Test of the Quantum Chaoticity Criterion for Diamagnetic Kepler Problem

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Abstract:

The earlier suggested criterion of quantum chaoticity, borrowed from the nuclear compound resonance theory, is used in the analysis of the quantum diamagnetic Kepler problem (the spinless charged particle motion in the Coulomb and homogenous magnetic fields).

1 Introduction

It is believed for decades that the main feature of the classically chaotic system is the instability of its trajectories to minor variations of the initial conditions. Since the concept of the trajectory in phase space does not apply in quantum mechanics, the possibility of quantum signatures of chaos is still opened to discussion. It was suggested [1] to look for the ”quantum signatures of classical chaos”. The only more or less generally accepted ”signature” found up to now is the Wigner level repulsion. In this paper we proceed with the illustration of our alternative suggestions [2-5] concerning the definition of chaos for the Hamiltonian quantum (and classical) systems.

According to Liouville-Arnold theorem in classical mechanics, the Hamiltonian system with \( N \) degrees of freedom is regular if it has \( M = N \) independent global integrals of motion. If the number \( M \) of global integrals becomes less than \( N \), the system becomes chaotic. The well known Noether’s theorem connects the existence of global integrals of the system with the symmetries of its Hamiltonian. According to this theorem, breaking the symmetry of the initially regular system decreases the number of its independent global integrals of motion. Thus the system becomes chaotic only in the case of such a symmetry-breaking which makes the number \( M \) of global integrals less than \( N \).

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Our first (and major) suggestion is to generalize this definition of chaoticity for the case of quantum systems. Since the concept of symmetry (unlike the trajectory) is universal for both classical and quantum mechanics, this generalization seems to be quite straightforward - one should simply substitute the integrals of motion by the corresponding 'good' quantum numbers, resulting from the symmetries of quantum Hamiltonian. This approach immediately allows to treat the only generally accepted signature of quantum chaos - Wigner’s level repulsion - as a signature of symmetry-breaking leading to chaos. Indeed, the general property of the highly symmetrical regular quantum system is the high degeneracy of its eigenstates. The immediate consequence of perturbation breaking the original symmetry is the removal of this degeneracy (in other words, Wigner’s level repulsion). It is worthwhile to remind that Wigner’s level repulsion was first observed for the resonance states of compound nucleus, whose only good quantum numbers are their energy and spin. This property comes from the fact that the symmetries of the nuclear mean field are destroyed by the pair-wise "residual" interactions [2–5].

Our second (rather technical) suggestion is to use the concept of spreading width $\Gamma_{spr}$ (and the related criterion $\varphi$) as a sensitive measure of symmetry-breaking of the Hamiltonian $H_0$ caused by the perturbation $V$. Indeed, consider a Hamiltonian $H$ of the non-integrable system as a sum:

$$H = H_0 + V$$

of the highly symmetrical regular Hamiltonian $H_0$ (say, of non-interacting particles or quasi-particles in the spherically-symmetrical mean field):

$$H_0 \psi_k = \epsilon_k \psi_k$$

and of the perturbation $V$ which destroys the symmetries of $H_0$ (the pair-wise particle-particle forces in nuclear case). Expand now the eigenstates $\psi_i$ of $H$ over the "regular" basis $\phi$:

$$\psi_i = \sum_k c^i_k \phi_k$$

and look for the probability $P_k(E_i) = |c^i_k|^2$ to find the original "regular" component $\phi_k$ in the different eigenstates $\psi_i$ (with eigenenergies $E_i$) of our nonintegrable system. It is obvious, that for sufficiently small perturbations $V$ the probability $P_k(E_i)$ is centered around the "original" energy $\epsilon_k$ and tends to saturate to unity over some characteristic energy interval $\Gamma_{spr}$ which is called "the spreading width" of the initially unperturbed state $\phi_k$. Various realistic models (see e.g. chapter 2 of ref.[6]) give the Lorentzian shape of the strength function energy dependence:

$$S_k(E_i) = \frac{|c^i_k|^2}{D} \approx \frac{\Gamma_{spr}}{2\pi (E_i - \epsilon_k)^2 + \Gamma^2_{spr}/4}$$
where $D$ is the average level spacing of the nonintegrable system. A slight generalization of the derivation given in ref. [6] allows [3,4] to express the spreading width in terms of the "mean square root" matrix element $\tilde{v} = \sqrt{\langle v^2 \rangle}$ of the interaction $V$ mixing the basic states $\phi$ (angular brackets imply averaging over all the basic components admixed by $V$ to a given one):

$$\Gamma_{spr} \sim \tilde{v} \sqrt{N_d}$$  \hspace{1cm} (5)

Here $N_d$ stands for the degeneracy rank of the initial level $\epsilon_k$.

Thus the system formally becomes nonintegrable as soon as $\Gamma_{spr}$ deviates from zero. However, while the ratio

$$\bar{\varepsilon} = \frac{\Gamma_{spr}}{D_0}$$  \hspace{1cm} (6)

(where $D_0$ is the level spacing of the initial regular system) is smaller than unity - the traces of the initial good quantum numbers are quite obvious as isolated maxima of the strength function. We can easily distinguish between the maxima corresponding to the different values of the originally good quantum numbers. This is the analogue of the classical "weak chaos" governed by the KAM theorem. When $\bar{\varepsilon}$ exceeds unity these traces of regularity disappear since it becomes impossible to distinguish between the successive maxima of the strength function corresponding to the different values of the original quantum numbers $k$. This situation is the quantum analogue of the smearing out and disappearance of the invariant tori. It means that we approach the domain of "global" or "hard" chaos.

Furrier transforming Eq. (4) one can show (see e.g. [6]) that $\Gamma_{spr}/\hbar$ defines the rate of decay of the "regular" states $\phi$ resulting from the instability caused by the perturbation $V$. One can even form the wave packets $|A>$ of the states $\phi_k$ and analyze the recurrence probabilities $P(t) = |\langle A(t)|A(0) \rangle|^2$. This analysis shows [3] the periodic recurrences with classical period $T$ modulated exponentially by the factor $\exp(-\Gamma_{spr}t/\hbar)$ arising from the above instability. Combining these results with the results of Heller’s wave-packet experience (see e.g. [7] or paragraph 15.6 of ref. [8]), one can show that the quantity $\Gamma_{spr}/\hbar$ transforms in the classical limit into the Lyapunov exponent $\Lambda$:

$$\frac{\Gamma_{spr}}{\hbar} \to \Lambda$$  \hspace{1cm} (7)

The corresponding classical limit for the dimensionless chaoticity criterion is:

$$\bar{\varepsilon} \to \frac{\Lambda T}{2\pi} = \frac{\chi}{2\pi}$$  \hspace{1cm} (8)

where $T$ is the classical period and $\chi$ is the stability parameter of the classical monodromy matrix (see, e.g. [8]).

Thus the particular quantity $\Gamma_{spr}$ and the parameter $\bar{\varepsilon}$ seem to be more accurate numerical measures of quantum chaoticity than the level distribution law - this is proved by the
nuclear physics experience [2-4] and by its application to one of the most popular in classical mechanics cases of transition from regularity to chaos - Hennon-Heiles problem [5].

2 Diamagnetic Kepler Problem

Another very popular model for studies of transition from regularity to chaos in classical mechanics is the non-relativistic hydrogen atom in the uniform magnetic field (see e.g. [8,10,14]) with the Hamiltonian:

$$H = \frac{p^2}{2m} - \frac{e^2}{r} + \omega l_z + \frac{1}{2}m\omega^2(x^2 + y^2)$$

(9)

Here the frequency \(\omega = eB/(2mc)\) is a half of the cyclotron frequency and \(B\) is the strength of the magnetic field acting along \(z\)-axis. The dimensionless field strength parameter \(\gamma = \hbar\omega/R\) (here \(R\) is the Rydberg energy) is usually combined with the electron energy \(E\) to produce the scaled energy \(\epsilon = E\gamma^{-2/3}\). When the scaled energy varies from \(-\infty\) (for \(B = 0\)) to \(0\) (for \(B = \infty\)) the regular motion of the system becomes more and more chaotic. The fraction \(R\) of available phase space covered by regular trajectories was calculated in ref. [9 - 10] as a function of scaled energy for the case of \(l_z = 0\) (see Fig.1), showing the rapid chaotisation of the system in the range \(-0.48 \leq \epsilon \leq -0.125\).

We analyzed the quantum analogue of this system (with the Hamiltonian (9)) on the same lines as it was done in [5] for the quantum Henon-Heiles problem, namely we traced the gradual destruction of the \(O(4)\) symmetry characteristic of the unperturbed motion in Coulomb potential by the external magnetic field \(B\). In other words, we traced the disappearance of the \(^*\)good\(^*\) quantum numbers (integrals of motion) which characterize the regular motion in this potential. In order to do this, we diagonalized the Hamiltonian matrix (9) in parabolic coordinates on the basis of purely Coulomb wave functions \(\phi_{n_1n_2m}\), whose eigenvalues in the unperturbed case are defined by the principal quantum number \(n\):

$$n = n_1 + n_2 + |m| + 1$$

and are highly \((n^2\) times) degenerate. Diagonalizing the Hamiltonian matrix, we defined the new eigenvalues \(E_i\) and the eigenstates \(\psi_i\) in terms of the expansion coefficients \(c_i^{\ell}\) (see Eq. (3)). As a next step, we plotted the energy distribution of Eq. (4) for the coefficients’ squares of the \(n\)-th shell over the \(^*\)new\(^*\) eigenstates. Fig. 2 shows the examples of these distributions for \(n = 10\), \(m = 0\) and the magnetic field \(\gamma\) equal to \(4 \cdot 10^{-4}\), \(6 \cdot 10^{-4}\), \(8 \cdot 10^{-4}\) and \(12 \cdot 10^{-4}\), respectively. In order to increase the statistical accuracy, we performed the averaging over all the components of the basis with the same \(n\) value, as it is usually done in nuclear physics and as it was done in the case of quantum Henon-Heiles problem [5].
Assuming now that the shape of these distributions is approximately Lorentzian, like in the
case of the neutron strength function in nuclear physics, we define $\Gamma_{spr}$ as the energy range
around the maximum where the sum of the squares of the coefficients $\sum_i |c_i|^2$ saturates to
0.5. Thus obtained values of $\Gamma_{spr}$ were divided then by the level spacing $D_0$ between the
adjacent maxima of the strength function to give the desired parameter $\alpha$. The plot of this
parameter versus the scaled energy $\epsilon$ is given in Fig. 1.

We see that our parameter reaches the critical value of $\alpha = 1$ at the critical scaled energy
$\epsilon \approx -0.45$ in fairly good agreement with the classical critical value $\epsilon \approx -0.48$ of refs. [9,10].
It is worthwhile to remind here that in the previous studies of the quantum diamagnetic
Kepler problem [11 - 14] the existence was pointed of the approximately good quantum
number $K$, corresponding to the eigenvalues of the operator $\Sigma$ built as a combination of the
Runge-Lenz vector $A$:

$$\Sigma = 4A^2 - 5A^2_z$$  \hspace{1cm} (10)

The eigenstates of this operator are obtained [12, 13] by prediagonalization of the unperturbed
Coulomb basis within a single manifold $n$ (which physically corresponds to the values of our $\alpha \leq 1$). The appreciable $K$-mixing (disappearance of the integral of motion $\Sigma$) starts
[13, 14] when $\gamma^2 n^7 \approx 16$. In our case of $n = 10$ this corresponds to the scaled energy
$\epsilon \approx -0.45$.

3 Conclusion

Thus we confirmed once more the plausibility of the suggested approach to quantum chaosici-
ity, based on its connection with symmetry-breaking of the regular motion which makes the
number $M$ of the system’s global integrals of motion less than the number $N$ of its degrees
of freedom. We had also demonstrated that the spreading width $\Gamma_{spr}$ and the dimensionless
parameter $\alpha$ might serve a good quantitative criterion of quantum chaoticiti. Likewise in
the case of Henon-Heiles problem [4], the critical scaled energy value $\epsilon_c$ when the parameter
$\alpha$ reaches unity corresponds to the onset of ”global” chaos on the classical phase portrait for
the diamagnetic Kepler problem. Here, however, the origin of the approximate regularity of
the perturbed system for $\epsilon \leq \epsilon_c$ is more evident. Although formally the external magnetic
field makes the system nonintegrable by reducing the number of global integrals of motion to
$M = 2$ (energy and $l_z$), the third approximate integral of motion ($\Sigma$) survives much longer
making the system practically regular.

We should add in conclusion that the importance of studying the particular example of
hydrogen atom in the uniformed magnetic field was stressed (see, e.g. [14]) because it ”is not
an abstract model system but a real physical system that can be and has been studied in the
laboratory”. These studies were indeed started in 1986 (see [15]). One should point, however, that atomic nucleus is also "not an abstract model", whose experimental and theoretical studies are going on for more than half a century. As we had already mentioned, Wigner developed his random matrix approach in order to describe the experimentally observed properties of compound nuclear resonances. Since those times nuclear physics accumulated a vast arsenal of theoretical methods which allow Schrödinger’s equation to be solved in some effective manner, even when the system is not integrable and its behavior is chaotic by the criteria of level repulsion. As shown in [2-4], most of them are based on the smallness of the chaoticity parameter æ, which seems to be the most important small parameter of nuclear physics.

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