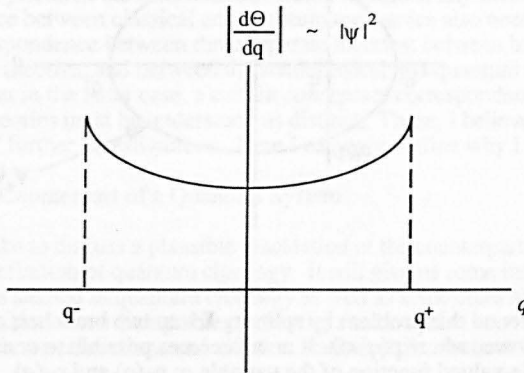


Figure 4.

But at the classical turning points  $q^-$  and  $q^+$ , the projection  $|\frac{d\Theta}{dq}|$  and hence, the density actually becomes infinite. These singularities are called caustics. (In higher dimensions they can take on a variety of different forms more complicated than the simple points in this example. These different forms can be classified by Rene Thom's catastrophe theory.) The existence and structure of the caustics are crucial elements in determining the form of the wavefunction associated with the surface  $\Sigma$ .

The second guiding physical principle involves determining the phase of the wavefunction. Here one appeals to the de Broglie relation  $\vec{p} = \hbar\vec{k}$  that relates the classical momentum to the wave vector of a locally plane wave. This introduces Planck's constant and has the effect of adding an oscillatory structure to the smooth classical background depicted in figure 4. The full construction yields a probability density  $|\psi|^2$  as shown in figure 5. The classical projection of figure 4 acts as the smooth envelope for the semiclassical oscillations.

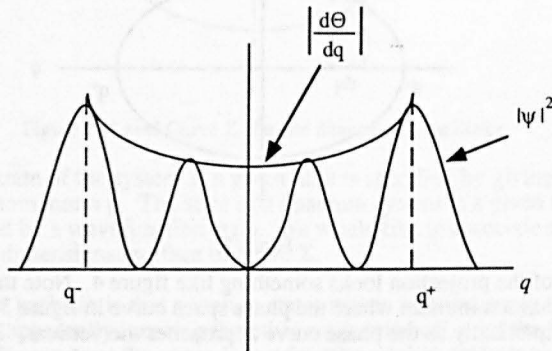


Figure 5.

Because of the singularity in the projection at the caustics, the construction just described actually breaks down in their neighborhood. In fact, there is a simple geometric criterion for determining the neighborhood in which the breakdown occurs. Consider figure 6. When the area enclosed by  $\Sigma$  and the line  $q=q'$  is on the order of  $\hbar$  the semiclassical formula breaks down and some way of dealing with the infinities becomes necessary.

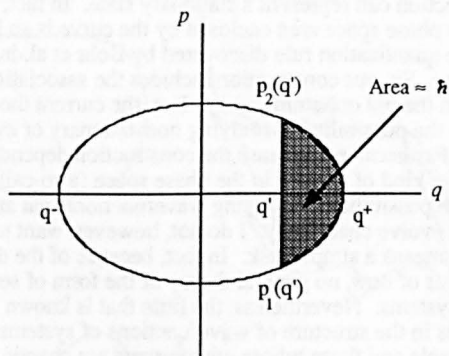


Figure 6.

There is a wonderful solution to this problem due to the Russian mathematician V. P. Maslov. (See Maslov, V. P. and Fedoriuk, M. V. (1981).) The idea roughly is to require that the association between waves and surfaces holds for momentum as well as position. In particular, we can, via a similar construction, come up with a momentum wavefunction  $\Psi(p)$  that will be valid in the neighborhood of the  $q$ -caustic ( $q^+$ ). This is possible because  $\Sigma$  is a smooth surface and cannot have points which would yield singular projections onto both the  $q$  and the  $p$  axes. One can then *define* the  $q$ -wavefunction in the bad neighborhood near the  $q$ -caustic to be the Fourier transform of the well-behaved  $p$ -wavefunction in that neighborhood.

So, we have succeeded in associating a wavefunction  $\Psi(q)$  with a phase space surface. The main question is why the association should be appropriate. Figure 7, helps to illustrate why.

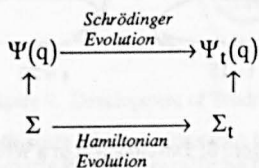


Figure 7.

Let  $\Sigma$  be an initial classical surface which evolves in time  $\Delta t$  into  $\Sigma_t$  according to the classical Hamiltonian equations of motion. If  $\Psi(q)$  is the initial wavefunction associated with  $\Sigma$  via the construction outlined above, then it will evolve in the same time interval into the wavefunction  $\Psi_t(q)$  according to the Schrödinger equation. The point is that *in the semiclassical limit* the association persists in time, so that the time evolved wavefunction  $\Psi_t(q)$  can be determined from the time evolved surface  $\Sigma_t$  by



the same recipe originally used to construct  $\psi(q)$  from  $\Sigma$ . In other words, if we solve the Schrödinger equation asymptotically to lowest order in  $\hbar$ , we see that *the association of the wave with the surface is time translation invariant*.

A few remarks on this construction are in order. If the surface  $\Sigma$  is an invariant surface (that is, if under the Hamiltonian evolution it remains unchanged) then the corresponding wavefunction can represent a stationary state. In fact, it will represent a stationary state if the phase space area enclosed by the curve is an integral multiple of  $\hbar$ . This is exactly the quantization rule discovered by Bohr et al. in the early days of the old quantum theory. So, our construction includes the associations with classical motions discovered in the old quantum theory. But, the current theory is much more general. It allows for the possibility of studying nonstationary or evolving states of “integrable” systems. Furthermore, because the construction depends *only* on the ability to identify a particular kind of surface in the phase space (a so-called Lagrangian surface), it *also* suggests the possibility of studying wavefunctions that are associated with classical surfaces that evolve chaotically. I do not, however, want to give the impression that this is by any means a simple task. In fact, because of the difficulties I am about to describe, there is, as of now, no general theory of the form of semiclassical wavefunctions for chaotic systems. Nevertheless, the little that is known suffices to suggest some general differences in the structure of wavefunctions of systems whose classical counterparts are integrable and those whose counterparts are chaotic.

Suppose the original curve  $\Sigma$  is not an invariant of the Hamiltonian evolution. Then it will evolve over time  $\Delta t$  into a new curve  $\Sigma_t$  which, since the Hamiltonian evolution is measure preserving, will enclose the same area as the original curve  $\Sigma$ . The shape of the new curve depends crucially on the type of motion (integrable or chaotic) under which its points evolve. There are basically two distinct morphologies for the evolution of 1-dimensional surfaces or curves. (In systems with more degrees of freedom—that is, with higher dimensional phase spaces—things are more complex.) Noninvariant curves evolving under integrable motion exhibit what Berry calls whorls; whereas those curves that suffer chaotic evolution develop tendrils. (Berry, et al. (1979), pp. 39ff.)

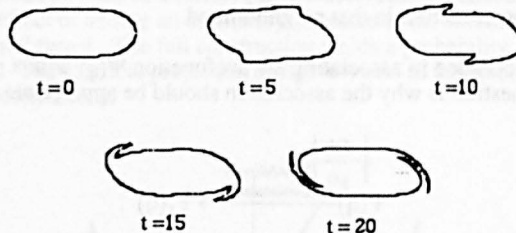


Figure 8. Development of a Whorl

Examples of whorls and tendrils can be seen, respectively, in figures 8 and 9. In the case of a whorl the curve  $\Sigma$  lies in a region surrounding an elliptic fixed point of the evolution. This is a region in phase space that contains stable trajectories that typically exhibit no more than linear separation from neighboring trajectories. Tendrils, on the other hand, develop when the initial curve  $\Sigma$  lies in a chaotic region near a hyperbolic fixed point. In such regions trajectories can be exponentially unstable. Since the area enclosed by the curve cannot change during evolution, it will develop long thin branches that swing violently back and forth as they are affected by the complex phase space structure associated with the presence of hyperbolic fixed points. One measure of the

difference in complexity of whorls and tendrils is the rate of increase in the length of the curves  $\Sigma_1$  under continuing evolution. For whorls it is expected that the curve's length will grow linearly with time, while for tendrils exponential growth is expected.

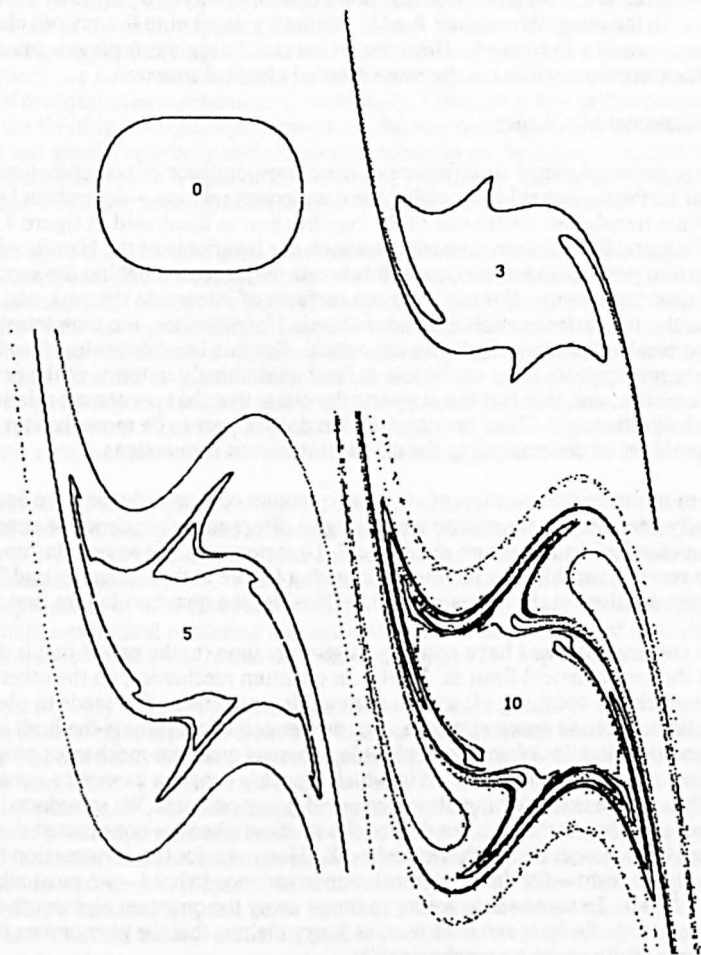


Figure 9. Development of Tendrils

It should be evident that both sorts of evolutions can lead to the development of more caustics. In the case of whorls it will generally be possible (that is, at least for reasonable times) to construct wavefunctions according to the recipe outlined above using Maslov's method to patch up the wavefunction at the caustics. However, for the chaotic evolutions that yield tendrils, caustics will proliferate rapidly. As soon as most caustics begin clustering on scales of order  $\hbar$ , the singularities can no longer be dealt with. The wavefunction will have undergone a transition to a new regime (a change in morphology)—one in which it can no longer be represented by superpositions of contributions from simple single-valued surfaces. The conjecture, which is quite well supported by computations, is that the semiclassical probability density will also undergo a change in morphology: For regular systems, the probability will be concentrated near



the caustics which mark the spatial boundaries of the classical motion; but, for chaotic systems the probability density will actually fall off in the neighborhood of the classical boundaries. Corresponding to these different regimes associated with integrable and with chaotic classical behavior one also notes two different roles played by Planck's constant: In the integrable regime  $\hbar$  adds oscillatory detail onto the smooth classical structure as we saw in figure 5. However, in the chaotic regime  $\hbar$  plays a smoothing role, which in effect, wipes out the more detailed classical structure.

## 5. Semiclassical Mechanics

The apparent physical significance of the correspondence of wavefunctions with classical surfaces—what I have called the counterpart relation—depends in large part on the time translation invariance of the construction as illustrated in figure 7. In the case of integrable evolution on surfaces which *are* invariants of the Hamiltonian, this construction persists indefinitely, and this is one major reason behind the successes of the old quantum theory. For noninvariant surfaces of integrable systems, and more importantly, for surfaces evolving under chaotic Hamiltonians, the time translation invariance breaks down rapidly as we have seen. But this breakdown itself, as I have tried to argue, appears to be explicable at least qualitatively in terms of the proliferation of caustics, and this fact too supports the claim that the counterpart relation has physical significance. Thus, the construction does appear to be more than an artifact of the problem of understanding the classical/quantum connections.

So, to return to the question of classical/quantum correspondence once again, have we finally been able to illuminate a meaningful *direct* correspondence or connection between classical and quantum mechanics? Unfortunately, the answer is “no.” There are two reasons for this, one having to do with a failure at the “quantum end,” the other with a failure at the “classical end.” Consider the quantum failure first.

The construction, as I have noted, persists over time (to the extent that it does) only in the semiclassical limit as  $\hbar \rightarrow 0$ . In quantum mechanics, on the other hand,  $\hbar$  is large relatively speaking. It acts as a smoothing parameter that tends to obscure detailed classical phase space structure. So, the semiclassical limit is the limit in which quantum considerations become negligible; whereas quantum mechanics proper is supposed to reign over the domain in which Planck's constant cannot be considered negligible. There is something almost magical going on here. We introduced the quantum of action  $\hbar$  through the de Broglie relation when we constructed the wavefunction  $\psi(\mathbf{q})$  associated with the surface  $\Sigma$ . However, for the construction to be physically relevant—for the time translation invariance to hold—we must take the limit as  $\hbar \rightarrow 0$ . In some sense we try to throw away the quantum element that was just introduced. So how can it be true, as Berry claims, that the phenomena being studied are “*fully* quantum mechanical”?

The magic comes because something is left after the limit gets taken, and it is this remainder that constitutes the problem with the “classical end.” When the limit is taken we do not simply recover the classical behavior that we started with since, as Berry notes, we are still talking about wavefunctions and discrete energy levels. And, these are definitely not classical dynamical concepts. The reason for the remainder is the singular nature or nonanalyticity of the  $\hbar=0$ , *classical* limit. Roughly, this means that quantum mechanics is not, for instance, like the special theory of relativity. That theory can mathematically and straightforwardly be related by perturbation to classical mechanics with the introduction of the dimensionless factor  $(v/c)^2$  as a perturbation parameter (relative velocity of the coordinate frames/speed of light)<sup>2</sup>. In the present case,  $\hbar$  cannot play an analogous role as a perturbation parameter. In other

words, one simply cannot compute “quantum mechanical quantities as classical quantities plus an expansion of corrections in powers of  $\hbar$ .” (Tabor 1989, pp. 229-230.) So, while the first “quantum reason” leads us to conclude that the phenomena being studied are not genuinely or fully quantum mechanical, this second problem relating to the nature of the limit suggests that they cannot be taken to be classical either. *In constructing a physically significant association between wavefunctions and classical surfaces, we have not established a direct correspondence or connection between classical and quantum mechanics.* (Incidentally, I think that this difference in the nature of the limiting relationships between on the one hand, quantum and classical mechanics and special relativity and classical mechanics on the other, is crucial for a proper understanding of a kind of intertheoretic reduction. However it is a difference which has, I believe, been insufficiently emphasized in the literature.)<sup>4</sup>

Given all of this, it seems quite reasonable to conclude that what is being studied and discussed at Quantum Chaos conferences is some third domain of behavior; namely, the semiclassical. To put the point rather picturesquely, semiclassical mechanics is the theory of the asymptotic border zone between quantum and classical mechanics. Many physicists and chemists appear to take semiclassical results to be more than just approximate solutions to quantum mechanical problems. In particular, they take the results to be genuinely explanatory and to further our understanding of a certain class of physical phenomena. Consider, as just one example, the following quote. In a discussion of the nature of semiclassical methods in chemical physics, W. H. Miller notes

Semiclassical theory plays an interpretive role; that is, it provides an understanding of the nature of quantum effects in chemical phenomena, such as interference effects in product state distributions and tunneling corrections to rate constants for chemical reactions. . . . The glory effect (an interference feature in the energy-dependence of total cross sections), for example, was first seen in completely quantum mechanical scattering calculations, *but was not understood until its semiclassical origin was realized.* (Miller 1986, p. 171. My emphasis.)

This quote not only suggests that semiclassical mechanics should be considered to be a theory in its own right separate from both classical and quantum mechanics, but it also suggests that there may be quite interesting correspondences between semiclassical and quantum mechanics. I would want to argue that a full understanding of the connections between classical and quantum mechanics requires studying the nature of the correspondences between, on the one hand, classical and semiclassical mechanics and, on the other, semiclassical and quantum mechanics. Regarding the latter semiclassical/quantum correspondence, it seems reasonable, in light of the above discussion, to argue, using Radder’s terminology, that some kind of *conceptual* correspondence obtains. The modern semiclassical theory, unlike its predecessor, Bohr’s old quantum theory, talks about wavefunctions, energy spectra, etc.—just the concepts that play a prominent role in modern quantum mechanics. While Radder appears to be correct in denying conceptual correspondence between classical mechanics and the new quantum mechanics as  $\hbar \rightarrow 0$  (Radder 1991, p. 209), such correspondence does exist between the semiclassical descendant of the old quantum theory and the new quantum theory.

The idea is that the semiclassical/quantum correspondence is something considerably more than just formal or numerical correspondence in certain domains of application. While the semiclassical theory may be incapable of yielding all the details of the quantum theory, it is more than a method for yielding approximate solutions to quantum mechanical problems. *In focusing on an underlying classical structure (the behavior of families of trajectories or surfaces), it is apparently describing something real that tends to be obscured by the quantum theory.* Perhaps one way to un-



derstand this is the following. In taking the  $\hbar \rightarrow 0$  limit we are essentially ignoring the dispersion typically associated with quantum evolutions; and in so doing, we are clearly idealizing. But, rather than obscuring the genuine mechanisms at work, this idealization actually brings them into focus.

Finally, there is a hope that further study of the nature of chaotic wavefunctions will lead to a general semiclassical theory comparable to that which exists for the integrable case. When that happens it may not be too far-fetched to suggest that it could lead to an extension or partial revision of quantum mechanics making it explicitly capable of incorporating the ubiquitous chaotic behavior present in the world.

### Notes

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<sup>2</sup>There are however, some integrable systems whose equations of motion are not separable, and which therefore do not easily lend themselves to integration by quadratures. The Toda lattice is an important example.

<sup>3</sup>For a more detailed and technical discussion than what follows here see Berry 1983 and the references therein.

<sup>4</sup>For a discussion of this see Batterman 1993.

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