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ENERGY CHARACTERIZATION OF CHAOS IN THE HYDROGEN ATOM IN A UNIFORM MAGNETIC FIELD.

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ABSTRACT

The kinetic energy possessed on the Poincare surface of section has been used as a measure of the degree of chaoticity in the case of the Hydrogen atom in a uniform magnetic field. Polynomial expressions have been obtained for the maximum, mean, range and standard deviation of the kinetic energy on the Poincare surface have been obtained as functions of the scaled energy of the system.

Key words: Kinetic energy, Poincare surface, Chaos

INTRODUCTION

The Hydrogen atom in a uniform magnetic field (of strength B) is described by the Hamiltonian

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

where z is the direction of the field, m_e is the reduced mass of the electron (of charge e) and the nucleus, and ω is half the cyclotron frequency, equal to $\frac{eB}{2m_e c}$. r is the radial distance of the electron from the nucleus of the atom, l_z the z component of the angular momentum of the electron in the Cartesian (x,y,z) coordinate system and p is the momentum of the electron. It has been shown (Friedrich and Wintgen (1989)), that the dynamics is equivalent to that given by the Hamiltonian:

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2}\left(p_1^2 + p_2^2\right) - \varepsilon\left(q_1^2 + q_2^2\right) + \frac{1}{8} q_1^2 q_2^2 \left(q_1^2 + q_2^2\right) \qquad (2)$$

where ε, the scaled energy $\left(\varepsilon = \frac{B}{B_0} = \frac{\hbar\omega}{\Re}\right)$ determines the degree of chaoticity of the system and $B_0 = m_e e^3 c / h^3$, the value of the magnetic field strength at which the oscillator energy equals the Rydberg energy, $\Re$ (Friedrich and Wintgen(1989)). q_1, q_2, p_1 *and* p_2 are the coordinates and momenta of the equivalent system respectively.

The dynamics of a bounded Hamiltonian system with a Hamiltonian $H(q_i, p_i)$ with $i = 1, 2$ and $|p_i|, |q_i| < \infty$, is determined by the Hamilton canonical equations of motion,

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \ i = 1,2 \qquad (3)$$

$$\frac{dq_i}{dt} = +\frac{\partial H}{\partial p_i}, \ i = 1,2 \qquad (4)$$

The equations of motion resulting from canonical equations define a mapping from the phase space onto itself, that is area preserving (Liouville's Theorem).

The trajectory of such a system is governed by some constants $I(q_i, p_i)$ of motion,

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$\frac{dI}{dt}=0$. If there are not sufficient numbers of such constants, then the system is deterministically chaotic. The pattern of chaos is furnished by mapping the trajectory onto a Poincare surface of section given by, say, $q_n = 0$, $p_n > 0$.

The degree of chaoticity of non-integrable systems has been measured by various authors (Henon and Heiles (1963), Mo (1972), Toda (1974), Brumer and Duff (1976), Noid *et al.* (1977), Chirikov (1979), Henon (1983), Harada and Hasegawa (1983), Schuster (1984)). Others include Chirikov and Shepelyansky (1984), Klimontovich (1987), Akin-Ojo (1993), Torcini (1996), Tiwari and Rao (1998). In the case of the Hydrogen atom in a uniform magnetic field, the degree of chaoticity is determined by the parameter ε.

There is a growing interest in the statistics of recurrences (Aframovich and Zalavsky (1998), Chirikov and Shepelyansky (1999) and Floriani and Lima (1999)). This has motivated this work, which attempts to find numerical measures of chaoticity on the Poincare surface of section. In particular, we investigate the variation of the total kinetic energy $\frac{p_1^2+p_2^2}{2}$ on the Poincare surface with the scaling parameter ε.

METHODOLOGY

The Runge Kutta method was used in solving the ordinary differential equations that resulted from the Hamiltonian:

$$\frac{d}{dt}p_1 = -\left(2\varepsilon q_1 + \frac{4q_1^3 q_2^2}{8} + \frac{2q_1 q_2^4}{8}\right) \qquad (5)$$

$$\frac{d}{dt}p_2 = -\left(2\varepsilon q_2 + \frac{4q_2^3 q_1^2}{8} + \frac{2q_2 q_1^4}{8}\right) \qquad (6)$$

$$\frac{d}{dt}q_1 = p_1 \qquad (7)$$

$$\frac{d}{dt}q_1 = p_1 \qquad (8)$$

For each scaled energy of the system, ε, a uniform mesh of initial points covering the Poincare surface was mapped out and the four measures of distance computed. Sixty initial points were considered in all cases. In each case, 300 intersections on the Poincare surface were observed.

RESULTS AND CONCLUSION

The randomness of some physical parameters associated with a system is a measure of the degree of its chaoticity. Thus, we expect a greater spread in the range and the standard deviation of the kinetic energy of the system. In addition, the more chaotic a dynamical system is, the more of the area it traverses on the Poincare surface. Thus, the mean and the range of the kinetic energy are expected to increase with the degree of chaoticity.

Fig. 1 shows the proportion of the surface of section covered by chaotic orbits, as reckoned using the meshes. This compares well with the result due to Harada and Hasegawa (1983) and is an indication that the sampling has truly reflected the dynamics of the system.

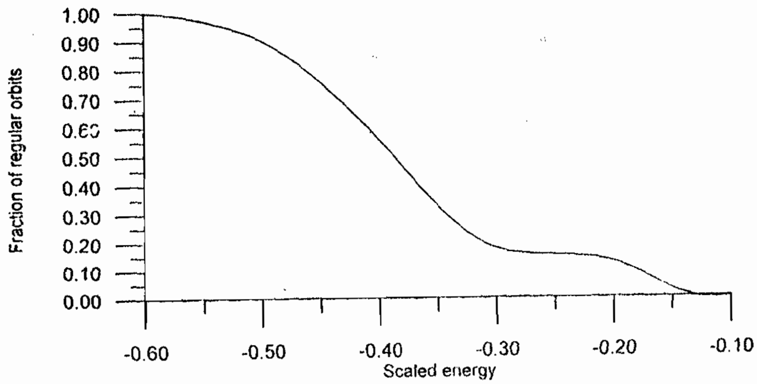

Fig. 1: Fraction of regular orbits in the surface of section as a function of scaled energy

The maximum, mean, range and standard deviation of the total kinetic energy on the Poincare surface are illustrated (together with lines of best fit) in Figs. 2 to 6.

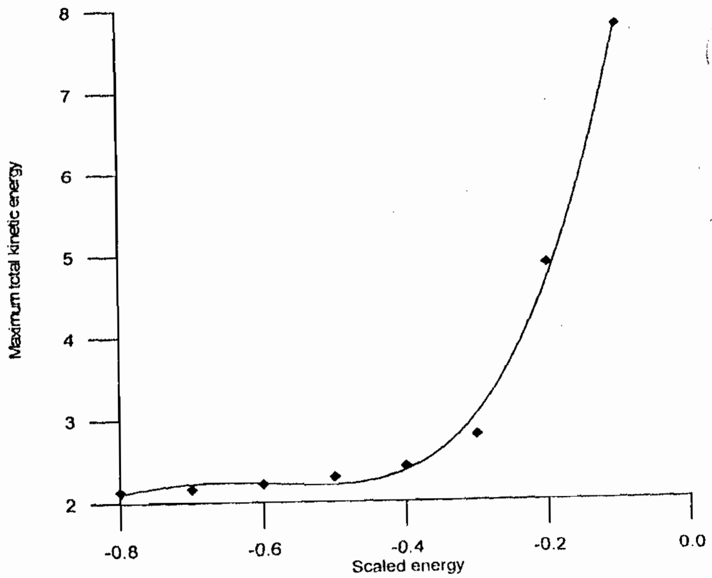

Fig. 2: Maximum kinetic energy against scaled energy

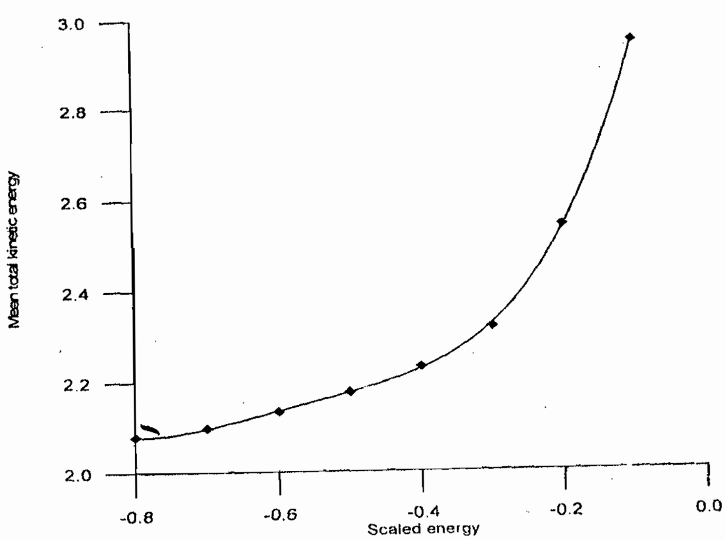

Fig. 3: Mean kinetic energy against scaled energy

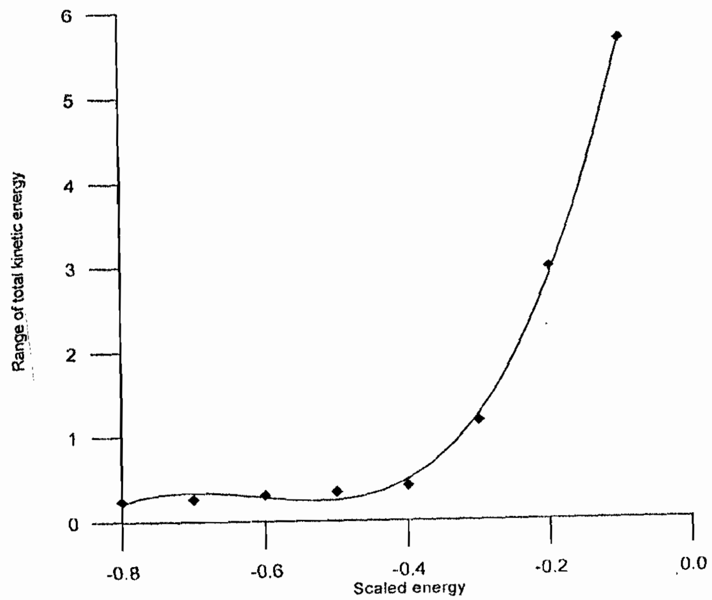

Fig. 4: Range of kinetic energy against scaled energy

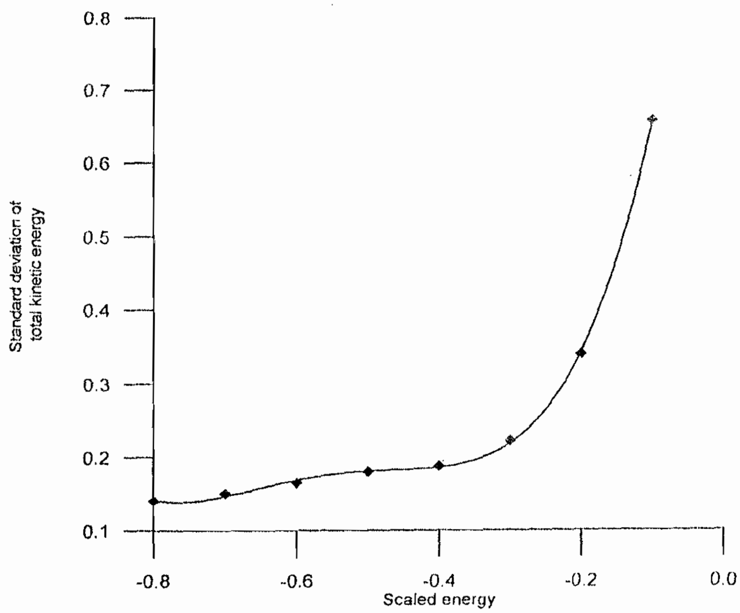

Fig. 5: Standard deviation of kinetic energy against scaled energy

The following expressions are the respective polynomial fits for maximum, mean, range and standard deviation of the total kinetic energy as functions of the scaled energy of the system.

$$49.614\varepsilon^4 + 143.787\varepsilon^3 + 150.008\varepsilon^2 + 67.435\varepsilon + 13.191$$
$$11.4678\varepsilon^4 + 26.7082\varepsilon^3 + 23.2929\varepsilon^2 + 9.41641\varepsilon + 3.68174$$
$$14.3072\varepsilon^4 + 71.5824\varepsilon^3 + 99.0971\varepsilon^2 + 53.1484\varepsilon + 10.0935$$
$$12.8913\varepsilon^4 + 28.9093\varepsilon^3 + 23.555\varepsilon^2 + 8.37202\varepsilon + 1.28571$$

Thus, the lines of best fit for each of the measures of the kinetic energy are all polynomials of degree four. All the parameters increase with the degree of chaoticity of the system, as measured by the parameter ε.

Our analysis has taken into consideration the values of ε between – 0.1 and -0.8. A search of the literature has not revealed that there has been any numerical measure obtained for a chaotic system on the Poincare surface.

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