Quantum Non-Integrability: An Analog to Classical Chaos

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Classical non-linear dynamics, and its descent into chaos, is a widely appreciated and well studied field in modern physics and mathematics; it's appeal spreading from those who have devoted their life to its study to even the most casual enthusiast. Knowledge of its analog at the quantum level, however, is not nearly as widespread. The purpose of this paper is to outline the basic physics behind this concept and to present simple examples which will display the correspondence between the classical and quantum limits. Particular attention will be given to quantum "billiard" systems and the recovery of known, unstable periodic orbits from the probability density in the limit that $\hbar \to 0$. Henceforth, the behavior these systems exhibit will be referred to as "quantum chaos"; a term which is concise, somewhat ambiguous, and entirely incorrect.

Classical Chaos and Non-integrability

Classically speaking, and in very simple terms, a non-integrable system is one in which there is no closed-form solution it dynamics. These systems, in many cases, can lead to chaos. Chaos, generally speaking, is the tendency of certain dynamical systems to display extreme sensitivity to initial conditions. These systems are deterministic (described completely and exactly by their initial conditions and equations of motion) and yet particles within them, with arbitrarily close initial conditions, have trajectories which will eventually and always diverge exponentially. Typically, chaos arises as a result of non-linearity in the equations of motion, but chaos may also arise from complicated boundary conditions or the geometry of the phase space. Chaotic systems are normally characterized by abstract methods such as determining bifurcations-- sudden qualitative changes in behavior as a particular parameter is tuned, measures of the rate of divergence of arbitrarily close initial conditions such as the Lyapunov exponent and phase space analysis using tools such as Poincare sections.

A non-linear system is not necessarily chaotic. There is a clear distinction between a non-linear system which displays so-called “normal” motion and one whose motion is chaotic. I will stop short of a rigorous definition of the distinction and say only that the difference is very intuitive: normal, or regular, motion “looks” like the particle is behaving normally or regularly while chaotic motion looks wild, unpredictable and almost entirely random. The dynamics of billiard balls confined to various differently shaped tables, illustrated in figure 1, provides a clear picture of this concept. Here the system is idealized; there is no friction, the billiard ball is a point particle and collisions with the perimeter are perfectly elastic. As you can see, there is a very distinct difference between the trajectory of the billiards in each situation. The dynamical description of the circle in this case is integrable, while the stadium's is not.

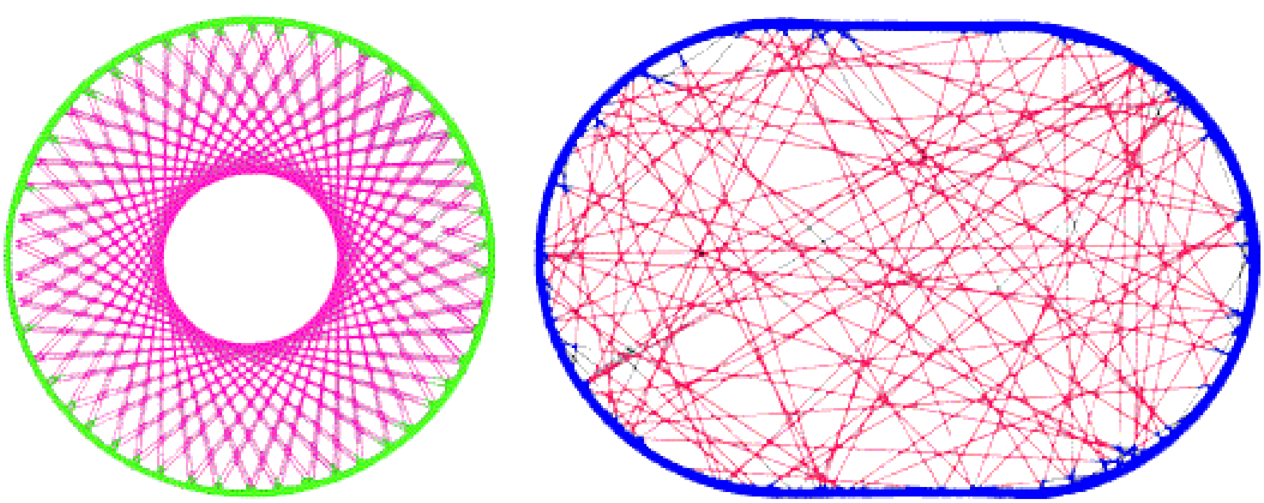


FIGURE 1.) Left: A circular billiard table displaying regular motion. Right: A stadium shaped billiard table displaying chaotic motion

Quantum-Classical Correspondence and its conflict with Chaos

The fundamental assumption (and flaw) of classical dynamics is that we may know, with arbitrary precision, the exact phase space description of a particle at any given time and, along with knowledge of the equations of motion, may completely determine its trajectory in the immediate future. With the development of quantum mechanics this idea has essentially been tossed out the window in favor of the probabilistic description of nature á la Heisenberg, Schrödinger, etc. However, the immense success of classical mechanics to describe the behavior of particles, whose trajectories have actions which are huge compared to Planck's constant, means that should we take the limit where $\hbar \rightarrow 0$, we must be able to recover the classical behavior of a macroscopic system from the quantum behavior of a microscopic system.

This presents a problem: how may we recover non-linear behavior from quantum mechanics when the fundamental equation describing it, the Schrödinger equation, is linear? Simply put, the Schrödinger equation **cannot** behave “chaotically” or unpredictably in the sense described by classical chaos theory. What is meant, then, by the term “quantum chaos” is “the quantum (probabilistic) analog of a classically (deterministic) chaotic system.” It is therefore evident that we must first approach the system from a classical perspective; analyze the chaos with known methods and then attempt to describe these using quantum mechanics. Then, in conjunction with the correspondence principle, should the energy of the microscopic system be sufficiently large we should expect to see a qualitative similarity between the quantum picture and the classical, chaotic picture. Methods for connecting these paradigms will be briefly discussed in the following sections.

Quantum "Phase-space" Representation

One of the primary difficulties in making a comparison between classical and quantum mechanics is that they are described using very different mathematics. Classical mechanics is described by ordinary differential equations acting on the phase-space while quantum mechanics involves partial differential equations acting on a space of probability distributions. One in-road is to compare the quantum mechanics with classical statistical mechanics, to find a probability distribution function which reduces to the classical probability distribution (Louisville) in the correspondence limit. This is, in general, very difficult due to the nature of uncertainty in quantum mechanics.

One method, proposed by Wigner, was introduced to study quantum corrections to statistical mechanics. He defined the so-called Wigner distribution as,

$$P(x,p) \stackrel{\text{def}}{=} \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} \psi^*(x+y)\psi(x-y)e^{2ipy/\hbar}\,dy$$

a "displaced" Fourier transform of the probability distribution. This representation was later shown to be exactly analogous to the classical probability density function in phase-space and that it can be used to compute expectation values of a quantum system. Interestingly, this function has negative values for states which are classically not allowed and is therefore sometimes referred to as a quasi-probability distribution, due to the fact that a true probability distribution is positive definite. However, these negative values vanish as we approach the correspondence limit and the classical mechanical probability distribution is recovered. Further exploration of this subject is interesting, but beyond the scope of this paper.

Semi-classical Quantization

Semi-classical quantization is, at its heart, an interference phenomenon. Wave-fronts follow the classical paths and form eigenfunctions when they interfere constructively. For integrable systems, classical motion may described on tori and produce the WKB quantization rule when constructive interference is accounted for. In likewise fashion, Gutzwiller showed that periodic orbits play a similar role for the quantization of chaotic systems. Using stationary phase analysis, he was able to show that the trace of the semi-classical Green's function connects the quantum spectrum with classical periodic orbits; the Fourier transform of the spectrum has sharp peaks at the periods of the orbits. The primary and most useful result of Gutzwiller's theory is an expression for the density of states, which is the trace of the semi-classical Green's function

$$g_c(E) = \sum_k T_k \sum_{n=1}^{\infty} \frac{1}{2\sinh\left(\chi_{nk}/2\right)}\, e^{i(nS_k - \alpha_{nk}\pi/2)}.$$

which involves a sum over all of the periodic orbits.

The orbits, however, are much too numerous to provide a one to one connection and other methods beyond the scope of this paper must be applied, based on the particular system of interest. The main takeaway from this brief section is that semi-classical quantization provides a connection between the classical picture and the quantum-mechanical eigenvalue spectrum.

Classical and Quantum Billiards

A connection may also be made between the classical trajectories and the quantum-mechanical *wave-function.* As mentioned earlier, it has been shown that classical billiard systems can display regular or chaotic behavior based simply on the shape of the boundary. It has also been shown that systems known as “quantum dots” may be classified by the motion of their corresponding classical billiard system, and properties such as their resistance are described through this analogy. It is counter-intuitive that quantum properties such as resistance can be related to a the dynamics of billiards, which are purely classical. Nevertheless, it has been shown that they are related and it would seemingly be fruitful to investigate the quantum mechanical behavior of systems analogous to the classical billiards. This is done, á la Eric Heller, by solving the Schrödinger equation for an infinitely deep, two dimensional square well of any shape of interest, such as the stadium.

Heller employed methods similar to those of Gutzwiller to study these systems. He was able to show, in the correspondence limit, that many of the eigenfunctions of irregular shaped wells showed anomalously high probabilities corresponding to classical periodic orbits. This phenomenon has been dubbed the “scarring” of the quantum-mechanical eigenfunctions and these scars represent both isolated and non-isolated periodic orbits; the distinction being that the isolated orbits are all qualitatively distinct while there are infinitely many non-isolated orbits that are locally identical. The qualitative difference in appearance of the scars corresponding to each type of orbit is that the eigenfunctions showing isolated orbits look nearly identical to the classical trajectory (figure 3), while those corresponding to non-isolated orbits (sometimes dubbed “superscars”) show smearing over the entire range of possible orbits (figure 2).

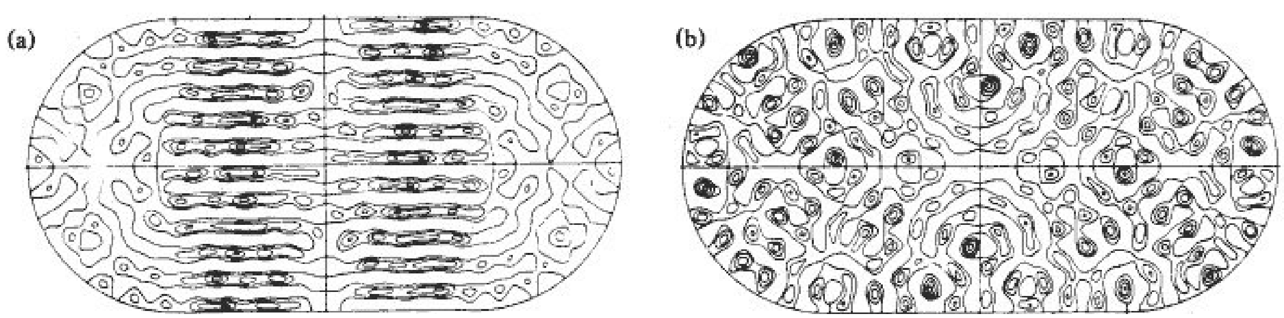


FIGURE 2) Left: Smeared orbits (superscars), the ball bounces back and forth from top to bottom. Right: Purely chaotic behavior

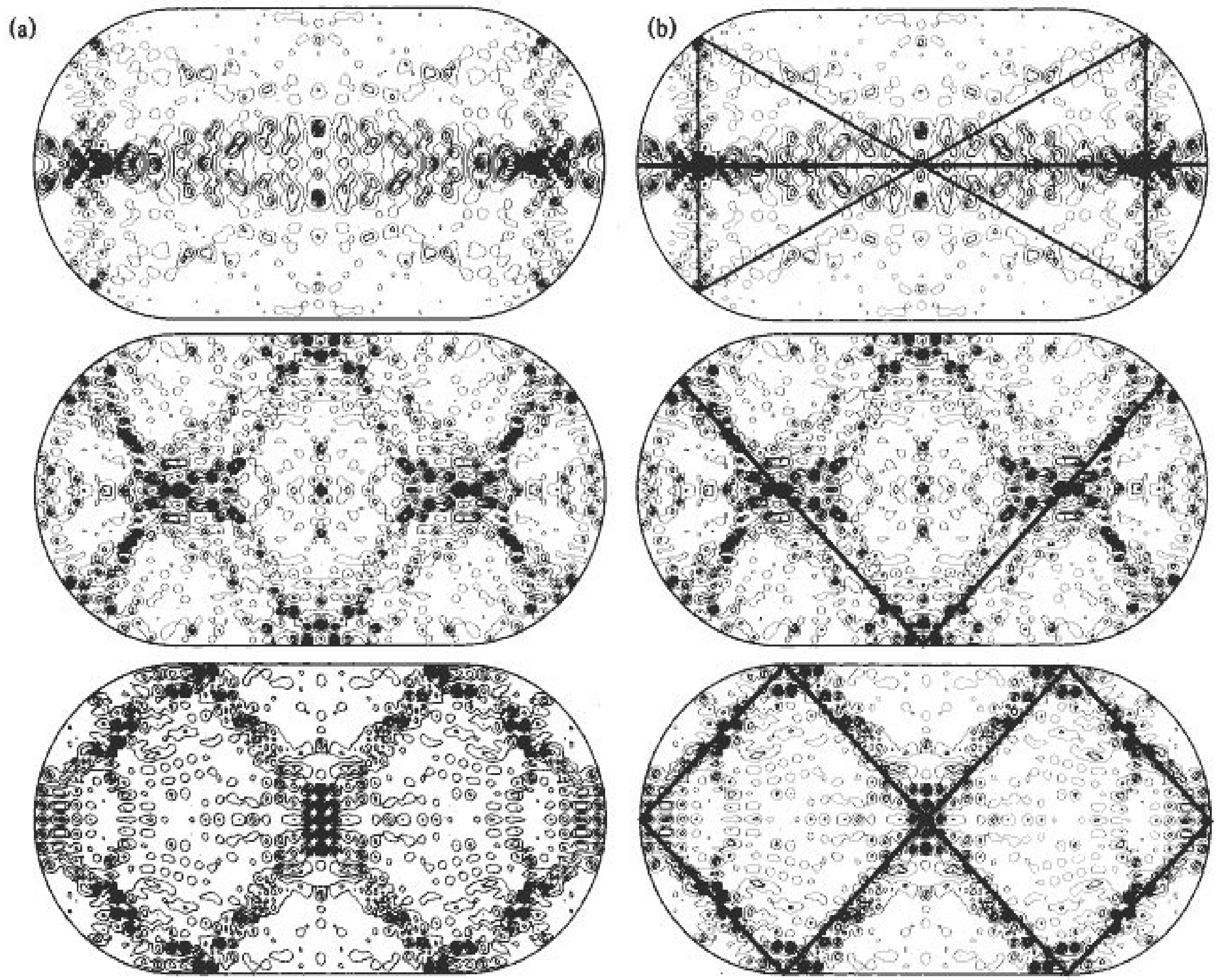
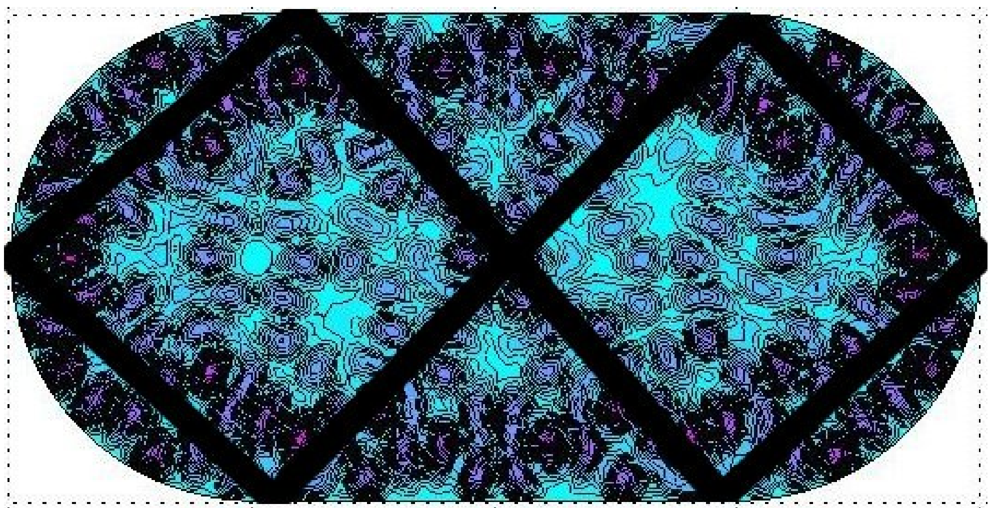


*FIGURE 3.) The left collumn shows the scarred states of the stadium, right column shows the corresponding **isolated** periodic orbits (from Heller, Phys Rev.)*

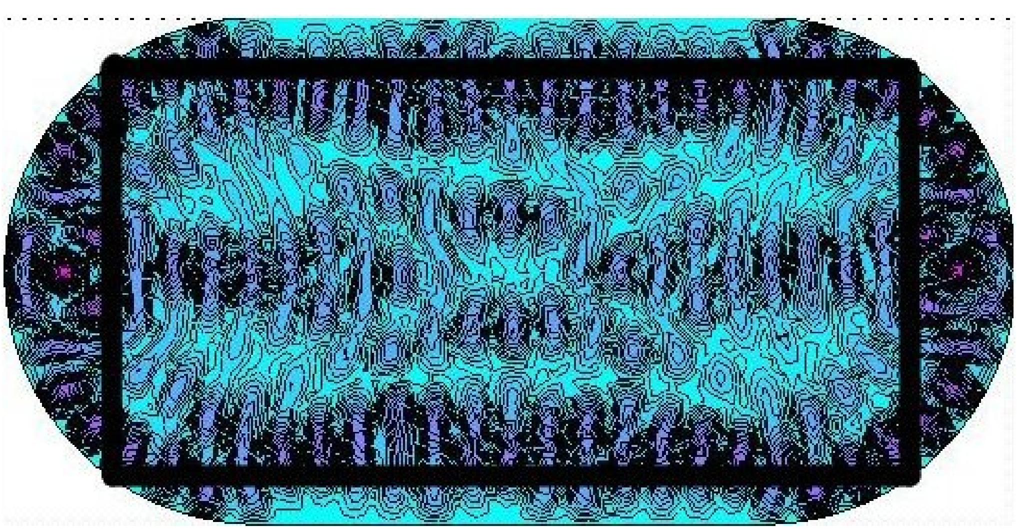
Clearly, the previous two sections show that a great deal of information about both the eigenvalues and the eigenfunctions may be extracted from knowledge of the periodic orbits of the analogous classical system.

<u>Quantum Billiards in Matlab</u>

Heller's work in the previous section involved much complicated mathematics, including matrix algebra, Green's function, density matrices and so on. I will show that the same eigenvalues and eigenfunctions may be obtained using Matlab's PDETool, for which only a cursory knowledge of the Schrödinger equation and a moderate proficiency in a program such as MS Paint is necessary. The input equation into pdetool is: $-\nabla\cdot(c\nabla u) + au = \lambda du$. Where I will set c=0.001, a=0 and d=1, and solve for the eigenfunctions and eigen values. The results are consistent with those of Heller and there are other orbits I have found in addition to those displayed previously.



The two square orbit shown by Eric Heller



Large, rectangular orbit. Corresponds to the trajectory where the tangent of the stadium corner is 45 deg to the incoming trajectory

These are just a few of the many periodic orbits that can be seen in in studies such as these.

Conclusions

It is evident that there are many conceptual leaps that must be made in order to understand the quantum manifestations of chaos. However, it is evident both from theory and from experiments, on systems such as quantum dots and quantum wires, that connections may be made allowing for the transition from quantum behavior to classical, chaotic behavior. Analysis may be done using quantum phase-space representations as well as quantization of chaotic systems through knowledge of their classically periodic orbits, which gives both eigenvalues and scars of the orbits in the quantum eigenfunctions. Thus, we may rest assured that the correspondence principle is safe.

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