COMPARISON BETWEEN CLASSICAL AND QUANTUM DYNAMICAL CHAOS

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Abstract

Quantum mechanical constants of motion which have no classical analogue are the source of discrepancy between the onset of chaos in classical and quantum dynamical systems. This difference can be measured by using objective criterions such as the classical and quantum Kolmogorov entropy. This difference is found to the lowest order in h.

1. INTRODUCTION

Recent advances in the theory of classical dynamics, particularly those concerning the onset of chaos in Hamiltonian systems (1-8), have stimulated two very different approaches to understanding the correspondence of quantum mechanics. One category of studies is concerned with the general relationship between classical and quantum mechanics (9-12) the nature of the transition between them, and with the development of convenient and accurate algorithms for so called semiclassical quantization. The second category of studies is related to attempts to improve understanding of intermolecular dynamics, in particular the relative rates of vibrational relaxation, isomerization, dissociation. In this second category the onset of chaos is often used to give theoretical justification for the use of statistical theories in intermolecular phenomena. It is usually assumed that the onset of chaos in the classical mechanical model, signals the onset of rapid intermolecular energy transfer in the corresponding quantum mechanical model. In turn this assumption presupposes that dynamical chaos in classical and quantum mechanical models of the same system, occur under nearly the same conditions, e.g. the nature of excitation and energy are similar, and that the existence of chaos in classical mechanics systems implies the existence of chaos in the corresponding quantum mechanical system (13-18). This study on the other hand argues that the onset of chaos in classical and quantum mechanics is different and that interference effects inherent to quantum dynamics, render it different from classical dynamics. Indeed when a common quantitative measure of chaos is

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J. Jortner and B. Pullman (eds.), Intramolecular Dynamics, 107–113.

employed, namely the Kolmogorov entropy (5,6,7,8,20) it is found that a bound quantum mechanical system cannot exhibit chaos even when the corresponding classical system does. This implies that dynamical predictions derived from classical mechanics must be interpreted with considerable care. In the proceeding sections explicit examples are presented where interference effects in quantum mechanics produce new constants of motion with no classical analogue. These new constants of motion restrict the quantum motion causing it to be non chaotic.

2. THE STANDARD MAPPING

When investigating chaotic dynamics, it is found that dynamical discrete mappings exhibit chaotic behavior and that explicit formulas for the Kolmogorov entropy can be obtained.

Chirikov and coworkers (22-24), have studied the classical and quantum dynamics associated with the abstract "standard mapping" defined by

$$\begin{aligned} \bar{P} &\equiv P + K\sin X \\ \bar{X} &\equiv X + \bar{P} = X + P + K\sin X \end{aligned} \qquad (1)$$

For this mapping there is a critical value of K for which the motion becomes chaotic. Numerical investigations find this value to be K = 0.989. This abstract mapping (5) is equivalent to that defined by the classical Hamiltonian

$$\begin{aligned} H &= \frac{P_\theta^2}{2m\ell^2} - m\ell^2\omega_o^2\cos\theta\,\delta_T(t/T) \\ \delta_T(t/T) &= \sum_{n=-\infty}^{\infty} \cos(2\pi t/T) \end{aligned} \qquad (2)$$

which describes a pendulum of fundamental frequency $\omega_o = (g/\ell)^{1/2}$ subject to periodic "kicks" with period T. The classical equation of motion now reads

$$\begin{aligned} \dot{P}_\theta &= -m\ell^2\omega_o^2\sin\theta\,\delta_T(t/T) \\ \dot{\theta} &= \dot{P}_\theta/m\ell^2 \end{aligned} \qquad (3)$$

Let θ_n and $P_{\theta n}$ be the values of θ and P_θ just before the n'th "kick". Integration of the equation of motion for time T gives

$$\begin{aligned} (P_\theta)_{n+1} &= (P_\theta)_n - m\ell^2\omega_o^2 T\sin\theta_n \\ \theta_{n+1} &= \theta_n + P_{n+1} = \theta_n + P_n - K\sin\theta_n \end{aligned} \qquad (4)$$

with the definition $P_n = P_\theta T/m\ell^2$, $K = \omega_0^2 T^2$, equations (4) reduce to the standard mapping form:

$$(P_\theta)_{n+1} = (P_\theta)_n - K\sin\theta_n$$
$$\theta_{n+1} = \theta_n + P_{n+1} = \theta_n + P_n - K\sin\theta_n \qquad (5)$$

In the limit $T \to 0$ for which the time between "kicks" vanishes the evolution is regular. As T increases away from zero the motion increasingly deviates from that of a pendulum Hamiltonian. For $0<K<1$ the momentum variation is bounded with $|\Delta P| = K^{1/2}$, and the motion is confined to simple invariant curves. For $K>1$ the simple invariant curves disappear and most mapping curves become chaotic point sets. For large K the classical motion becomes diffusion like with $<P^2> = (K^2/2)t$. For this model the Kolmogorov entropy can be calculated (24) and for $K >> 1$ is $h = \ell nK$, which is positive.

The quantum mechanical analogue motion of the same Hamiltonian, is strikingly different. Numerical integration of the equation of motion reveals no transition to chaos when K exceeds one (22-23). Moreover, for certain choice of parameters, the motion becomes periodic. The profound difference between the classical and quantum motion can be explained by the introduction of new quantum mechanical constants of motion which have no classical analogue. The first of these constants is the modulus momentum operator

$$\hat{C}_1 = \exp\{ih^{-1}\alpha\hat{P}\} \qquad (6)$$

where α is a constant to be defined later. To check whether $\hat{C}_1$ is a constant of motion one has to prove

$$[\hat{C}_1, \hat{H}] = 0 \qquad (7)$$

Calculating the commutation relation of $\hat{C}_1$ with any periodic potential where period is $2\pi\beta$

$$[\ell^{ih^{-1}\hat{P}}, \sum_{k=-\infty}^{\infty} A(k)\ell^{ikX/\beta}] = \sum_{k=-\omega}^{\infty} A_k[\ell^{ih^{-1}\alpha\hat{P}}, \ell^{ik\hat{X}/\beta}] \qquad (8)$$

One finds using the identity $\ell^A\ell^B = \ell^B\ell^A\ell^{-[A,B]}$. For each Fourier component

$$[\ell^{ih^{-1}\alpha\hat{P}}, \ell^{ik\hat{X}/\beta}] = 1 - \ell^{i2\pi\alpha/\beta} \qquad (9)$$

This proves that C is a constant of motion if $\alpha = \beta$. It can be noted that $\hat{C}_1$ is not Hermitian, which means that there is no direct observable that we can associate with it. Moreover when $h \to 0$ or where the correspondence to classical mechanics should be, the operator $\hat{C}_1$ loses its meaning.

Another quantum mechanical constant of motion is the modulus energy

$$\hat{C}_2 = \exp\{ih^{-1}T\hat{H}\} \tag{10}$$

which is a time dependent constant of motion. To prove that this operator is a constant of motion one can use the formalism of Pfeifer and Levine (25) which defines an extended time dependent Hilbert space. In this space the energy operator is defined by

$$\hat{H} = i\frac{\partial}{\partial\tau} \tag{11}$$

Using the commutation relation with the time operator and taking into account that the potential is periodic in time the proof that the modulus energy is a constant of motion is a repetition of equations (7),(8) and (9).

These two constants of motion severely restrict the quantum evolution. Combined together these two constants of motion serve as selection rules which give

$$\frac{1}{2m\ell^2}(m_1P_o+(P_\theta)_n)^2 = m_2E_o+E_n \tag{12}$$

where m_1 and m_2 are integers and E_o and P_o are the initial energy and momentum. The meaning of the selection rule is that the dynamics is periodic or quasiperiodic, depending on the periodicity match of the time and space. A periodic solution is possible whenever the periods of momentum and energy match

$$T = \frac{m\ell^2}{h}2\pi n \tag{13}$$

when n is an integer.

Otherwise a quasiperiodic solution is obtained where the amplitude of the wavepacket is concentrated around the integers which are restricted by the selective rule. Because there is no exact match the amplitude grows to higher and higher values of energy. Eventually the system will obtain infinite energy.

To conclude this comparison the quantum dynamical evolution is quasiperiodic restricted by non classical constants of motion. As a consequence the quantum evolution has zero Kolmogorov entropy in contrast to the classical system.

3. THE LINEAR MAP

After considering the previous "standard map" for which the quantum evolution was regular, one asks under what conditions does a quantum map become chaotic. The linear map supplies an example where some kind of quantum chaos does exist, and there is a close correspondence between the quantum and classical map. This mapping is defined by

$$
\begin{aligned}
q_{n+1} &= q_n + \frac{P_n}{\mu}T \\
P_{n+1} &= P_n - TV'(q_{n+1})
\end{aligned}
\tag{14}
$$

Now if $V(q) = \frac{1}{2}\omega^2 q^2$, one obtains the linear map $X_{n+1} = MX_n$

$$
M = \begin{pmatrix} 1 & T/\mu \\ -\mu\omega^2 T & 1-\omega^2 T \end{pmatrix}
\tag{15}
$$

As can be expected for linear systems, the quantum and classical maps are similar where the main difference is that P and q are operators in the quantum version. In order to integrate the equations of motion the eigenoperators and eigenvalues of M are calculated,

$$
M\hat{I}_{12} = \lambda_{12}\hat{I}_{12}
$$

$$
\hat{I}_{12} = \hat{q} + \beta_{12}\hat{P}
$$

where (16)

$$
\lambda_{12} = 1 - \frac{1}{2}\omega^2 T^2 \pm i\omega T\left(1 - \frac{1}{4}\omega^2 T^2\right)^{1/2}
$$

and

$$
\beta_{12} = \pm i/\mu\omega\left(1 - \frac{1}{4}\omega^2 T^2\right)^{1/2}
$$

Because the map is area preserving $\lambda_1 \cdot \lambda_2 = 1$ and the operator $\hat{N} = \hat{I}_1\hat{I}_2$ is therefore an invariant of motion, representing the area preserving property. Writing $\hat{N}$ explicitly one finds

$$
\hat{N} = P^2 + \omega'^2 q^2
$$

where (17)

$$
\omega' = \frac{\mu^2\omega^2}{\left(1-\frac{1}{4}\omega^2 T^2\right)^{1/2}}
$$

The motion is periodic for real ω' and becomes chaotic quantum mechanically and classically when ω becomes imaginary and the spectrum of $\hat{N}$ becomes continuous.

The dynamics of the map can be analysed by examining the operators $\hat{I}_1$ and $\hat{I}_2$

$$\hat{I}_{1n} = \hat{I}_{10}\lambda_1^n$$
$$\hat{I}_{2n} = \hat{I}_{20}\lambda_2^n \qquad (18)$$

One finds that the motion is expanding in $\hat{I}_1$ and contracting in $\hat{I}_2$. Classically the measure of the degree of stochasticity is obtained from the rate by which neighbouring trajectories diverge, which is in this case λ_1. In order to define the Kolmogorov entropy one has to define a compact space. This is usually done by implying periodic boundary conditions on phase space with the result of

$$h = \ell n\lambda_1 \qquad (19)$$

Considering the quantum mapping implying periodic boundary conditions will completely change the dynamics to a regular type. This is an example of how the non local character of quantum mechanics influences the onset of chaos.

Seeking a quantum measure of stochasticity for the non compact system consider an initial Gaussian density operator which is diagonal in the $\hat{I}_1$ representation

$$\hat{P} = \exp\{\bar{X}(\hat{I}_1-\alpha)^2 + \gamma\} \qquad (20)$$

The entropy associated with the measurement of the operator $\hat{I}_1$ is now considered as a measure of stochasticity

$$S(\hat{I}_{1n}) = n\ell n\lambda_1 + \frac{1}{2}\ell n 2\pi e\bar{X}_o \qquad (21)$$

As can be seen this entropy is linear in the time step. Now the measure of stochasticity is defined as the entropy increase per time step, which for this mapping is:

$$h(\hat{I}_1) = \ell n\lambda_1 \qquad (22)$$

which is identical to the classical Kolmogorov entropy and that has a few of the properties of the Kolmogorov entropy.

To conclude this work the differences and similarities between classical and quantum systems were examined for model systems. The significance of these models is similar to the Hopff model of motion on a surface with negative curvature everywhere, which serves a model in which to compare real dynamical systems. It seems that a wavepacket has to spread exponentially in order to reach the onset of quantum chaos.

ACKNOWLEDGMENT

Work supported by the Bat-Sheva Foundation. The Fritz Haber Research Center is supported by the Minerva Gesellschaft für die Forschung, mbH, München, BRD.

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