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LETTER TO THE EDITOR

Correspondence between classical and quantum chaos for hydrogen in a uniform magnetic field

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Abstract. It is shown, by numerical computations, that the classical and the quantal critical energy of a hydrogen atom in a uniform magnetic field, characterising the onset of irregular motions, approximately coincide. This result is obtained by applying a simple scaling property of the classical Hamiltonian, valid only for $L_z = 0$ (the angular momentum component along the field vanishes), to the numerically deduced relative areas of the irregular region of Poincaré surfaces of section.

The hydrogen atom in a uniform magnetic field is a typical example of a non-integrable Hamiltonian system, hence it is very difficult to elucidate over all quantum-mechanical energy levels of the system for arbitrary strengths of the magnetic field.

Thus, some interesting problems exist in connection with this system:

(i) the unique ground state having a binding energy logarithmically divergent with an increase in the field strength (Avron *et al* 1981, Patil 1981);

(ii) the appearance of quasi-Landau levels in the vicinity of the ionisation threshold (Edmonds 1970, Gay *et al* 1980);

(iii) the connection between the Rydberg and the Landau levels (Robnik 1980, Kuroda *et al* 1982);

(iv) the existence of an approximate symmetry (Zimmerman *et al* 1980, Delande and Gay 1981, Robnik 1981, Clark 1981).

The latter two problems, in particular, have received special attention in recent years as major exploring points in connection with the non-integrability of the system.

Delande and Gay (1981), in their analysis of the quadratic Zeeman effect, argued the problems speculatively in the context of classical non-integrable systems, suggesting that it would be worth while investigating the corresponding classical trajectories. Robnik (1981) performed such computations, and his result exhibited a general feature of the Poincaré mapping analogous to the one for the well known nonlinear oscillator, namely the Hénon–Heiles system (Ford 1975). It can be seen from his results that the classical Kepler motion in a uniform magnetic field possesses a substantial region of irregularity in the diagram of the energy E against magnetic field B, which is located over the regular region of the approximate symmetry and also below that of the escape motion. The result should naturally lead one to anticipate a structure of the quantal energy spectrum of the same system reflecting such coexistence of regular and irregular motions.

This letter sets out to show that we have just obtained an affirmative answer to the above assumption. This is obtained from our own numerical analyses by Robnik type classical computation, which is designed, however, for the special situation when the constant of motion of the angular momentum component along B vanishes, i.e. L_z $(\equiv m) = 0$.

According to Robnik's indication (1981), the classical Kepler motion, in a uniform magnetic field under the condition of the constant of motion L_z (or quantum number m) equal to zero, is an exceptional case as regards the general feature of the irregular region to exist, as outlined above, because this feature was obtained from the Poincaré mapping analysis together with a scaling property of the classical Hamiltonian in terms of m (regarding it as a continuous parameter) that is valid only for $m \neq 0$. To be more precise, let γ denote the well known parameter representing the field strength $(\frac{1}{2}\hbar\omega_c/Ry)$. The constant surface of energy E, when expressed as a function of γ and m, was shown to satisfy

$$E(\gamma, m) = m^{-2}E(\gamma m^3, 1). \tag{1}$$

However, this is valid only for $m \neq 0$: if $m = 0$, due to the absence of the centrifugal potential, the effective two-dimensional potential of the Hamiltonian in cylindrical coordinates has no minimum. Thus, by considering a limiting procedure, $m \to 0$, of the curve of the critical energy E_c against γ (the boundary of the regular and the irregular regions), Robnik concluded that the critical energy is merged into the escape energy in this limit, implying the disappearance of the irregular region in the E against B diagram for the $m = 0$ case. This seems to be one of the main reasons why Robnik was not able to compare his result with the quantum-mechanical optical spectra for the diamagnetic Lyman series $(16 \leqslant n < \infty, m = 0)$ calculated by Clark and Taylor (1980). Here, we show our result of the classical phase orbits computed directly for $m = 0$, verifying the real existence of the classical chaos characterised by the critical energy $E_c < 0$; direct evidence that the irregular portion of the spectrum seen in the result of Clark and Taylor is indeed the quantal correspondence to the classical chaos.

The classical Hamiltonian in the cylindrical coordinate system of the Kepler motion with the quadratic Zeeman term is given by

$$H = \tfrac{1}{2}(p_\rho^2 + p_z^2) + (m^2/2\rho^2) + \tfrac{1}{8}\gamma^2\rho^2 - (\rho^2 + z^2)^{-1/2}, \tag{2}$$

where atomic units are used and the constant of motion L_z is set equal to m. This Hamiltonian, as a function of four canonical variables $p_\rho, \rho; p_z, z$ and two parameters m and γ, satisfies the scaling property (Robnik 1981)

$$H(p_\rho, p_z, \rho, z; \gamma, m) = m^{-2}H(mp_\rho, mp_z, m^{-2}\rho, m^{-2}z; \gamma m^3, 1)$$

resulting in the relation (1) for the constant value E of the Hamiltonian with $m \neq 0$.

On the other hand, the Hamiltonian (2) for the special case $m = 0$ is shown to have the following scaling property:

$$H(p_\rho, p_z, \rho, z; \gamma, m = 0) = \gamma^{2/3}H(\gamma^{-1/3}p_\rho, \gamma^{-1/3}p_z, \gamma^{2/3}\rho, \gamma^{2/3}z; 1, m = 0), \tag{3}$$

from which, in place of (1), we obtain the relation

$$E(\gamma, m = 0) = \gamma^{2/3}E(1, m = 0). \tag{4}$$

Figures 1(a)–(c) exhibit some examples of Poincaré surfaces of section at the plane $z = 0$ with $p_{z|z=0} \geqslant 0$ for $m = 0$ and $\beta \equiv \frac{1}{2}\gamma = 1$. A characteristic point of these figures is that the Hill region (the intersection of the invariant surface $H(p, q) = E$ with $z = 0$ on which the mapping is made) is unbounded along the p_ρ axis up to $\pm\infty$ owing to the absence of the centrifugal potential, as contrasted to the compact Hill region for

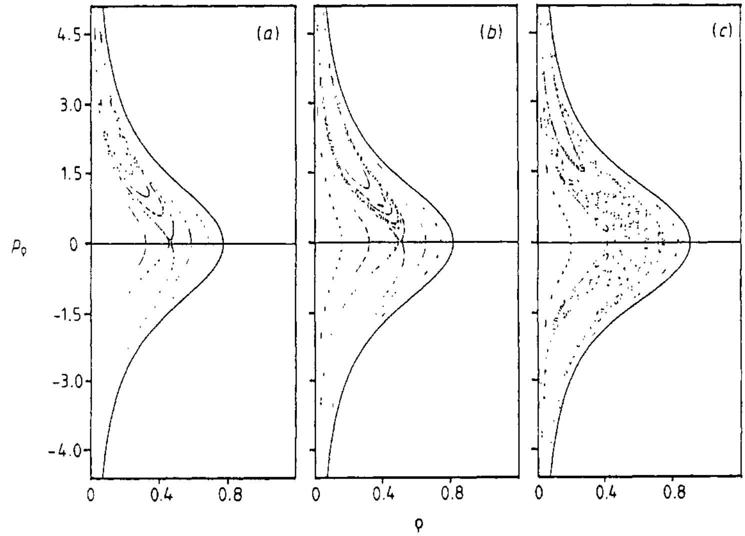

Figure 1. Poincaré surfaces of section inside the Hill region for the Hamiltonian (2) with $m=0$, $\beta=1$ ($\gamma=2$) and energies (*a*) -1.0, (*b*) -0.9 and (*c*) -0.7 in atomic units. The region $|p_\rho|>5.1$ is cut off.

$m=1$. It means that for any negative value of the energy E there exist some phase-orbit solutions of the equation of motion, associated with the Hamiltonian (2), with $m=0$. Because of this singular nature of the equation of motion, the ordinary Runge–Kutta method of integration is found to break down near $\rho=z=0$. To avoid this difficulty we adopted the Adams method with double precision (available from FACOM-SSL II subroutine library), and found it necessary to revise the trajectories in order to satisfy the conservation of the energy set up for each initial data.

For the value of energy $E=-1.0$ (atomic unit) the Hill region is filled up with tori and a separatrix is seen to exist dividing the region into three parts (figure 2(*a*)). The phase flows resemble those of double-well potential systems. For $E=-0.9$ (figure 2(*b*)) there appear a stochastic layer around the separatrix and some resonances of orbits that look like chains. Thus, we can conclude that the critical energy E_c, the onset of the irregular motions, is about -0.9 for $\beta=1$ ($\gamma=2$).

From the above numerical analyses, it can be seen that the critical energy E_c for the irregular region exists, in fact, even for $m=0$, whereas Robnik asserted that this was not the case. However, an important difference exists in the nature of the irregular regions between the case of $m\neq0$ and of $m=0$: Robnik's result indicates that in the former case the curve of the critical energy $E_c(\gamma)$ as a function of γ possesses a minimum at the value

$$\gamma_{\min}=2.5\ \mathrm{m}^{-3} \tag{5}$$

showing that in both limits, $\gamma\to0$ and $\gamma\to\infty$, the motion becomes regular with the Hamiltonian being approximately integrable. For $m=0$, our result indicates, from (4), simply that

$$E_c(\gamma)=\gamma^{2/3}E_c(1). \tag{6}$$

Thus, the critical energy always decreases to $-\infty$, as $\gamma\to\infty$, without reaching a minimal

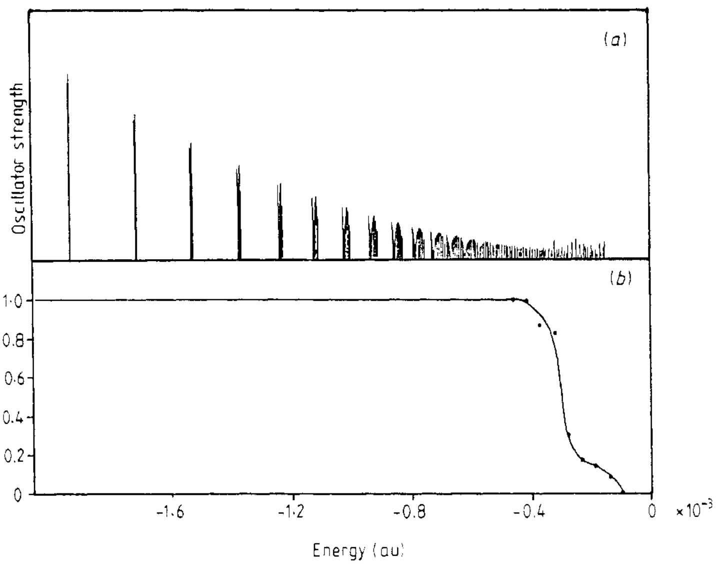

Figure 2. (*a*) The oscillator strengths for $\Delta m=0$ transitions from the ground state to the Rydberg states after Clark and Taylor (1980). The lowest line corresponds to the $n=16$ levels perturbed by the quadratic Zeeman part. (*b*) The ratio of the area of total regular regions to that of the Hill region for each Poincaré surface of section calculated from figure 1(*a*)–(*c*) etc. (The cut-off regions are ignored.)

value (as formally consistent with the relation (5)). This is a specific feature of the classical Hamiltonian (2) with $m=0$, and contradicts the quantum-mechanical result that for $\gamma \gg 1$ the low-lying spectrum of the energy eigenvalues of the same system becomes regularly behaved (Hasegawa and Howard 1961), where the aspect of the divergence of energy against γ is concentrated to the ground-state energy.

It may be expected, on the other hand, that in a weak field regime $\gamma \ll 1$ of the quadratic Zeeman perturbation on the Rydberg states the quantal energy spectrum would show behaviour reflecting the coexistence of the regular and irregular motions of classical dynamics that would be in accordance with (6). We have tested this expectation by comparing our numerical data of the Poincaré surfaces of section (i.e. by calculating an area ratio of the irregular region to the total one of each surface of section plotted in the figures) with the quantum-mechanical optical spectra provided by Clark and Taylor (1980). Their figure 1 yields the best profile for comparison because this is the dipole excitation spectrum polarised along B of the Lyman series so that, apart from the relative intensity of each peak, the profile reflects the energy eigenvalue spectrum of the perturbed Rydberg series with $m=0$. Figures 2(*a*)–(*b*) show this comparison by applying the scaling law (6) (actually, $E_c(\gamma=2\beta)=(2\beta)^{2/3}E_C(2)$ in order to be consistent with Clark and Taylor) to the unscaled data. From this comparison, therefore, we have good reason to justify that the irregular portion of the energy spectrum calculated by Clark and Taylor provides a real example of quantum chaos.

The non-integrability of the classical Kepler motion in a uniform magnetic field is analogous to that of a two-particle Toda lattice with a varying mass ratio investigated by Casati and Ford (1975): the E_c against γ curve for $m \neq 0$ demonstrated by Robnik is in reasonable agreement with their result for the curve of E_c against mass ratio.

The problem of quantising such non-integrable systems is considered important (see e.g. Percival 1977), but at present no clear-cut prescription is available for defining the quantal critical energy. Recently, Saitô *et al* (1981) presented an explicit comparison of the classical E_c with the quantal energy spectrum for the Hénon–Heiles system, showing that the onset of a group of spread degenerate levels merging into the adjacent one is nearly identical to the classical E_c. A group of spread degenerate levels of the Rydberg series merging into the adjacent one (see Clark and Taylor 1982) may be identified, therefore, as the quantal critical energy, which we demonstrate here to coincide approximately with the classical E_c.

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