

de Broglie–Bohm formulation of quantum mechanics, quantum chaos and breaking of time-reversal invariance

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Abstract. A recently developed unified theory of classical and quantum chaos, based on the de Broglie–Bohm (Hamilton–Jacobi) formulation of quantum mechanics is presented and its consequences are discussed. The quantum dynamics is rigorously defined to be chaotic if the Lyapunov number, associated with the quantum trajectories in de Broglie–Bohm phase space, is positive definite. This definition of quantum chaos which under classical conditions goes over to the well-known definition of classical chaos in terms of positivity of Lyapunov numbers, provides a rigorous unified definition of chaos on the same footing for both the dynamics. A demonstration of the existence of positive Lyapunov numbers in a simple quantum system is given analytically, proving the existence of quantum chaos. Breaking of the time-reversal symmetry in the corresponding quantum dynamics under chaotic evolution is demonstrated. It is shown that the rigorous deterministic quantum chaos provides an intrinsic mechanism towards irreversibility of the Schrödinger evolution of the wave function, without invoking ‘wave function collapse’ or ‘measurements’.

Keywords. de Broglie–Bohm quantum mechanics; quantum chaos; Lyapunov numbers; time-reversal invariance.

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1. Introduction

Deterministic chaos in classical macroscopic systems is understood as the property of exponential divergence of initially adjacent trajectories in the phase space (of coordinates and conjugated momenta) and is universally characterized by a non-vanishing positive Lyapunov number. Such a behaviour, apparent in numerous (non-integrable) classical systems, has led to the introduction of the problem of chaos in quantum dynamics by Percival [1], Berry and Tabor [2], and Casati *et al* [3], some two decades ago. Considerable efforts have been made since towards an appropriate definition and meaning of the concept of quantum chaos [4–6], and a rich heuristic literature has emerged (see, e.g. [6–12]) which has provided much insights into the similarity and difference of the behaviour of the two dynamics, but, on the whole, a rigorous unified definition of quantum chaos on the same footing as classical chaos, remained elusive. This state of affairs may be summarised by the following two questions:

1. Can quantum chaos be rigorously defined?
2. Does quantum chaos exist?

Clearly, the second of the above two questions is unambiguous only if the answer to the first question is positive. Below we shall give positive answers to both the questions and discuss certain implications of the existence of quantum chaos on the problem posed by the existence of the time-reversal invariance of quantum mechanics and the occurrence of irreversible evolutions of quantum systems. Finally, we shall give an intrinsic solution to the problem of quantum irreversibility in the presence of quantum chaos without invoking influences from outside the system such as from 'baths', 'environmental dephasing', 'wave function collapse' or 'measurements'.

2. A unified definition of classical and quantum chaos

Under the spell of the conventional wisdom of quantum mechanics which forbids thinking about a single valued space-time trajectory of a quantum particle, quantum chaos is often thought to be undefinable with equal rigor and on the same footing as the classical chaos. A consequence of this belief has been the subsequent controversies and confusions when discussing 'quantum chaos'. This led M V Berry [2] to introduce the concept of 'quantum chaology' with the definition: 'Quantum chaology is the study of semiclassical, but non-classical, behaviour characteristic of systems whose classical motion exhibits chaos'. This definition depends on the rather unsharp notion of 'semiclassical behaviour', but succeeded in calming down the controversies in the field of investigation, and led to the flourishing of various heuristic and restricted criteria for recognising 'quantum chaological' behaviour, e.g. level-separation statistics, diffusive growth of energy, behaviour of the survival probability, etc. But a rigorous, unified, and generally applicable definition of quantum chaos, on the same footing as the classical chaos, remained unavailable. The above mentioned difficulty faced by the conventional quantum wisdom could, of course, have been overcome if one systematically employed the long existing Hamilton–Jacobi (de Broglie–Bohm) formulation of quantum mechanics, which is, in terms of the predictions of the results of measurements, completely equivalent [13–16] to the conventional quantum mechanics. Indeed, using this formulation systematically, a rigorous definition of quantum chaos, unifying it with that of the classical chaos, has recently been given [17,18]. This unification is achieved in terms of the same concept of positive Lyapunov numbers, associated with the classical as well as the quantum trajectories and their Euclidean distance in the classical or the quantum (de Broglie–Bohm) phase space. Before going further, let us briefly indicate the salient features of the resulting unified theory of quantum chaos below.

The wave function (say, of a particle of charge q in an electromagnetic field) is governed by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi = \hat{H} \psi, \quad (1)$$

where the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m} \left(\nabla - \frac{iq}{\hbar c} \mathbf{A} \right)^2 + q\phi + V, \quad (2)$$

\mathbf{A} and ϕ are the vector and the scalar potential respectively, and V is an external poten-

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tial. Substitution of the wave function in the form $\psi = R \exp(iS/\hbar)$ in (1) yields the generalized Hamilton–Jacobi equation

$$\partial S/\partial t + m\mathbf{v}^2/2 + q\phi + V + Q = 0, \quad (3)$$

and the continuity equation (with the density $P = R^2$),

$$\partial P/\partial t + \nabla \cdot (P\mathbf{v}) = 0, \quad (4)$$

where $\mathbf{v} = (\nabla S - (q/c)\mathbf{A})/m$ denotes the velocity field, and $Q = -\hbar^2(\nabla^2 R)/(2mR)$, appearing in (3) is the so-called quantum potential. The associated quantum trajectories of the particle are then governed by the de Broglie–Bohm equation of motion [13]

$$m\dot{\mathbf{x}}(t) = m\mathbf{v}(\mathbf{x}, t) = \nabla S(\mathbf{x}, t) - (q/c)\mathbf{A}(\mathbf{x}, t), \quad (5)$$

or, equivalently, by the quantum Newton equation [13]

$$m\ddot{\mathbf{x}}(t) = q\mathbf{E} + (q/c)\mathbf{v} \times \mathbf{B} - \nabla(V + Q). \quad (6)$$

It is important to note that the consistency of the above de Broglie–Bohm formalism of quantum mechanics with the conventional formulation is ensured by the fact that the Born probability density $|\psi(\mathbf{x}, t)|^2$ at a time t is identical to the density distribution $P_{\{\mathbf{x}(t)\}}(\mathbf{x}, t)$ of the ensemble of the quantum trajectories $\{\mathbf{x}(t)\}$, which evolves uniquely from an initial distribution of positions $\{\mathbf{x}(0)\}$, $P_{\{\mathbf{x}(0)\}}(\mathbf{x}, 0) = |\psi(\mathbf{x}, 0)|^2$. Another important consequence of this formulation of quantum mechanics is the existence of a non-negative phase space distribution function, given by (see [16])

$$f(\mathbf{p}, \mathbf{x}, t) = P(\mathbf{x}, t)\delta(\mathbf{p} - \nabla S(\mathbf{x}, t)). \quad (7)$$

From eq. (5) or its equivalent (6) it can be seen that the quantum dynamics is completely describable in the configuration space, since the momentum distribution is given as soon as the initial quantum state is specified in the configuration space. This simplicity of the quantum phase-space distribution is expressed by the factorizability of the Bohmian phase space distribution function, given explicitly by eq. (7). It is also to be noted from eq. (6) that a unique condition for the passage of the quantum dynamics to the classical dynamics follows whenever $\nabla Q = -\frac{\hbar^2}{2m}\nabla\left(\frac{\nabla^2 R}{R}\right) \rightarrow 0$. Under this condition the quantum Newton equation of motion (6) goes over exactly to the classical Newton equation for all classical trajectories, satisfying the same initial conditions. This permits us to give a unified definition [17,18] of the Lyapunov exponent λ for both classical and quantum mechanics:

$$\lambda = \lim_{\substack{t \rightarrow \infty \\ d(0) \rightarrow 0}} t^{-1} \ln(d(t)/d(0)), \quad (8)$$

where $d(t)$ is the Euclidian distance in the phase space of two initially adjacent trajectories. Thus, the Lyapunov exponent (8) in connection with the equation of motion (6) yields a rigorous and unified definition of classical and/or quantum chaos in a given region of phase space. Consequently, the answer to question No. 1 posed at the outset is: Yes.

3. Examples of regular and chaotic quantum dynamics

Before answering the second question also positively, we give an example of exact quantum evolution in terms of Bohmian trajectories and compare it with the evolution of the corresponding classical trajectories. To this end we show the dynamics of ionization (transition

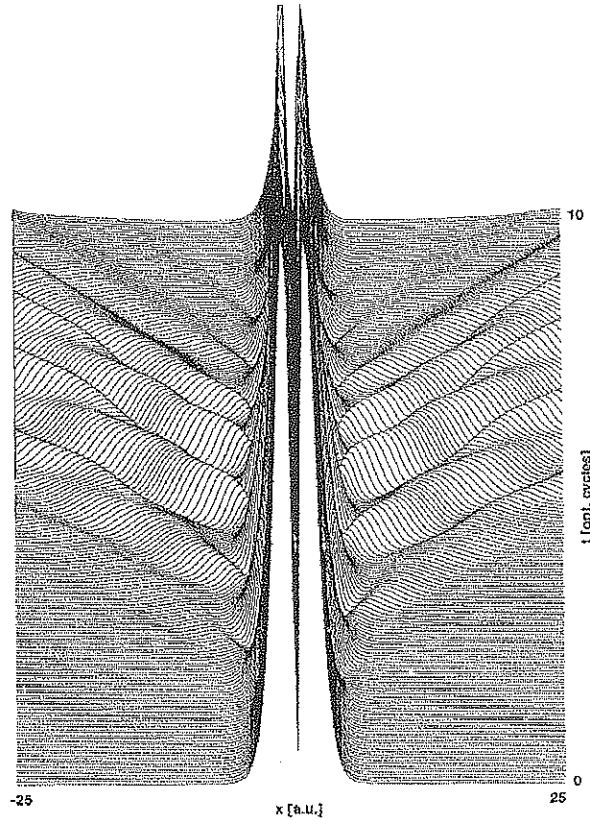


Figure 1. Probability density of (1D) atomic hydrogen in an intense laser field (5 optical cycles \sin^2 turn-on/off), $E = 0.5$, $\omega = 1$, initial state: $n = 1$.

to the continuum) of a 1D model hydrogen atom, initially in a bound state, and acted upon by a linearly polarized light field [19] at high (non-perturbative) intensities. The Hamiltonian of the system reads ($m = e = \hbar = 1$)

$$\hat{H}_\alpha(x) = \lim_{\alpha \rightarrow 0} \left[-\frac{1}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{|x| + \alpha} - x f(t) E_0 \sin(\omega t) \right], \quad (9)$$

where ω is the laser frequency, E_0 is the peak amplitude of the electric field, and $f(t)$ is the envelope of the light field including a sine-squared turn-on/off over five optical cycles. Figures 1 and 2 show the Born probability density of the electron and the corresponding distribution of the quantum ensemble of Bohmian trajectories, respectively, obtained from a numerical simulation of trajectories with an initial ensemble of positions given by the state with the principal quantum number $n = 1$ of the unperturbed atom, and propagated according to the evolution eq. (17) of the system. For the sake of comparison, in figure 3 we show the time-evolution of the corresponding classical ensemble of trajectories.

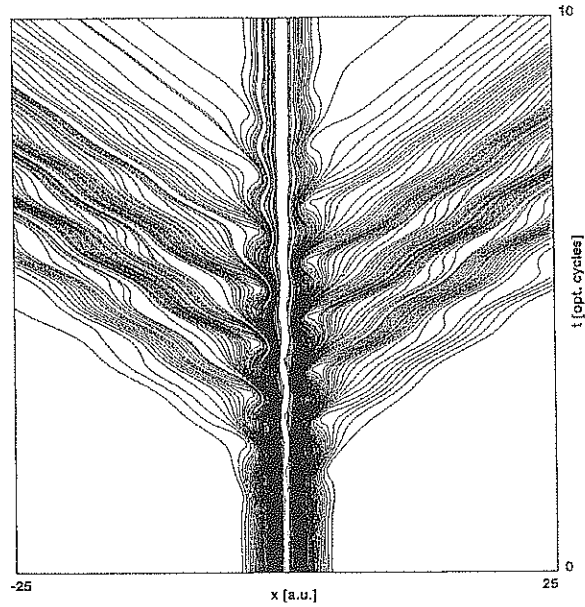


Figure 2. Quantum ensemble of trajectories of (1D) atomic hydrogen in the intense laser field (5 optical cycles \sin^2 turn-on/off), $E = 0.5$, $\omega = 1$, initial state: $n = 1$.

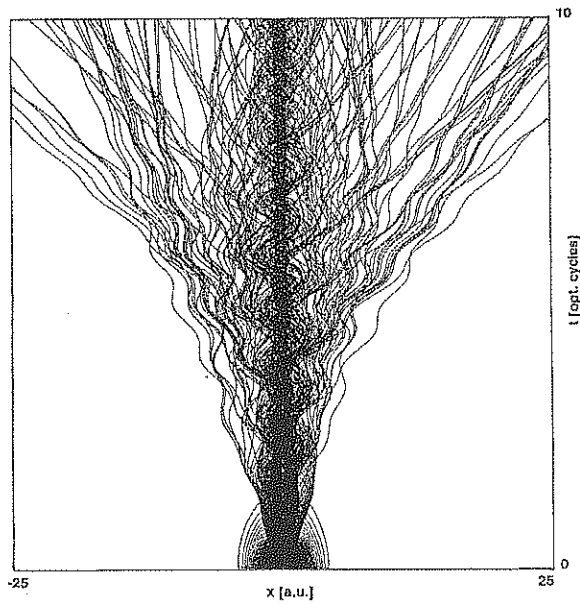


Figure 3. Classical ensemble of trajectories of (1D) atomic hydrogen in an intense laser field (5 optical cycles \sin^2 turn-on/off), $E = 0.5$, $\omega = 1$.

It becomes evident that, in contrast to the classical motion (figure 3), the quantum motion, shown in figures 1 and 2, is a highly ordered process. In fact the motion is regular since the calculated Lyapunov exponent has been found to tend to zero. We note further that the classical trajectory density (cf. figure 3) bears virtually no correlation with the quantum probability density, whereas the quantum trajectory density (figure 2) reproduces the Born probability density (figure 1), as it must.

We now come to the second question posed at the outset, which can be answered positively as soon as the existence of quantum chaos can be shown rigorously, strictly speaking even in a single case. To this end we shall next analyse a 2D quantum system, consisting of a charged particle moving under spatially periodic boundary conditions in a rectangle of dimension $[0, L] \times [0, L]$, $L = 1$, that is subjected to a (time-) periodic electromagnetic field, given by the vector potential (in the following we assume $m = q = 1$)

$$\mathbf{A} = -c \mathbf{V} \mathbf{x} \delta_\tau(t), \tag{10}$$

where $\delta_\tau(t) = \sum_{j=-\infty}^{\infty} \delta(t - j\tau)$, τ is the period length, and $\mathbf{x} = (x, y)^T \text{ mod. } 1$. We define matrix \mathbf{V} in (10) via the transformation matrix [20]

$$\mathbf{M}(K) = \exp(\mathbf{V}) = \begin{pmatrix} 1 & K \\ 1 & K+1 \end{pmatrix}, \tag{11}$$

where $\det \mathbf{M}(K) = 1$ ensures the corresponding map to be area preserving, and the system parameter K is assumed to vary on the real axis. The scalar field ϕ may be chosen in analogy with [21,22] to yield the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2} \nabla^2 - \frac{i\hbar}{2} (\nabla \cdot \mathbf{V} \mathbf{x} + \mathbf{x} \mathbf{V} \cdot \nabla) \delta_\tau(t). \tag{12}$$

It will be shown below that the parameter K , appearing in (11), controls the nature of evolution of the wave function of the system in time. In the special case $K = 1$, the system represents the quantum realization of Arnold's cat map [23], due to Weigert [21,22], that has been shown [24] to exhibit deterministic quantum chaos in terms of a positive Lyapunov exponent λ . Note that this realization of a quantum cat map differs from those introduced by Hannay and Berry [25], and Ford *et al* [26] that are defined in one-dimensional configuration space and are confined within finite domains of both space and momentum dimensions.

To be able to investigate the transition from regular to irregular quantum dynamics analytically, we consider below the so-called resonant case with a kick-period of length $\tau = L^2/\hbar\pi$. In this case the free evolution operator $U_0(\tau) = \exp(i\hbar\tau\nabla^2/2)$ returns the wave function at the end of a period to its value at the beginning of the period. The time evolution of the periodically kicked system is then obtained by the repeated application of the evolution operator

$$\hat{U}(\mathbf{V}) = \exp((\nabla \cdot \mathbf{V} \mathbf{x} + \mathbf{x} \mathbf{V} \cdot \nabla)/2) \tag{13}$$

on an initial state $\psi_0(\mathbf{x}, t_0^+)$. An algebraic calculation similar to that in [22,24] shows that the wave function at the time immediately before the $(n + 1)$ th kick, t_{n+1}^- , as well as immediately after the n th kick, t_n^+ , is given by

$$\psi(\mathbf{x}, t_{n+1}^-) = \psi(\mathbf{x}, t_n^+) = \psi_0(\mathbf{M}^{-n} \mathbf{x}, t_0^+). \tag{14}$$

de Broglie–Bohm formulation

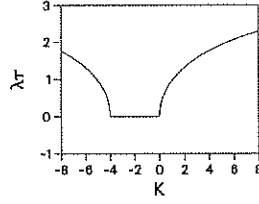


Figure 4. Dimensionless quantum Lyapunov number $\lambda\tau$ versus system parameter K , showing the domains of regular ($\lambda\tau = 0$), $-4 \leq K \leq 0$, and chaotic dynamics ($\lambda\tau > 0$), $K < -4$ and $K > 0$.

The equation of motion of the system is obtained from (5) and (10) to be $\dot{\mathbf{x}}(t) = \nabla S(\mathbf{x}, t) + \mathbf{V}\mathbf{x} \delta_\tau(t)$. It can be seen from (14) that for all real initial states $\psi_0(\mathbf{x}, t_0^+)$, the wave function $\psi(\mathbf{x}, t_n^\pm)$ remains real and hence the gradient of the phase vanishes immediately before and after the n th kick for all n :

$$\nabla S(\mathbf{x}, t_n^\pm) = 0. \quad (15)$$

Integrating the corresponding equation of motion (5) piecewise, in the interval $t_n^- \leq t \leq t_n^+$, one obtains the coordinates at the time immediately after the n th kick, t_n^+ :

$$\mathbf{x}(t_n^+) = e^{\mathbf{V}} \mathbf{x}(t_n^-) = e^{\mathbf{V}} \mathbf{x}(t_{n-1}^+) \pmod{1}, \quad (16)$$

where the last equality follows from the free propagation between two successive kicks under the resonance condition mentioned above. Given an initial coordinate $\mathbf{x}(t_0^+)$, repeated application of (16) yields (with $\exp(\mathbf{V}) = \mathbf{M}(K)$)

$$\mathbf{x}(t_n^+) = [\mathbf{M}(K)]^n \mathbf{x}(t_0^+) \pmod{1}. \quad (17)$$

From (17), the separation between two neighbouring coordinates is given by

$$\Delta \mathbf{x}(t_n^+) = [\mathbf{M}(K)]^n \Delta \mathbf{x}(t_0^+). \quad (18)$$

The Euclidean phase space distance is given by $d(t_n^+) = |\Delta \mathbf{x}(t_n^+)|$. The Lyapunov exponent, defined by (8), then becomes

$$\lambda = \lim_{\substack{t_n^+ \rightarrow \infty \\ d(t_0^+) \rightarrow 0}} \frac{1}{t_n} \ln \frac{d(t_n^+)}{d(t_0^+)} = \lim_{n \rightarrow \infty} \frac{1}{n\tau} \ln \|\mathbf{M}(K)\|^n, \quad (19)$$

where the last equality follows from (18), and $\|\cdot\|$ stands for the matrix norm (e.g. [27]). Thus, from the eigenvalues of the matrix $\mathbf{M}(K)$, given by

$$\gamma_\pm(K) = (K + 2)/2 \pm \sqrt{(K + 2)^2/4 - 1}, \quad (20)$$

we finally obtain from (19) the quantum Lyapunov exponent

$$\lambda = \tau^{-1} \ln |\gamma(K)|, \quad (21)$$

where $|\gamma(K)|$ is the greater of $|\gamma_+(K)|$ and $|\gamma_-(K)|$. It can be seen from eqs (20) and (21) that for $-4 \leq K \leq 0$, λ is zero, establishing that the dynamics of the system is regular in this domain. For parameter values $K < -4$ as well as $K > 0$, the quantum Lyapunov

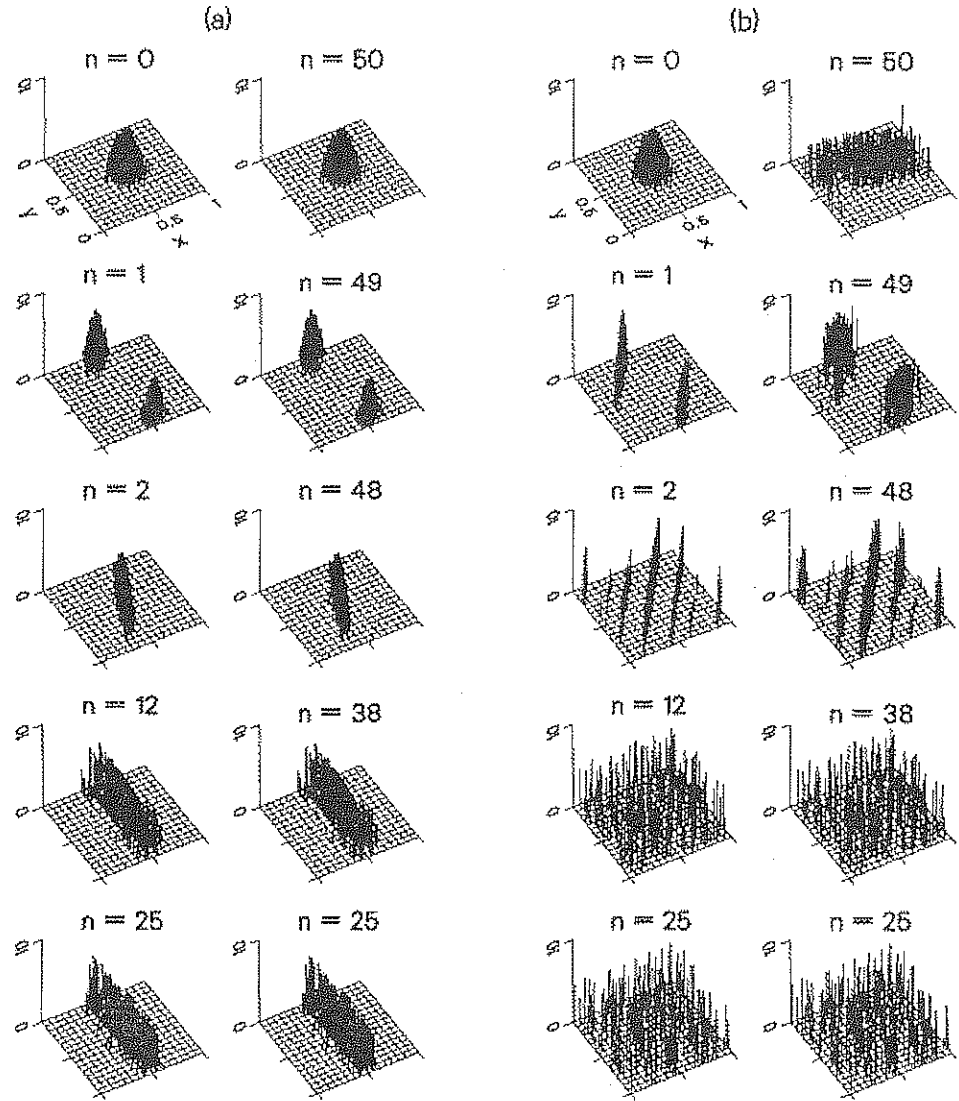


Figure 5. Evolution of the wave function, starting with a Gaussian function and propagating up to the 25th period; then time-reversing and propagating another 25 periods backward ($n = 26 \dots 50$). (a) regular case with $K = 0$, and (b) chaotic case with $K = 2$. In case (a), the wave function maintains time-reversibility and returns to its initial state, whereas in case (b), the time-reversal symmetry is broken (cf. text).

exponent λ is positive definite, proving that the dynamics in these domains is rigorously

chaotic. This regular to chaotic transition as a function of K is depicted in figure 4. It is seen clearly from this figure that the critical values of the parameters for this transition are at $K = 0$ and $K = -4$. One important consequence of the chaotic evolution is the long-time unpredictability of the dynamics. This fact can reflect itself in the breaking of the time-reversal symmetry of the quantum evolution in the chaotic region, whenever the latter cannot be followed with infinite precision. To test this prediction based on the analytical demonstration of deterministic chaos given above, we show below the results of numerical simulations of the propagation of the wave function of the system at a sequence of kick periods $n\tau$, starting with the Gaussian wave function

$$\psi(\mathbf{x}, t_0^+) = \sqrt{N} \exp\left(-a^2/2 \left((x - 1/2)^2 + (y - 1/2)^2\right)\right) / 2$$

$$0 \leq x \leq 1, \quad 0 \leq y \leq 1, \quad (22)$$

where $a = 10$ and the normalization factor $N = 31.830\dots$. Figures 5(a) and (b) show the evolution of the wave function during the first 25 kicks (the left-hand columns in (a) and (b), from above downward), as well as the time-reversed evolution from the 25th period backward (the right-hand columns in (a) and (b), from below upward). Figure 5(a) corresponds to $K = 0$, and therefore to the critical regular value of the quantum Lyapunov exponent $\lambda = 0$. In this regular domain one expects a stable evolution in time both for the forward and the backward propagations. This is indeed what is seen to be the case in this figure; not only the forward evolution remains regular in time, but also the time-reversed evolution after the 25th kick brings back the wave function to its initial state. Figure 5(b) corresponds to a value of $K = 2$ that lies in the chaotic domain with $\lambda > 0$. It can be seen that not only the wave function of the system becomes visibly chaotic with time (left-hand column of figure 5(b)) but also, on backward propagation from the 25th period, the system fails to return to its initial state (see right-hand column of figure 5(b)), showing a breakdown of the time-reversal symmetry in the chaotic region. It should be noted here that this breakdown occurs already at the level of the wave function itself.

4. Breaking of the time-reversal invariance

We have seen from the illustrations (figure 5a and b) of the time evolutions of both the regular and the chaotic case that in the presence of quantum chaos (positive Lyapunov number) the time-reversal symmetry of the wave function is broken. The significance of this result can be appreciated on considering the connection between the Lyapunov number λ of the dynamical evolution with the notion of algorithmic information, which are related, according to the Alekseev–Brudno theorem [28] as $\lambda = \lim_{t \rightarrow \infty} I(t)/t$, where $I(t)$ is the information needed to record a stretch of the trajectory exactly (without loss of accuracy) in the interval of time t . In the long run, for a positive definite value of λ , the need for information increases without bound (independent of the previous amount of available information) and the evolution cannot be followed exactly neither in the forward nor in the backward direction of motion, resulting in the breaking of the time-reversal symmetry. Thus, the presence of the quantum chaos (and similarly the presence of the classical chaos) provides an intrinsic mechanism for the origin of irreversibility in the realisation of quantum (and similarly of classical) dynamics. The length of time $t_{\text{critical}} = n_{\text{critical}}\tau$ over which the evolution can be recorded (not just imagined!) is given by the Chirikov

condition: $\tau = \lambda|t_{\text{critical}}|/|\ln(\mu)| \leq 1$, where μ is the accuracy of recording. One may estimate therefore that for an accuracy $\mu \approx 10^{-14}$ and $\lambda\tau \simeq 1.32$, as in the case of figure 5(b), the critical time is about $n_{\text{critical}} \approx 24$ periods, which is essentially the same as seen in figure 5(b).

5. Conclusion

A unified theory of classical- and quantum chaos is developed based on the de Broglie–Bohm formulation of quantum mechanics. The quantum chaos is defined in terms of the positivity of the Lyapunov number associated with quantum trajectories, on the same footing as in classical dynamics, which characterises universally the extreme sensitivity of chaotic motion to the initial conditions in both the dynamics. An example is given proving the existence of quantum chaos in a simple quantum system and showing the breaking of the time-reversal symmetry of the wave function as a consequence; it demonstrates that rigorous quantum chaos provides an intrinsic mechanism towards quantum irreversibility (and hence a possible basis for the derivation of quantum statistical mechanics), independently of the presence of any influence from outside the system, such as that of ‘baths’, ‘environmental dephasing’, ‘wave function collapse’, or ‘measurements’.

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