Chaos with Few Degrees of Freedom

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As a mathematician, astronomer, and physicist, Poincaré was the first to study the phenomenon of chaos in classical mechanics, in particular the three-body-problem of the Moon orbiting around the Earth under the perturbation of the Sun. His work helps us to understand atomic and molecular physics, because our intuition in these areas is always based on a classical picture for the motion of the nuclei and electrons. The Moon's motion was found to be multi-periodic by the early observers; Newton explained the main frequencies and calculated the lowest terms in the corresponding Fourier expansion. But inspite of ingenious efforts, like the work of Hill involving as a starting point a periodic orbit of the full problem, Poincaré showed that perturbation theory is unable to guarantee the convergence of the Fourier expansion. In this traditional representation, the lunar trajectory would be restricted to a four-dimensional invariant torus although the available phase-space has eight dimensions.

The invariant tori are destroyed because of increasing phase-lock due to perturbations, whenever the system is close to a resonance. The KAM-theorem gives a mathematical criterion for this loss, which is best seen in a surface of section for such simple systems as the Anisotropic and the Diamagnetic Kepler Problem (AKP and DKP). Instead of invariant tori, the flow in phase space involves a double foliation where each trajectory is the intersection of one leaf from the unstable foliation with a leaf from the stable foliation. Neighboring trajectories drift exponentially away from each other in the future along the unstable leaf, and approach each another in the stable leaf coming from the past. This situation, called "hard chaos", also allows for a symbolic description of each trajectory in terms of a simple code like binary sequences in the AKP.

Einstein showed that the usual connection with quantum mechanics is valid only for the case of "regular behavior", i.e. the presence of invariant tori. For classically chaotic systems, VanVleck's expression for the propagator seems to be the best starting point, provided it is summed over all the classical trajectories that go from the source to the detector. Its trace becomes a sum over periodic orbits, which lends additional weight to Poincaré's emphasis on their importance in classical mechanics. In trying to understand the trace of an operator as a function of time, or the scattering phase-shift as a function of momentum, one runs into almost-periodic functions. They are able to mimic locally any arbitrary smooth function provided the spectrum of frequencies, although discrete, is rich enough. This unexpected, but smooth behavior can be seen as a symptom of quantum chaos, in contrast to the fractal nature of classical chaos.

Introduction

The main topic of this conference, as expressed in the title, is a question: Quantum and Chaos: How Incompatible? Since I was instructed by the organizers to present an introduction for the non-experts in the audience, I will not try to give a definite answer to this question; rather, I will try to offer some preliminary considerations that should help in putting the later talks of this program into perspective.

When I speak about perspective, I mean the effort to see what is happening now as part of a development that may be at least one century in the making. To be precise, it started with the work of the great French mathematician-astronomer-physicist Henry Poincaré in the 1880's and 1890's, more than a hundred years ago. For a long time, mathematicians remembered him for his work in topology, including his discussion of surfaces of constant negative curvature, whereas physicists gave him credit for almost discovering special relativity ahead of Albert Einstein. Only astronomers seemed aware of his new approach to celestial mechanics, in particular the three-body-problem, either Sun-Earth-Moon or Sun-Jupiter-asteroid, and the stability of the solar system in general.

Poincaré discovered that our intuition had been misled for the two centuries since Newton had found the laws of motion and universal gravitation. I will give you the most immediate example, the motion of the Moon around the Earth as perturbed by the Sun: each body is assumed to be rigid, and spherically symmetric so that we can treat each as if all the mass were concentrated in the center. Such a dynamical system has three times three equal nine degrees of freedom, but there are ten constants of motion, i.e. ten different functions of the configuration coordinates and momenta whose values do not change with time. There are the six parameters that determine the motion of the center of mass, the three components of the angular momentum, and the total energy. We are left with four degrees of freedom for the internal motions.

Multiperiodic motion

More than two thousand years of observations of the Moon's motion in the sky, followed by two hundred years of hard work by the best theoretical physicists in the 18-th and 19-th century, had shown the following: The internal motions of a three-body system look like the internal motions of four coupled pendula. There are four fundamental frequencies, call them $\omega_0, \omega_1, \omega_2, \omega_3$, which are characterized by their periods $T=2\pi/\omega$, namely

T_1= tropical month (the time for the Moon to move from equinox to equinox) =27.32158 days;

T_2= anomalistic month (perigee to perigee)=27.55455 days;

T_3= draconitic month (node, i.e. intersection with the ecliptic, to node)=27.21222 days;

measured in mean solar days. The fifth decimal corresponds to 1 second of time, and was correctly known to the Greeks. By combining the tropical month with the period for the Sun returning to the spring equinox,

T_0=tropical year=365.2422 days,

we can figure out the second most familiar period in this system, the average time between new moons which turns out to be 29.53059 days.

The motion of the Moon can be written as a Fourier series in these four frequencies where all the various linear combinations with integer coefficients occur. For this purpose, we define four angles that vary linearly with time, $\chi_i=\omega_i t+\chi_{i0}$

where $i=0, 1, 2, 3$. Then we can write any configuration coordinate or momentum of the system, e.g. the distance r of the Moon from the Earth, as a Fourier series of the following type,

$$r=a\sum_{k_0,k_1,k_2,k_3} C_{k_0,k_1,k_2,k_3}\cos(k_0\chi_0+k_1\chi_1+k_2\chi_2+k_3\chi_3)\,, \tag{1}$$

where k_0, k_1, k_2, k_3 are any integers. Also, we require that the coefficients C_{k_0,k_1,k_2,k_3} be real, and satisfy the relation $C_{k_0,k_1,k_2,k_3}=C_{-k_0,-k_1,-k_2,-k_3}$. A function of this type is called multi-periodic; although its structure is very simple, it raises many questions.

First we have to find the coefficients C. Before Newton's great treatise, the Mathematical Principles of Natural Philosophy, appeared in 1687, the coefficients were obtained from the observations in the sky. The process was a precursor to what we call Fourier analysis of a time series today. The Greeks had already found a term that couples the radial motion, i.e. the angle χ_2, with the angular distance of the Moon from the Sun, i.e. the difference $\chi_1-\chi_0$. Tycho Brahe at the end of the 16-th century found several other coupling terms of this kind; but nobody could explain or predict how big they are, because the laws of motion and universal gravitation were not understood.

Newton was the first to calculate not only the basic frequencies, but also the coefficients C. He was followed by a long and distinguished line of mathematician-astronomer-physicists who invented various procedures for computing the coefficients. All these methods come under the heading of perturbation theory, and resemble very much what we learn in beginning quantum mechanics. The coefficients C are functions of very few small parameters that describe the physical situation and the initial conditions for the Moon in its orbit around the Earth. The most important of these is the ratio $m=T_1/T_0$ which is about 1/13; others are the eccentricity and the inclination of the lunar orbit with respect to the orbit of the Earth around the Sun.

The calculation of the coefficients C occurs in a stepwise fashion: the lowest powers of the parameters and the simplest combinations of frequencies come first, higher powers and more complicated combinations of frequencies are obtained on the basis of the earlier results. It is generally not possible to find the general expression for an arbitrary term, or even to estimate its rate of convergence. At each step we average over some perturbation with a sinusoidal time-dependence; that leads to dividing by the corresponding combination of frequencies. Therefore, whatever method is used, there is always the danger of the small denominators: e.g. in the lunar problem we have the relation,

$$\frac{2\pi}{3\omega_1-2\omega_3-\omega_2}=24331 \text{ days}\,,$$

almost a factor 1000 bigger than the prevailing periods of some 27 days, as you can check from the figures above. It means that all of a sudden, a sixth-order (from $3+2+1=6$) term in the expansion has an unexpected factor 1000.

Laplace thought that nobody would ever be able to calculate the coefficient that goes with this particular small denominator. Deprit and Rom,[1] however, did get the

lowest order approximation for it, with the help of a computer doing the algebra. We have a similar situation in quantum electrodynamics (QED) where the fourth order correction in the fine-structure constant $\alpha = e^2/\hbar c$ was calculated by Kinoshita[2] at Cornell University. By his own account he had to evaluate 891 Feynman diagrams, all of which are complicated many-dimensional integrals that only a machine can do. Laplace was right, no human being is able to carry out the calculation. Ironically, with all these technical refinements we are now back where the Greeks were 2000 years ago: we have the numerical values of the coefficients from perturbation theory, but we do not understand them.

This phenomenon of small denominators pervades all of classical mechanics, as soon as we push any approximation to higher order. Poincaré[3] showed that the expansion in powers of the parameter m in the lunar problem will eventually lead to a divergence of the perturbation procedure. On the other hand, Kolmogoroff tried to find a criterion for guaranteeing that a perturbation expansion in a particular dynamical system converges; the proof for his idea was given by Arnold and Moser in 1963. I will try to explain some simple aspects of the KAM-theorem (for Kolmogoroff-Arnold-Maser, cf. Ref. 4)), because they are basic to our understanding of chaos in classical mechanics, and that in turn is important for the difficulties we face in quantum mechanics. To this end, we have to speak about phase space.

Phase space

The idea of phase space is already found in the two introductory chapters of Newton's Principia. The first chapter is entitled "Definitions", and the Second Definition states in modern English:

The momentum is the product of the mass and the velocity.

It is understood that the velocity is the rate of change with time of the position of a particle, or more generally, of the configuration of the dynamical system. The Second Definition, slightly turned around, states that "the rate of change of the configuration with time has the same direction and equals the momentum divided by the mass". E. g. if the system rotates, the configuration coordinate is an angle, the mass is the moment of inertia, and the momentum is the angular momentum.

The second chapter is entitled "Axioms or Laws of Motion", and the Second Law says, again in modern English:

The rate of change of the momentum with time has the same direction and is proportional to the applied force.

Again the Second Law is quite general, and occurs in many different forms. In the case of the rotating body, the second law of motion becomes: "The rate of change of the angular momentum with time has the same direction and is proportional to the applied torque."

Notice that Newton does not state the Second Law in the form in which most textbooks offer it, namely the infamous "force equals mass times acceleration". Also, Newton is a careful logician: the relation between velocity and momentum is a matter of definition, whereas the relation between the change of momentum and the

force is a profound Law of Nature. Therefore, we can expect the Second Law to remain valid under circumstances that Newton could not even dream about, while the Second Definition may change. E. g. in a semiconductor, the velocity of a conduction electron is related to its momentum by an anisotropic tensor; in a magnetic field, an additive term appears which is the electromagnetic vector-potential; even more esoteric are the corrections that come from special relativity, or the change of mass in a rocket.

The Second Definition and the Second Law have a superficial symmetry: the change in the configuration coordinate depends mostly on the momentum, while the change of momentum depends mostly on the configuration coordinates. Moreover, both relations can be interpreted as first-order ordinary differential equations, where the functions to be found come in natural pairs; each degree of freedom has a configuration coordinate and a conjugate momentum. Therefore, it is best to represent the development of the dynamical system in a space, called phase space, that has twice as many dimension as the number of degrees of freedom.

Equations of motion

This idea then leads to the method that was first suggested by Hamilton, and worked out by Jacobi; it is the basis for both, classical as well as quantum mechanics. The first thing to do is to list the conjugate pairs of configuration coordinates q and momenta p; these are the coordinates in phase space. If we study a single particle in Cartesian coordinates, we will write $q=(x, y, z)$ and $p=(u, v, w)$ or if we use polar coordinates, $q=(r, \theta, \phi)$ and $p=(N, M, L)$.

The second thing we have to do is to write the total energy of the system as a function of these variables, p and q (and the time-variable t), namely the Hamiltonian $H(p, q, t)$. In all the cases that come up at this conference, the Hamiltonian is simply the sum of the kinetic energy and the potential energy. As an example, I will write down the expression in Cartesian coordinates for a particle with mass m_0 and electric charge e, in the presence of an electromagnetic vector-potential $\boldsymbol{A}(x, y, z, t)$ and an electro-static field $V(x, y, z, t)$,

$$H=\frac{1}{2m_0}\left(\left(u-\frac{e}{c}A_x\right)^2+\left(v-\frac{e}{c}A_y\right)^2+\left(w-\frac{e}{c}A_z\right)^2\right)+eV(x, y, z, t)\,. \tag{2}$$

At this point, the physical problem is already fully defined; we have no more choices left: all we have to do now is to apply the standard rules, either of classical mechanics or of quantum mechanics.

If we want to treat the problem in classical mechanics, we write down the Second Definition and the Second Law, which now have become,

$$\frac{d\boldsymbol{q}}{dt}=\frac{\partial H}{\partial \boldsymbol{p}}\,,\quad \frac{d\boldsymbol{p}}{dt}=-\frac{\partial H}{\partial \boldsymbol{q}}\,. \tag{3}$$

These equations define a flow in phase space, because they tell us at every point in which direction and how fast, both for the configuration coordinate q and for the momentum p, the system will move. All the little arrows of direction that are

attached at every point in phase space, can be tied together to form continuous curves that fill out the whole space without ever intersecting one another. But let me warn you: writing down the Hamiltonian H for any problem, and then the corresponding differential equations (3), is nothing! Our real task is either to construct an explicit solution like the multiperiodic function (1), or, if that does not work, to understand at least qualitatively the flow in phase space. Poincaré was the first to tackle this last job.

His results were so unusual that we are still struggling to understand what happens in a system with an arbitrary number of degrees of freedom. Therefore, I will immediately restrict the further discussion to systems with two degrees of freedom. There are many interesting problems that can be reduced in this manner. The anisotropy of the mass-tensor for the conduction electrons in a semiconductor still has rotational symmetry around the direction of large mass; similarly, when we apply a constant magnetic field to an atom, we still maintain circular symmetry around the direction of the field. Every continuous symmetry of this kind has the effect of making the corresponding momentum a constant of the motion, in this case the angular momentum around the symmetry axis. The equations of motion (3) are thereby reduced from three pairs to two coupled pairs and one decoupled pair.

The Hamiltonian for the electron in the neighborhood of the donor impurity with angular momentum 0 around the heavy axis is simply,

$$H(u, v, x, y)=\frac{u^2}{2m_1}+\frac{v^2}{2m_2}-\frac{e^2}{\kappa\sqrt{x^2+y^2}}, \tag{4}$$

where the ratio of the effective masses m_1/m_2 is about 5 for silicon, and the dielectric constant κ is about 11; this system is called the Anisotropic Kepler Problem (AKP). The Hamiltonian for the electron in the hydrogen atom with an external magnetic field B, and an angular momentum 0 around the direction of this magnetic field has an equally simple Hamiltonian,

$$H(u, v, x, y)=\frac{u^2+v^2}{2m_0}-\frac{e^2}{\sqrt{x^2+y^2}}+\frac{e^2B^2}{8m_0^2c^2}y^2, \tag{5}$$

it is called the Diamagnetic Kepler Problem (DKP). In both these examples, the coordinate x is the distance along the axis of rotation, and y is the distance from this axis.

No work is done by outside forces on the electron either in the neighborhood of a donor impurity in a semiconductor, or in the hydrogen atom which is placed in a magnetic field. Therefore, the value of the Hamiltonian does not depend explicitly on the time t; its value remains the same depending on the initial conditions, $H(p, q)=E$. In trying to understand the flow in phase space, we can restrict our attention to one particular energy-shell; the four-dimensional phase-space gets reduced to a three-dimensional submanifold. Now we can try to imagine what the flow looks on the energy-shell; at worst, it is like a bowl of tangled spaghettis.

Invariant tori

At best, however, the system is multiperiodic, with no more than two frequencies, ω_1 and ω_2 for each trajectory. An expression like (1) is valid for any of the coordinates in phase space, always with the same two frequencies. It is not difficult to see that a particular trajectory lies on a two-torus, i.e. a two-dimensional submanifold of the energy-shell with the topology of a torus; such a torus in phase space will be called "invariant torus" henceforth. This idea of an invariant torus in phase space can be generalized immediately: since experience shows that we need only four frequencies in the case of the Moon, we can say that the Moon moves on a four-torus that is embedded in the eight-dimensional phase-space. For reasons that are not at all obvious, Nature has done us a great favor by restricting the Moon-Earth-Sun system to such a four-torus rather than take advantage of the full eight dimensions of phase-space.

The presence of invariant tori in phase space seems to indicate the existence of a hidden constant of motion, whereby the energy-shell gets further broken up into submanifolds of smaller dimension. But Poincaré showed that in the gravitational three-body-problem like the Moon-Earth-Sun, no function that is analytic in the phase-space coordinates as well as in the masses, can be an integral of motion, except the ten obvious ones from the energy-momentum tensor. If there is any constant of motion hidden in the lunar trajectory, it cannot be an analytic function of the phase-space coordinates, but perhaps some terrible, poorly converging expression. Therefore, our efforts to use perturbation theory, i.e. power series expansions, will yield only limited results, but never a complete solution.

No general criterion is known by which one could decide for a particular dynamical system whether its phase space breaks up into invariant tori or not. Poincaré had no practical way of finding out, nor did Kolmogoroff, Arnold, and Moser. They relied on proving or disproving the convergence of the perturbation expansion. But since the late 1950's the astronomers, starting with G. Contopoulos[5] and continuing with C. Heiles and M. Hénon,[6] have used an idea of Poincaré in conjunction with modern computers. They tried to understand the trajectories of stars in the average gravitational field of a galaxy. The presence or absence of a "third integral" in addition to the energy and the angular momentum around the axis of the galaxy changes the distribution of stellar velocities in the neighborhood of the solar system.

Surface of section

Poincaré obviously found it difficult to visualize the three-dimensional content of a bowl of noodles. Therefore, he proposed to make a two-dimensional cut in such a way that no noodle is tangent to this "surface of section" Σ. In order to describe the surface of section Σ we can now choose internal coordinates (p_2, q_2) that form a conjugate pair of momentum and position, while the energy $E=p_1$ and the time $t=q_1$ form the other conjugate pair in a system with two degrees of freedom.

Any pair $(p_{2,0}, q_{2,0})$ serves as the initial condition for a trajectory to start at time

$t=0$ in Σ. This trajectory will eventually intersect Σ again in a point $(p_{2,1}, q_{2,1})$ at the time t_1, always at the fixed energy E, of course. This process can be carried out very efficiently on a computer by the numerical integration of the equations of motion (3). Also we can continue to integrate beyond the time t_1 to the second intersection with Σ in $(p_{2,2}, q_{2,2})$ at the time t_2, and so on. With equal ease, we can go backwards to $(p_{2,-1}, q_{2,-1})$ at time to t_{-1}, with the preceding intersection in $(p_{2,-2}, q_{2,-2})$ at time t_{-2}, etc.

A simple consequence of Liouville's theorem is the fact that the map of Σ into itself, from $(p_{2,0}, q_{2,0})$ to $(p_{2,1}, q_{2,1})$, preserves the element of area $d\Sigma=dp_2dq_2$. This preservation of the area in the surface of section is essentially equivalent with the combination of Newton's Second Definition and Second Law of Motion. Therefore, many mathematicians restrict themselves to the study of these area-preserving maps, as a valid substitute for Poincaré's original map of Σ.

The basic character of this map can be presented very vividly in multicolored splendor with the help of modern computer technology. In the (p_2, q_2)-plane, the consecutive points of intersection of a particular trajectory with the surface of section Σ, ..., $(p_{2,-2}, q_{2,-2})$, $(p_{2,-1}, q_{2,-1})$, $(p_{2,0}, q_{2,0})$, $(p_{2,1}, q_{2,1})$ $(p_{2,2}, q_{2,2})$, ..., are plotted in the same color. Even a casual look at the plot shows immediately whether these points lie on a smooth curve or whether they scatter so badly that no sensible smooth curve can be drawn through them. These two possibilities seem to mingle in a very intimate, fractal manner.

If there exist as many constants of motion as degrees of freedom, e.g. an angular momentum in addition to the energy in our system with two degrees of freedom, then Σ gets completely covered with smooth curves. The multiperiodic expansion (1) becomes a valid solution of the equations of motion; the smooth curves in Σ are the intersections of the corresponding invariant tori with Σ. Each invariant torus is characterized by the two frequencies ω_1 and ω_2. The ratio of the two frequencies varies continuously from one invariant torus to a neighboring one.

As soon as we introduce a perturbation, however, some of these smooth curves in Σ and their corresponding invariant tori are destroyed. The origin for this destruction is the phase-locking mechanism: wherever the two frequencies ω_1 and ω_2 of a particular two-torus are resonant, i.e. the ratio ω_1/ω_2 is a simple rational number, the perturbation will cause a whole open neighborhood in phase space to force its two frequencies into the same rational relation. The most striking case of phase-lock is the rotation of the Moon which is tightly coupled to her motion around the Earth so that we always see the same side of the Moon.

Classical chaos

The extent of any particular phase-lock in phase space depends on the type and strength of the perturbation, as well as on how close any frequency-ratio is to being rational. Kolmogoroff, Arnold, and Moser showed that the loss of invariant tori is a process that depends smoothly on the strength of the perturbation. Such a loss can be limited to small regions in phase space that are too small to be noticed in any practical calculation, or a fortiori in any measurement.

On the other hand, the calculations for the simple Hamiltonian (4) show that for

a mass-ratio larger than 2, no invariant tori are left in phase space.[7] The progressive destruction of invariant tori in the Hamiltonian (5), as the magnetic field B is raised, can be seen quite clearly from the multicolored plots. I like to call "hard chaos" this condition of the phase space in (4); there is nothing left over from the description of a dynamical system that we were taught in our courses, and that most of us probably keep on teaching. On the other hand, the phase space for (5) looks like an intimate mixture of invariant tori and chaotic regions; I like to call this latter condition "soft chaos".

Hard chaos is the opposite extreme to what you might call "regular behavior", that is the condition where all of phase space is covered with invariant tori. I am convinced that most dynamical systems live in the intermediate condition of "soft chaos" which is a mixture of regular behavior and hard chaos; but our ability to describe such systems effectively is still very poor. The KAM-theorem shows that regular systems are not generic; their structure can be destroyed by an arbitrarily small perturbation. Hard chaos, on the other hand, is generic; it is stable against sufficiently small perturbations. Therefore, it should receive priority in our research compared to regular behavior; meanwhile we must work to understand soft chaos better than we do now.

Without going into details, I want to mention that the phase space for a system with hard chaos has also a very characteristic structure. There are two foliations, i.e. two families of smooth two-dimensional submanifolds where each family covers the entire phase space. Each leaf from one family intersects the leaves from the other family in a transverse manner; obviously, the intersection of two leaves belonging to different families is a submanifold of dimension one: it is a particular trajectory, i.e. a solution of the equations of motion (3). Moreover, each trajectory can be uniquely characterized by a code, e.g. an infinite string of binaries whose interpretation is quite closely related to the appearance of the trajectory. E.g. in the Anisotropic Kepler Problem (AKP), each binary simply records the sign of the consecutive intersections of the trajectory with the x-axis.

Many physicists are surprised to find that the trajectories in such a simple dynamical system as the AKP should be in a one-to-one relationship with infinite sequences of 0's and 1's. The AKP seems to be closer to tossing a coin than to a regular machine which repeats ad infinitum what it did in the past. The two leaves whose intersection defines the trajectory are called the stable and the unstable leaf, because they play special roles. If instead of starting at the point $(p_{2,0}, q_{2,0})$ of Σ we choose a nearby initial condition (p'_2, q'_2), this neighboring trajectory will drift away exponentially from the original one while approaching the unstable leaf. If we follow these two trajectories back into their past, the neighboring one again drifts away exponentially from the original one, but it does so by approaching the stable leaf. Every trajectory in hard chaos is exponentially unstable in this manner.

Periodic orbits

The existence of a stable and an unstable leaf whose intersection defines a trajectory becomes very striking when we look at a trajectory that closes itself

smoothly in phase space. Such a solution of the equations of motion (3) appears in phase space as a simply closed loop; it is called a periodic orbit. If its initial condition in Σ is $(p_{2,0}, q_{2,0})$, then for some positive integer n we have $(p_{2,n}, q_{2,n})=(p_{2,0}, q_{2,0})$. Of course, the same equality also holds for the intersections $2n, 3n, \ldots$, as well as for $-n, -2n, -3n, \ldots$. The periodic orbit is a fix-point for some power of the Poincaré map of Σ into itself.

Again it comes as a surprise to many physicists that a system with hard chaos has many periodic orbits. In the case of the AKP a periodic orbit defines a binary sequence that repeats itself, and vice versa a repeating binary sequence defines a periodic orbit. That leads essentially to 2^n periodic orbits of length n, i.e., which close smoothly after n intersections with the surface of section Σ. In a regular system only those trajectories are periodic whose frequency ratio is a rational number. Therefore, the total number of PO's in regular systems grows only as a power of their period, i.e. their time for smooth closure, whereas in chaotic system their number grows exponentially with their period.

Poincaré[8] felt that the periodic orbits in any dynamical system contained the secret for understanding the system. He said in the third chapter of his great treatise, "The New Methods of Celestial Mechanics":

"What makes these periodic solutions so valuable, is that they offer, in a manner of speaking, the only opening through which we might try to penetrate the fortress which has the reputation of being impregnable."

He died in the same year 1913 when N. Bohr succeeded in explaining the spectrum of the hydrogen atom on the basis of classical mechanics by restricting the values of the angular momentum to multiples of $\hbar$. Four years later, Einstein[9] gave a more general interpretation to Bohr's "quantization rules". Nobody appreciated Einstein's paper until 40 years later, and even then it took another ten years for physicists to read the last paragraph where Einstein quotes Poincaré.

Semi-classical quantum-mechanics

Einstein first discusses the example of a particle moving in a circularly symmetric potential, and he finds that it moves on an invariant torus in phase space. Then he explains that all the various schemes for quantizing a dynamical system are based on the assumption that the phase space is foliated into invariant tori, and the rule for finding the energy levels is the following: On each torus define two topologically independent contours, C_1 and C_2, and calculate in any canonical coordinate-system the contour integrals over $p_1dq_1+p_2dq_2$; then find the energies where both contour integrals are integer multiples of Planck's quantum,

$$\int_{C_1} \boldsymbol{p}d\boldsymbol{q}=2n_1\pi\hbar\,, \qquad \int_{C_2} \boldsymbol{p}d\boldsymbol{q}=2n_2\pi\hbar\,. \tag{6}$$

Until after his death in 1955, Einstein was still the only physicist who knew anything about invariant tori.

But he also realized that they were the exception among systems in classical

mechanics, and he quotes Poincaré in the last paragraph of his paper of 1917 to claim that his own quantization scheme was of no use in three-body problems. He had no suggestion about how to quantize those systems where no invariant tori were available to do the job. Some efforts were made to tackle such problems, in particular the spectrum of the helium atom which was the obvious candidate after the hydrogen atom had been explained. But without understanding the classical behavior of the three-body-problem, there was no chance of making any progress.

Finally in 1925/26 Heisenberg and Schrödinger were able to formulate the correct version of quantum mechanics. It is important to appreciate what happened in less than twelve months, after the best people in the field had tried for about 25 years. At the same time, we have to realize that quantum mechanics has undergone nothing more than purely technical improvements and some rather straightforward generalizations. Nevertheless, the success of the original idea has been overwhelming; no experiment has been found to contradict quantum mechanics.

Its fundamental recipe is extremely simple. First, we have to write down a Hamiltonian, $H(u, v, x, y)$, exactly the same as in classical mechanics, such as (4) for the AKP and (5) for the DKP, as long as the electronic spin is disregarded. (Of course, the inclusion of the spin is very significant, but it is no more than a technical matter.) Then, we reinterpret the definition of the energy, $E=H(u, v, x, y)$ in terms of operators in a Hilbert space, by making the following assignments,

$$E \to i\hbar\frac{\partial}{\partial t}, \quad u \to -i\hbar\frac{\partial}{\partial x}, \quad v \to -i\hbar\frac{\partial}{\partial y}. \tag{7}$$

That leads to the time-dependent Schroedinger-equation for the wave function $\psi(x, y, t)$, e.g. for the AKP,

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m_1}\frac{\partial^2\psi}{\partial x^2}-\frac{\hbar^2}{2m_2}\frac{\partial^2\psi}{\partial y^2}-\frac{e^2}{\kappa\sqrt{x^2+y^2}}\psi. \tag{8}$$

Finally, we need a few rules to establish the relations between the mathematics and the experimental measurements.

Let me emphasize what I said before: These three initial steps in solving a particular problem like the AKP or the DKP are nothing! Nor is the further step that may be necessary occasionally when the Hamiltonian has some obvious symmetries, such as rotations or the interchange of identical particles. We can all learn how to reduce the Hamiltonian accordingly, and should get no credit for doing it correctly. We are then left with trying to understand the dynamics of special problems like the AKP, DKP, or the helium atom, not to mention QED or QCD where we are still groping in the dark.

Right at the beginning of modern quantum mechanics, Brillouin, Kramers, and Wentzel found a simple method for writing approximate solutions of Schroedinger's equation like (8) with the help of classical trajectories. It is important to realize that the WKB-method works only for systems with one degree of freedom, or systems that have as many constants of motion as degrees of freedom, and where the variables can be separated. Keller[10] was the first to point out the connection between WKB and the existence of invariant tori in phase space, as well as Einstein's quantization rules

(6). Starting with VanVleck,[11] however, there were some isolated efforts to solve Schroedinger's equation on the basis of classical trajectories, without worrying about their dynamical nature. But the mathematical results were always limited to short times, and were obtained without any awareness of classical chaos.

Until less than 25 years ago, nobody took up Einstein's challenge, as formulated in the last paragraph of his 1917 paper: find the quantum-mechanical energy-spectrum on the basis of classical mechanics, even when there are no invariant tori. The solution lies in a method that I started studying in 1967,[12] and that led to a very general result[13] which is now known as the trace formula. Its derivation is technically involved, and will not be given in this paper; for a general account cf. Ref. 14). In order to convey some idea about its origin, however, we will discuss a related topic that is more general, and a little easier to present to a non-expert audience.

Riding with the quantum wave on a classical trajectory

The propagator $K(q, t; q', t')$ is the probability amplitude for a system to start in the configuration q' at time t', and be found in the configuration q at the time t. It is a special solution of Schroedinger's equation that vanishes for times $t<t'$, and therefore requires a special δ-function excitation on the right-hand side,

$$\left(i\hbar\frac{\partial}{\partial t}-H(-i\hbar\partial/\partial q, q, t)\right)K(q, t; q', t')=\delta(q-q')\delta(t-t')\,. \tag{9}$$

If we can calculate the propagator for a particular dynamical system, we are able to find the quantitative answer to any problem, e.g., we get the response to some weak, external electro-magnetic pulse if we know the state of the system at time t'.

Such a process can be viewed in an almost purely classical picture: The system moves from the configuration q' at time t' along a classical trajectory to the configuration q at the time t, and carries with it the VanVleck probability-amplitude,

$$K_c(q, t; q', t')=(2\pi i\hbar)^{-n/2}\sqrt{|\partial^2 R/\partial q\partial q'|}\exp[(i/\hbar)R(q, t; q', t')-i\phi]\,. \tag{10}$$

The crucial ingredient into this expression is the action, also called Hamilton's principal function, because he was the first to use it,

$$R(q, t; q', t')=\int_{t'}^{t}(\boldsymbol{p}d\boldsymbol{q}-H(\boldsymbol{p}, \boldsymbol{q}, t)dt)\,, \tag{11}$$

which is also the integral over the Lagrangian along the classical trajectory from q' at t' to q at t. We have assumed n degrees of freedom; the vertical bars under the square-root sign in (10) imply the n by n determinant for the matrix of mixed derivatives. Finally, the angle ϕ in (10) is a special phase that has to do with the caustics along the trajectory: a fan of trajectories all of which start in q' at time t', going off in slightly different directions, may collapse at certain later times; it is as if there was a wall from which the system is reflected, and looses the phase $\pi/2$ every time that happens. At the same time the determinant of mixed derivatives becomes infinite and changes sign, so that the classical propagator (10) is certainly not a good approximation to the propagator K.

VanVleck's amplitude has a simple interpretation. The determinant under the square-root, including the normalization by $(2\pi\hbar)^n$, is a probability measure,

$$P_c(q, t; q', t') = (2\pi\hbar)^{-n} |\partial^2 R/\partial q \partial q'| . \tag{12}$$

It tells us the likelihood for the classical system to start in a small volume $d^n q'$ near q' at time t', and arrive in the small volume $d^n q$ near q at time t. The quantum-mechanical probability-amplitude has an absolute value equal to the square-root of the classical probability, and a phase angle equal to Hamilton's principal function. Even the phase loss coming from the caustics along the way is obtained from a more detailed investigation of classical trajectories.

We have to ask ourselves how the VanVleck's amplitude (10) compares with the quantum-mechanical propagator $K(q, t; q', t')$ which is a solution of (9). If we consider for simplicity's sake a conservative system where the time does not appear explicitly in the Hamiltonian, as in the AKP or the DKP, the propagator depends only on the time-difference, $t-t'$; equivalently, we can set $t'=0$ without loss of generality. If $t>0$ is very small, there is only a finite number of classical trajectories from q' to q, unless the potential energy increases very steeply. As the t increases, there are more and more different trajectories; each of them passes a number of caustics before reaching q, and the phase-angle in (10) has to be adjusted accordingly. We shall assume that the propagator becomes approximately the sum over the individual contributions (10) from each classical trajectory.

The information contained in this sum over classical trajectories is, therefore, analyzed as if it was similar to the exact formula for $t>0$,

$$K(q, t; q', 0) = \sum_j \psi_j(q) \psi_j^x(q') e^{-iE_j t/\hbar} , \tag{13}$$

where $\psi_j(q)$ is the eigenfunction belonging to the eigenvalue E_j of the Hamiltonian. The right-hand side is a Fourier expansion in time that yields a set of frequencies $\omega_j = E_j/\hbar$ with the Fourier coefficients given by the product of the eigenfunctions $\psi_j(q)\psi_j^x(q')$. Does the sum over the VanVleck amplitudes (10) as a function of t have such a structure, when it is Fourier analyzed?

Trace formulas

Rather than to answer this general question, we try a simpler, preliminary test which might also be more directly related to a measurement. As an example, take an experiment where the dipole-moment D_{op} is obtained as a function of time, so that we would like to know the function,

$$\sum_j (j|D_{\text{op}}|j) e^{-iE_j t/\hbar} = \sum_j D_j e^{-i\omega_j t} = \int d^n q [D_{\text{op}} K(q, t; q', 0)]_{q=q'} . \tag{14}$$

Notice that we are really calculating the trace of the operator product $D_{\text{op}}K$. The last expression in (14) is an integral over configuration space that we can try to evaluate even when the propagator $K(q, t; q', 0)$ is replaced by its classical approximation, i.e., the sum over the VanVleck amplitudes (10).

Let us consider what happens when we calculate the trace of (10) in the special

case where D_{op} is the identity. We have to find a classical trajectory that goes from the initial configuration q' to the final configuration q in the given time t, except that the two configurations are now the same, i.e., $q'=q$. Such a trajectory forms a loop in configuration space, but the initial momentum p' is generally different from the final momentum p, i.e. the initial and the final directions of motion are different. Such loop-trajectories in configuration space are not hard to find; moreover, the configuration $q'=q$ can be moved continuously while keeping the time t fixed and deforming the closed loop-trajectory accordingly. The energy E of the loop-trajectory changes continuously in this process; the explicit calculation may not be easy.

The expression (10) is good only in the classical limit where $\hbar$ is small compared to the integral (11). As we change the initial-final configuration $q'=q$ in order to do the integration in the trace (14), the value of the integral (11) varies. The exponent in (10) changes rapidly, while the determinantal factor varies slowly. Therefore, we can apply the method of steepest descent, i.e., the main contribution to the integral over $q'=q$ comes from the configuration space where the action integral (11) over the loop-trajectory is stationary with respect to the variation of $q'=q$. The standard argument from classical mechanics shows that the initial momentum $p'=p$, the final momentum, i.e., only those loop-trajectories matter that close smoothly, the periodic orbits.

The quantum-mechanical trace (14) is thereby approximated by

$$\sum_{\text{periodic orbits}} A_{po}\exp\left[\frac{i}{\hbar}\int_{po}(\boldsymbol{p}d\boldsymbol{q}-Hdt)-\nu\pi/2\right], \tag{15}$$

where ν counts the caustics along the periodic orbit. The amplitude A_{po} depends not only on the operator D_{op}, but very importantly on the character of the periodic orbit. As a general rule, the less stable the orbit, the smaller the amplitude A_{po}. Since a classically chaotic system has many periodic orbits, one might have hoped that the amplitude A_{po} guarantees the convergence of the sum over periodic orbits in (15). But that does not happen; the convergence of (15) is conditional, and depends crucially on the cancellation due to the phase-factor.

The sum over the VanVleck amplitudes, or in particular, the trace formula in one or the other of its different versions, does provide some of the essential features of quantum mechanics, in spite of its purely classical origin. The sum of the classical probabilities for the different classical trajectories converges absolutely, whereas the sum over the VanVleck amplitudes depends critically on the phase relations as expressed in the action integral occurring in the phase factor. I am convinced that with the proper skill we will be able to extract most of the qualitative information about quantum dynamics, including its chaotic features, from simple expressions of this kind.

What is quantum chaos ?

The contrast between classical and quantum mechanics shows up in this context in a way that is directly related to the issue of chaos. If we ask for the probability

that certain events occur in a classical problem, e.g., getting from the source to the detector in a scattering experiment, we have to add up the classical probabilities (12). The resulting sum is generally convergent, although individual terms may have strong singularities, and appear as well as disappear rather unexpectedly. Such singularities with a fractal structure become especially noteworthy when we study the events as a function of the energy E rather than of the time t, as we have done sofar. For an experimentalist, this erratic behavior is quite unphysical, and shows that some fine details in classical mechanics cannot be real.

The semiclassical expression (15) however does not have this chaotic character; it will tend to smooth over the rough spots, particularly when viewed as a function of the energy E. What happens now, however, is a more subtle expression of chaos, that we can study with the help of an expression like the center term in (14), or (15), with the proper modifications if we want to talk about, e.g., the scattering amplitude as a function of the wave vector. We now have a function,

$$f(t)=\sum_j a_j e^{-i\lambda_j t}\,, \quad \sum_j |a_j|^2<\infty\,, \tag{16}$$

where the coefficients a_j are complex; the frequencies λ_j are real, and ordered according as their absolute value. (The sum over j may represent either a sum over quantum-mechanical energy-levels, or a sum over classically periodic orbits.) Such a sum is reminiscent of the Fourier expansion (1) for the coordinates of a multiply periodic classical system like the Moon-Earth-Sun. But there is a profound difference: the set of frequencies λ_j is infinite and linearly independent, i.e., there exists no finite set of frequencies ω_l such that every λ_j becomes a linear combination of the ω's with integer coefficients.

Almost periodic functions

Such functions were first studied by H. Bohr, the younger brother of Niels, at about the same time as his older brother explained the spectrum of the hydrogen atom. Unfortunately, Harald called these functions "almost periodic", by which is meant that they repeat themselves with a certain precision ε provided one shifts the independent variable t far enough, from t to $t+\tau(\varepsilon)$. The technical definition of almost periodic is a little more complicated, but there is a very readable explanation[15] in a small book by H. Bohr himself that was translated into English after WWII:

Given $\varepsilon>0$, there exists a length $L(\varepsilon)$ such that every interval $(a, a+L)$ contains a translation number $\tau(\varepsilon)$ such that $|f(t+\tau)-f(t)|\leq\varepsilon$.

Can such functions be represented in the form (16) ? Before answering, we need the definition of what Bohr called a "trigonometric polynomial", $s(t)$. It is a finite sum over trigonometric functions with arbitrary frequencies and amplitudes,

$$s(t)=\sum_{n=1}^{N} a_n e^{i\mu_n t}\,, \tag{17}$$

where again the coefficients a_n are arbitrary complex, and the freqencies μ_n are real. Such trigonometric polynomials form a linear space, whose closure we call $A\{s(t)\}$.

In both definitions, almost periodic function as well as trigonometric polynomial, the measure of the difference between two functions or, equivalently, the limit for defining the closure, has to be specified. There are two main possibilities: Bohr originally assumed uniform pointwise convergence, whereas later on Besicovitch and Bohr remade the theory by adopting convergence in the L^2-norm. In either case, one gets the main theorem:

A function $f(t)$ is almost periodic if and only if it belongs to the closure $A\{s(t)\}$ of trigonometric polynomials.

A function like (16) is, therefore, almost periodic in the later sense; I would like to give it the name "almost periodic B^2", to remind everybody of the two names, Bohr and Besicovitch, as well as the L^2-norm of the required limit.

These functions at first look like a straightforward generalization of the multiply periodic functions (1) that appear in classical mechanics when there are invariant tori in phase space. But there is an example (cf. Ref. 16)) of an almost periodic function that not only reproduces itself with any required precision, but also approximates locally any arbitrary smooth function, i.e., a function with a convergent power-series expansion. Bohr's idea of Almost-Periodicity does not convey what actually happens; such functions are wild in spite of having a discrete and enumerable spectrum; they manage to imitate, at least locally, any smooth behavior, like a good actor who can play any character and convince any audience.

The theory of almost-periodic B^2-functions is very difficult because the linear space of trigonometric polynomials is not separable, i.e., it does not have a denumerable base like a good Hilbert-space. Such functions appear even in the simplest quantum-mechanical expectation-values (traces) as functions of the time or the energy whenever their classical equivalent is chaotic. Therefore, I want to propose them as the most obvious expression of chaos in quantum mechanics, the quantum-mechanical equivalent of the fractal structure of classical phase space, a partial answer to the question that forms the title of this conference.

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