QUANTUM CHAOS, CLASSICAL RANDOMNESS, AND BOHMIAN MECHANICS

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Abstract. It is argued that dynamical chaos in quantum mechanics arises solely from the collapse rule applied in measurements. As such it is quite distinct from classical (deterministic) chaos, which arises from the dynamical law itself. It is shown, however, that if the particles of a quantum system are regarded as "real," i.e., if their positions are made part of the state description, one obtains a formulation of quantum theory, Bohmian mechanics, in which "quantum chaos" also arises solely from the dynamical law. Moreover, this occurs in a manner far simpler than in the classical case.

KEY WORDS: Quantum chaos; quantum randomness; sensitive dependence on initial conditions; Bohmian mechanics; Bernoulli system; hidden variables.

1. Introduction

A characteristic feature of chaotic classical dynamical systems is the randomness or unpredictability of their behavior. Randomness and unpredictability are also, of course, characteristic features of quantum phenomena. However, they are not to be found in the quantum dynamics, the Schrödinger evolution, itself. This evolution is very regular, in fact preserving distances in Hilbert space. Thus it can have no sensitive dependence on initial conditions, the hallmark of classical chaos: A (small) variation $\delta\psi_0$ in the initial wave function

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$$\psi_0 \longrightarrow \psi_0 + \delta\psi_0$$

leads to the variation $\delta\psi_t$

$$\psi_t \longrightarrow \psi_t + \delta\psi_t$$

at later times whose magnitude does not change with time

$$\|\delta\psi_t\| = \text{const.}$$

After all, the evolution is unitary! (Here

$$\|\delta\psi\|^2 = \int |\delta\psi(q)|^2 \, dq.)$$

In orthodox quantum theory randomness arises only in connection with measurements. And, however measurements may manage to produce randomness, the point we wish now to emphasize is that the Schrödinger dynamical system itself does not (much) contribute to it. (We do not discuss here the randomness which emerges as a quantum system approaches, in the classical limit, a chaotic classical one; we discuss here only random behavior which is already exhibited in microscopic systems. In particular, we do not address issues such as the manifestations of classical chaos in the semiclassical regime, for example in the asymptotic distribution of the eigenvalues of the Hamiltonian. Of course, quantum randomness on the microscopic level is readily elevated to the macroscopic (classical) level when sensitive dependence on initial conditions is present on the latter level.)

2. Two examples

We shall consider here two elementary examples:

1) Simple scattering (see Fig. 1).

We are trained to see the scattering process in quantum theory as one in which, for example, a particle with an initially more or less definite momentum emerges after scattering with a random momentum, and this is of course what we find if we take into account the effect of measurement upon the final, scattering state. However, the Schrödinger evolution by itself leads to no randomness; a wave packet coming in evolves into a definite spread out wave coming out. And a small change in the incoming state leads only to a small change in the final state.

Let us remark that it would not help here if we were to include the measurement device as part of our Schrödinger system. The spreading and lack of randomness will remain, elevated, however, to the macroscopic level.

2) Simple periodic motion.

Consider a particle in one dimension in a (symmetric) double-well potential V (Fig. 2), for example, $V(q) = \lambda(q^4 - q^2)$. The ground state ψ_{sym} (Fig. 3) is symmetric under reflection through the origin, and has energy E_0. The first excited state ψ_{asym} (Fig. 4) is antisymmetric (odd) and has energy E_1 (a little larger than E_0). Assume that the central barrier is so large ($\lambda \gg 1$) that the combinations

$$\psi_R = (\psi_{sym} + \psi_{asym})/\sqrt{2}$$

and

$$\psi_L = (\psi_{sym} - \psi_{asym})/\sqrt{2}$$

are (approximately) supported on the right and left, respectively.

Focus on the evolution beginning in the initial state $\psi_0 = \psi_R$. We have that, up to a time-dependent phase, the time evolved state is given by

$$\psi_t = (\psi_{sym} + e^{-i\omega t}\psi_{asym})/\sqrt{2},$$

which is periodic, with period $T = 2\pi/\omega$ where $\hbar\omega = \Delta E = E_1 - E_0$.

Now from a dynamical systems perspective a single periodic orbit can lead to no randomness, regardless of what property we choose to observe. But suppose, for this quantum system in the state described, we measure

$$\sigma = \mathrm{sign}(q) \approx |\psi_R\rangle\langle\psi_R| - |\psi_L\rangle\langle\psi_L|,$$

i.e., we "see" whether the state is ψ_R or ψ_L, and suppose we do this at times

$$t = \tau, 2\tau, 3\tau, 4\tau, \ldots$$

where $\tau = T/4$ is a quarter-period. Note that if the system were left undisturbed, i.e., for the pure Schrödinger evolution, we would have that

$$\psi_t = \psi_{R,L}, \psi_L, \psi'_{R,L}, \psi_R, \ldots$$

at these times, where $\psi_{R,L} = (\psi_{sym} - i\psi_{asym})/\sqrt{2}$ and $\psi'_{R,L} = (\psi_{sym} + i\psi_{asym})/\sqrt{2}$ assign equal probability to $\sigma = +1$ and $\sigma = -1$. Thus when we *measure* σ at time τ we will find that $\sigma = +1$ with probability $\frac{1}{2}$, with the system projected into the state ψ_R, and $\sigma = -1$, with probability $\frac{1}{2}$, with the system projected into the state ψ_L. Whichever outcome we obtain at time τ, we may repeat the analysis to obtain the same statistics for the outcome at time 2τ. Iterating, we find that the outcome at any time $n\tau$ is a Bernoulli $(\frac{1}{2}, \frac{1}{2})$ random variable, independent of all previous outcomes. We thus find the most random of processes, a Bernoulli process, arising from (what without "measurement" is) a periodic motion.

Of course, and this is the point, for orthodox quantum theory this randomness arises somehow from the effect of measurement—not from the behavior of the dynamical system, the periodic motion, describing the unmeasured system. In fact, we would go further and say that, at best, in orthodox quantum mechanics the randomness is put in by hand! We would thus like to suggest—particularly in view of the fact that it is fashionable nowadays to look for the quantum manifestations of classical chaos—that a comparison of classical and quantum chaos would be easier if the quantum dynamics, like the classical, were itself responsible for randomness, and it did not have to be put in by hand, in a rather mysterious way at that. But we have argued that, however nice it would be, this is simply not the case.

3. Bohmian mechanics

The situation is quite different in the formulation of quantum theory proposed in a tentative, incomplete form by de Broglie [5], and in a more definitive form by Bohm [3]. Bohm's theory, which we shall call *Bohmian mechanics,* can be regarded as based on the following contention: The wave function ψ for a system of one or more *particles* should not be regarded as the complete description of this system, since its most important feature, the *positions* of the particles themselves, should be included in this description.

For Bohmian mechanics the *complete* state for a system of N particles is given by

$$(Q, \psi)\,,$$

where

$$Q = (\mathbf{Q}_1, \ldots, \mathbf{Q}_N) \in \mathbb{R}^{3N},$$

with $\mathbf{Q}_1, \ldots, \mathbf{Q}_N$ the positions of the particles, and

$$\psi = \psi(q) = \psi(\mathbf{q}_1, \ldots, \mathbf{q}_N)$$

is the wave function of the system. Note that we use Q for the *actual* configuration and q for the generic configuration space variable.

As for the time evolution, since (Q, ψ) is indeed the "state," the present specification, say (Q_0, ψ_0), must determine the state (Q_t, ψ_t) at later times; thus the evolution is defined by first-order differential equations: Schrödinger's equation

$$i\hbar \frac{\partial \psi_t}{\partial t} = H\psi_t$$

for ψ, and an evolution equation for Q of the form

$$\frac{dQ_t}{dt} = v^{\psi_t}(Q_t)$$

where

$$v^{\psi} = (\mathbf{v}_1^{\psi}, \ldots, \mathbf{v}_N^{\psi}) \tag{1}$$

is a vector field on configuration space $\mathbb{R}^{3N}$. Thus the role of the wave function ψ here is to generate the motion of the particles, through the vector field on configuration space,

$$\psi \longrightarrow v^{\psi},$$

to which it is associated.

Moreover, the detailed form of v^{ψ} is determined by requiring space-time symmetry—Galilean covariance. This leads rather directly, as the simplest possibility, to

$$\mathbf{v}^{\psi} = \frac{\hbar}{m} \operatorname{Im} \frac{\boldsymbol{\nabla}\psi}{\psi}$$

for a one particle system (note that the $\boldsymbol{\nabla}$ is suggested by rotation invariance, the ψ in the denominator by homogeneity, the Im by time-reversal invariance, and the constant in front is precisely what is required for covariance under Galilean boosts) and to

$$\mathbf{v}_k^{\psi} = \frac{\hbar}{m_k} \operatorname{Im} \frac{\boldsymbol{\nabla}_k \psi}{\psi} \tag{2}$$

for many particles.

We've arrived at **Bohmian mechanics**: For a nonrelativistic system of N particles (for simplicity ignoring spin) the *state* is given by (Q, ψ) and the *evolution* by

$$\frac{dQ_t}{dt} = v^{\psi_t}(Q_t)$$

$$i\hbar \frac{d\psi_t}{dt} = -\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \boldsymbol{\nabla}^2_{\mathbf{q}_k} \psi_t + V\psi_t$$

with v^{ψ} given by (1) and (2). Bohmian mechanics is a fully deterministic theory of particles in motion, but a motion of a highly nonclassical, non-Newtonian sort. Nonetheless, in the limit $\frac{\hbar}{m} \to 0$, the Bohm motion Q_t becomes more and more like the classical. Moreover, although in orthodox quantum theory the notion of quantum observables as self-adjoint operators plays a fundamental role, while this notion does not appear at all in the *formulation* of Bohmian mechanics, it can nonetheless be shown that Bohmian mechanics not only accounts for quantum phenomena—this was essentially done by Bohm [3,4] in 1952 and 1953—but also embodies the quantum formalism itself—self-adjoint operators, randomness given by $\rho = |\psi|^2$, and all—as the very expression of its empirical import [6,7].

In order to get some feeling for how Bohmian mechanics is related to orthodox quantum theory, let's consider briefly the two-slit experiment. How does the electron know, when it passes through one of the slits, whether or not the other slit is open so that it can adjust its motion accordingly? The answer is rather trivial: The motion of the electron is governed by the wave function. When both slits are open, the wave function develops an interference profile, and it should not be terribly astonishing for this pattern to be reflected in the motion of the electron which it generates.

But for Bohmian mechanics what is special about the familiar distribution $\rho = |\psi|^2$? Consider the ensemble evolution $\rho \to \rho_t$ arising from the Bohm motion. ρ_t is the ensemble to which the Bohm evolution carries the ensemble ρ in t units of time. If $\rho = \rho^\psi$ is a functional of ψ (e.g., $\rho^\psi = |\psi|^2$) we may also consider the transformation $\rho^\psi \to \rho^{\psi_t}$ arising from Schrödinger's equation. If these evolutions are compatible,

$$\left(\rho^\psi\right)_t = \rho^{\psi_t},$$

we say that ρ^ψ is **equivariant**. In other words, the equivariance of ρ^ψ means that under the time evolution it retains its form as a functional of ψ.

$\rho^\psi = |\psi|^2$ is equivariant. This follows immediately from the observation that the quantum probability current $J^\psi = |\psi|^2 v^\psi$, so that the continuity equation

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho v^\psi) = 0$$

is satisfied by the density $\rho_t = |\psi_t|^2$. As a consequence,

If $\rho(q, t_0) = |\psi(q, t_0)|^2$ at some time t_0, then $\rho(q, t) = |\psi(q, t)|^2$ for all t.

What about the *physical* significance of $\rho = |\psi|^2$? It turns out that when a system has wave function ψ, its configuration is random, with distribution $|\psi|^2$. Now what this really means, and why this is so, we cannot go into here (for this, see [6]). Let us just say that the assertion can be regarded as roughly analogous to the Gibbs postulate of statistical mechanics: Compare **quantum equilibrium**

$$\rho = |\psi|^2,$$

whose complete justification [6] in fact turns out to be remarkably easy, with **thermodynamic equilibrium**

$$\rho \sim e^{-\beta H},$$

whose complete justification is remarkably difficult (and as yet nonexistent).

As far as the general problem of the existence of chaos in quantum theory is concerned, note that there is nothing in Bohmian mechanics which would preclude sensitive dependence on initial conditions, of Q_t on Q_0 and ψ_0, and hence positive Lyapunov exponents. Observe, in this regard, that the evolution equation for Q, i.e., v^{ψ}, will typically be highly nonlinear—both as a functional of ψ, and, more importantly, as a function of Q.

4. Examples revisited

Let's now reconsider the two examples from a Bohmian perspective:

1) For the scattering example we find that the randomness out emerges rather trivially from randomness in the initial configuration. The behavior here (see Fig. 5) is more or less like a typical classical scattering—the sort of event which may generate separation of trajectories and positive Lyapunov exponents for classical dynamics.

2) Concerning motion in the double-well potential, let us for simplicity consider the idealization ($\lambda \ggg 1$) in which ψ_R (ψ_L) is completely supported by $\{q > 0\}$ ($\{q < 0\}$). We are now employing (the obvious [$d = 1$] version of) Bohmian mechanics to study the motion of a single particle in 1 dimension. Since trajectories in 2 dimensions (1 space and 1 time) cannot cross, it follows that, with initial state ψ_R, initial positions Q in the "left half" $(0, b)$ ("right half" (b, ∞)) of the support $(0, \infty)$ of ψ_R will evolve to a position $Q(\tau)$ on the left (right) of the origin at time τ. In fact, by equivariance, we have that the boundary b of these two intervals is determined by

$$\int_0^b |\psi_R(q)|^2 \, dq = \frac{1}{2}$$

When an (ideal) measurement of σ is performed at time τ, the result is $\text{sign}(Q(\tau))$. Thus the result of the measurement of σ at time τ is governed by which of the two intervals happens to contain the initial position Q. Moreover, the position $Q(\tau)$ is not changed by this measurement. However, the "effective wave function" is changed: It follows from a detailed analysis of measurement in Bohmian mechanics that after this measurement, the future behavior of the system will be governed by either ψ_L or ψ_R as appropriate; i.e., at time τ the wave function of the system will effectively collapse to ψ_L (ψ_R) if $Q(\tau) < 0$ ($Q(\tau) > 0$)—see [3,7] for details. We wish to emphasize, however, that our point here is not to explain how collapse comes about, but to point out that the randomness associated with the collapse (or with the result of the measurement) derives here solely from randomness in the initial position, while for quantum orthodoxy there is absolutely nothing from which this randomness can be said to derive!

Continuing in this way, we find that the result of each successive measurement (of σ at times $n\tau$) corresponds to successive divisions into "left" and "right" subintervals of already "existing" intervals. The possible outcomes for the first n measurements correspond to 2^n intervals of initial positions. In fact, we may consider an (unconventional) binary expansion

$$Q = .x_1 x_2 x_3 \ldots \tag{3}$$

of the initial configuration, based on these successive binary subdivisions. Here x_i is 1 or 0 according to whether the result σ_i of the i-th measurement is $+1$ or -1, $\sigma_i = (-1)^{x_i+1}$. Thus the randomness in the sequence of outcomes here—and the infinite amount of information to which this randomness corresponds—arises in the usual chaos theory, symbolic dynamics, sort of way—from the infinite amount of information contained in each real number, i.e., in the detailed initial configuration. And while the analysis here is far simpler than is usually required to prove the existence of "chaos" for various standard models, and indeed is rather trivial, we remind the reader that the model considered here, arising as it does from nonrelativistic quantum theory, is a good deal more "physical" than the systems normally subjected to rigorous mathematical analysis in dynamical systems theory.

Note that $x_1, x_2, x_3, \ldots$ form a sequence of independent, identically distributed random variables on the space $(0, \infty)$ equipped with the probability measure given by $|\psi_R|^2$. It thus follows from the law of large numbers that for almost every initial position Q, with respect to ($|\psi_R|^2$ and hence with respect to) Lebesgue measure on $(0, \infty)$, the results of our sequence of measurements lead to empirical distributions charateristic of our Bernoulli process. In this sense the randomness which emerges from the infinite sequence of measurements is intrinsic to the dynamical system itself, and does not much depend upon what might be considered an arbitrary choice of initial probability distribution.

A final observation about this example: Let ϕ be the map from $\mathbb{R} \setminus \{0\}$ to itself which carries $Q(\tau)$ to $Q(2\tau)$ (see Fig. 6). Then it is easy to see (in the approximation which we are considering) that for all $n > 0$

$$Q((n+1)\tau) = \phi(Q(n\tau))$$

Moreover, by equivariance, the map ϕ preserves the probability distribution μ given by
$(|\psi_R|^2 + |\psi_L|^2)/2 = |\psi_{R,L}|^2 = |\psi'_{R,L}|^2$. It follows easily from the preceding discussion that the (noninvertible) dynamical system defined by ϕ and μ is isomorphic to a one-sided $(\frac{1}{2}, \frac{1}{2})$ Bernoulli shift—with the isomorphism defined by a coding similar to the one mentioned above, i.e., by the coding which associates $Q(\tau)$ with the sequence $x_1, x_2, x_3, \ldots$ arising from (3) above. (Thus it is isomorphic to $x \to 2x$ (mod 1).)

5. Hidden variables

We urge the reader to reflect upon the contrast between what we have described here—the ease with which randomness emerges in Bohmian mechanics—and the heuristic argument, as described by Wigner [8], that convinced von Neumann of the impossibility of a deterministic version of quantum theory employing "hidden variables." Referring to an alternating sequence of spin measurements, of σ_x followed by σ_z followed by σ_x..., Wigner (von Neumann) says

> ...all measurements succeeding the first one give the two possible results with a probability $\frac{1}{2}$. If these results are, fundamentally, all determined by the initial values of the hidden parameters, the outcome of each measurement should give some information on the initial values of these parameters. Eventually, it would seem, the values of the "hidden parameters" which determine the outcomes of the first N measurements would be in such a narrow range that they would determine, if N is large enough, the outcomes of all later measurements. Yet this is in contradiction to the quantum-mechanical prediction.

We conclude with a quotation from John Stuart Bell.

> Although ψ is a real field it does not show up immediately in the result of a single 'measurement,' but only in the statistics of many such results. It is the de Broglie-Bohm variable Q that shows up immediately each time. That Q rather than ψ is historically called a 'hidden' variable is a piece of historical silliness. [1]

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Figure captions

Fig. 1. Schematic wave fronts for simple scattering from a fixed central target.

Fig. 2.

Fig. 3.

Fig. 4.

Fig. 5. Two Bohmian trajectories for simple scattering.

Fig. 6. The action of ϕ. The motion $Q(t)$, $\tau \leq t \leq 2\tau$, is governed by v^{ψ_t} with $\psi_\tau = \psi_L$ (resp., ψ_R) for $Q(\tau) < 0$ (resp., $Q(\tau) > 0$).