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Hydrogen atom in a strong magnetic field: on the existence of the third integral of motion

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Abstract. The problem of the existence of the third integral of motion for the classical Hamiltonian describing a hydrogen atom in a magnetic field is studied by numerical methods. It is found that the third integral is isolating for all initial conditions for which the energy is lower than a critical energy, beyond which the phase orbits are unstable and the Hamilton system can behave stochastically. This critical energy depends upon the strength of the magnetic field and the value of the z component of the angular momentum. The critical energy approaches the (classical) ionisation energy in the weak-field and strong-field limits, while it is lowest in the transition region. The consequences for the quantum mechanical energy spectrum of the hydrogen atom are discussed: the existence of this approximate dynamical symmetry would allow for close anti-crossings of levels, and might facilitate the analytic calculations of the energy levels below the critical energy. In discussion of the correspondence diagram a criticism of an earlier paper is given.

1. Introduction

The problem of the hydrogen atom in an arbitrarily strong magnetic field has recently received more attention than ever before. In atomic physics new experimental and theoretical results on highly excited atoms in magnetic fields have been obtained (see the review by Rau (1980)) and in astrophysics much of the accumulated observational material on strongly magnetic white dwarfs (reviews by Angel (1977, 1978)) as well as on x-ray binaries (see review by Börner (1980), Kundt (1981)) requires a better theoretical understanding of atoms in magnetic fields. In the case of white dwarfs the polarisation measurements in the optical continuum, made by Kemp *et al* (1970), revealed magnetic fields $B \leqslant 5 \times 10^8$G, while the discovery by Trümper *et al* (1978) of an electron cyclotron line in the x-ray spectrum of Her X-1 confirmed the theoretical prediction $B \simeq 5 \times 10^{12}$G for the surface magnetic field of a neutron star (cf Mazets *et al* 1981). Other lines, such as FeXXVI, have been observed in x-ray binaries (Pravdo 1978). A study of the properties of matter in strong magnetic fields is therefore of great importance for astrophysics, where magnetic fields can have strengths by a factor of 10^7 in excess of those available in a laboratory (Latal 1975).

Theoretical understanding of the hydrogen atom stands naturally at the very beginning of the structure of matter in strong magnetic fields. However, although the simplest this problem turns out to be difficult enough. (See the review by Garstang (1977).) For instance, the two-body problem in a magnetic field was solved correctly only a few years ago (Avron *et al* 1978), and it has been shown that the N-body problem

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can be reduced to the $(N-1)$-body problem iff the total charge of the system vanishes. But even when one assumes an infinite mass for the nucleus of the hydrogen atom, thus restricting the discussion to the one-particle system, the symmetry breaking presents great difficulties, since it leads to the non-integrability of the Hamiltonian. As a consequence little can be done analytically: perturbational methods are good only in the weak-field region (Zeeman region) (Schiff and Snyder 1939), variational methods work only for the ground state (Yafet *et al* 1956); in the strong-field limit (Landau region) the adiabatic approximation together with a perturbation method can be used, but only for the lowest states (Canuto and Kelly 1972). Numerical works (Smith *et al* 1972, Praddaude 1972, Rau and Spruch 1976, Simola and Virtamo 1978, Wunner and Ruder 1981, Kara and McDowell 1980) improved the accuracy of the earlier estimates, but they still gave poor information on higher levels, on the spectrum in the intermediate region, and they still scatter in energy values by at least 10%. A very elegant analytical method has been recently presented by Mlodinow and Papanicolaou (1979). The method is based on the $1/N$ expansion (N = dimension of the configuration space), and has the advantage of being applicable to arbitrary field strengths, but it is still hard to obtain results for higher levels. Among other methods which have been attempted is the semiclassical quantisation (Angelie and Deutsch 1978). This was able to predict the spectrum in accordance with experiments only for the levels close enough to the zero-field ionisation limit (see Rau (1980) and references therein). Perhaps the results could be improved when using a more advanced method such as that developed by Gutzwiller (1978, 1980), who studied the semiclassical quantisation of systems with ergodic behaviour. An important paper promising more rapid progress has been published quite recently by Zimmerman *et al* (1980). There a numerical calculation of highly excited energy levels of a hydrogen atom in a magnetic field of intermediate strength has been reported. The accuracy of the method (diagonalisation of the Hamilton operator in the spherical basis) has been tested for the case of the Stark effect (for which analytical results are known due to existence of the Lenz–Pauli vector as an independent constant of motion). The result was a discovery of approximate level crossings (within a term group of given parity and angular momentum L_z, which are the only known constants of motion beyond energy). Now, if parity and L_z were the only existent symmetries of the hydrogen atom in a magnetic field, then according to the Neumann–Wigner (von Neumann and Wigner 1929) non-crossing rule, the levels could not cross. The existence of level crossings (or approximate crossings, i.e. close anti-crossings) led them to the conjecture that an additional, as yet unrecognised, dynamical symmetry of the Hamiltonian must exist. According to their results, the symmetry should be approximate and more effective as the energy of a level increases.

The hydrogen atom in a magnetic field is neither the first nor the last non-integrable Hamilton system whose quantisation is to be done. Note, however, that even our understanding of the non-integrable classical Hamilton systems is rather poor in general, since the Kolmogorov–Arnold–Moser (KAM) theory (Whiteman 1977, Arnold and Avez 1968; see also the excellent review by Berry (1978)) applies only to nearly integrable systems, i.e. to systems with a weak perturbation, to which the quantum mechanical perturbation theory can also be successfully applied. There is no exact theory which could predict the behaviour of a given system which is far from integrable (Zaslavskii and Chirikov 1972, Chirikov 1979). But there are numerical experiments (Henon and Heiles 1964, Casati and Ford 1975, Ali and Somorjai 1980) which give us a clue to what has to be done (Percival 1979, Berry 1982). Similarly, the semiclassical quantisation methods for non-integrable Hamiltonians are not far from the ideas put

forward by Einstein, although some progress has been made (Gutzwiller 1980, Neveu 1977, Berry 1980, 1982). As explained in the case of the hydrogen atom, the correct full quantisation of non-integrable systems is also at the beginning. Since the hydrogen atom in a strong magnetic field is a very important problem because of the applications, and since it is comparatively better studied than any other nonlinear quantum system, it seems appropriate to study the correspondence between the classical system and its quantal analogue.

The philosophy of this analogy is to find the integrals of motion of the classical Hamiltonian, in particular the third integral $I_3(p, q)$. This is the essential result of this paper, where I_3 is discovered by a numerical experiment. Once we have some insight into the nature and existence conditions of I_3, we can use an algebraic approach (see e.g. Gustavson (1966), where a series of canonical transformations using a computer to do all the algebraic operations has been performed) to construct $I_3(p, q)$. When the dynamical symmetry announced by Zimmerman *et al* (1980) is constructed we may use it to approximately separate the Schrödinger equation for the hydrogen atom in a magnetic field. All attempts to construct I_3 by elementary methods failed, and the construction using a method proposed above remains as a future plan.

It turns out that this problem is even more attractive than it seems at first glance, because the Hamilton system is rich enough to display a stochastic behaviour (known since Henon and Heiles (1964)) which is currently of interest for physicists dealing with nonlinear phenomena (Zaslavskii and Chirikov 1972, Whiteman 1977, Rabinovich 1978, Helleman 1980, Berry 1982).

2. The classical Hamiltonian and its properties

We assume an infinite mass for the proton and consider the classical motion of the electron in the Coulomb field and in a magnetic field. When the trivial paramagnetic term is transformed away (which can be done by using a uniformly rotating frame, a fact well known from the Larmor theorem, cf Landau and Lifshitz (1965)), the (non-relativistic) Hamiltonian can be written in the following dimensionless form:

$$H = \tfrac{1}{2}\boldsymbol{p}^2 + \tfrac{1}{8}\gamma^2\rho^2 - 1/r. \tag{1}$$

Here $\rho^2 := x^2 + y^2$ and all lengths are measured in units of Bohr radius, the energy is measured in units of $2E_{\mathrm{H}}$, E_{H} being the ionisation energy of the hydrogen atom in a vacuum, while the magnetic field strength is measured in units of the critical magnetic field B_0, at which the Landau energy equals E_{H}, so that $\gamma := B/B_0$, $B_0 = \alpha^3 e/r_0^2 = 2.35 \times 10^9$ G (α is the fine structure constant, e the elementary charge, r_0 the classical electron radius, $r_0 = e^2/mc^2$). (See also Garstang (1977).) The choice of these non-classical units has been made merely to achieve a direct analogy with the quantum mechanical problem. Except for the energy $E = H(\boldsymbol{p}, \boldsymbol{r})$ the z component of the angular momentum, denoted simply by L, is the only constant of motion which derives from the geometrical symmetries via Noether's theorem. If this is accounted for, the Hamiltonian can be 'reduced' in cylindrical coordinates (ρ, φ, z) as follows:

$$H_r = \tfrac{1}{2}(p_\rho^2 + p_z^2) + L^2/2\rho^2 + \tfrac{1}{8}\gamma^2\rho^2 - (\rho^2 + z^2)^{-1/2}. \tag{2}$$

The problem of classical motion has now been reduced to the study of orbits in a four-dimensional phase space (ρ, p_ρ, z, p_z). The Hamilton equations read $\dot{\rho} = p_\rho$, $\dot{p}_\rho = L^2/\rho^3 - \frac{1}{4}\gamma^2\rho - \rho(\rho^2 + z^2)^{-3/2}$, $\dot{z} = p_z$, $\dot{p}_z = -z(\rho^2 + z^2)^{-3/2}$.

The equipotential lines of the (effective) potential

$$U(\rho, z) := L^2/2\rho^2 + \tfrac{1}{8}\gamma^2\rho^2 - (\rho^2 + z^2)^{-1/2} \tag{3}$$

for $L = \gamma = 1$ are plotted in figure 1. In general, the potential is minimal for $z = 0$ and $\rho = \rho_0$, where

$$\tfrac{1}{4}\gamma^2\rho_0^4 = L^2 - \rho_0.$$

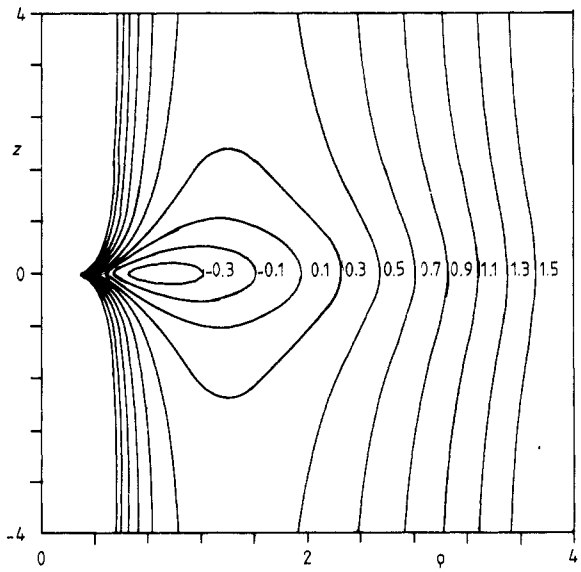

Figure 1. Equipotential lines of the potential $U(\rho, z)$ from equation (3) with $\gamma = L = 1$. The numbers refer to the value of the potential. In this case $E_{\min} = \min U = -0.394\,3046$ and $E_{\text{esc}} = 0.5$.

We define $E_{\min} := U(\rho_0, 0)$. The potential lines are closed for all energies E higher than $E_{\min}$ and smaller than the escape energy E_{esc} at which the potential lines open asymptotically and the particle can escape to infinity in the z direction. A simple calculation shows $E_{\text{esc}} = \frac{1}{2}\gamma|L|$. (Note, however, that the escape energy E_{esc} does *not* coincide with the quantum mechanical ionisation energy $E_{\text{ion}} = \frac{1}{2}\gamma(|L| + 1)$, which is higher by exactly the Landau energy. The reason is the quantum mechanical zero-point energy, which in this case equals the Landau energy $\gamma/2$. The particle is still transversally bounded after it has escaped the Coulomb potential well.)

Our central question is whether a third integral I_3 of motion exists or not. To decide this question a study of Poincaré mappings generated by the Hamilton system seems to be the best approach (see Henon and Heiles 1964). For a reader not familiar with this method a brief explanation is given. The idea is to take a surface Σ in phase space Φ. Each point on Σ uniquely defines initial conditions which determine (together with the Hamilton equations) a unique phase orbit. Now, the map of a point from Σ is defined as the point at which the phase orbit going through the initial point returns to Σ for the first time. This mapping can be shown (Whiteman 1977, Berry 1978) to be an area preserving continuous bijection, i.e. an area preserving homeomorphism, or simply a Poincaré mapping. In fact to each Hamiltonian H and a given surface Σ in phase space

Φ there corresponds a Poincaré mapping $f_{H,\Sigma}$, so that a Hamiltonian flow in Φ generates a family of Poincaré mappings. Consider a given mapping $f_{H,\Sigma}$. If H is conservative, so that the energy $E = H(p, q)$ is a constant of motion, then for a fixed value of E the intersection of the invariant surface $H(p, q) = E$ = constant with Σ will be in general a certain $(2N-2)$-dimensional region D, which we call Hill's region (cf Churchill *et al* 1978). If the motion is bounded in phase space, then Hill's region D will be compact, and the Poincaré mapping is defined on a compactum. We shall denote it simply by f_D (assuming that the Hamiltonian H and Φ are fixed). Then the following properties are of primary interest: fixed points, invariant curves and invariant regions of f_D and its iterates f_D^n, $n = 1, 2, 3, \ldots$. Namely, a fixed point of f_D^n corresponds uniquely to a strictly periodic orbit in phase space, an invariant curve corresponds to a quasiperiodic motion of the phase point on an invariant two-dimensional surface in the phase space, while an invariant region, which is not covered by invariant curves, corresponds to an ergodic component.

3. The numerical experiment

We now apply this method to the Hamiltonian H_r from equation (2). Note that because the energy E is constant a phase orbit can be plotted in a three-dimensional space for which we choose (ρ, p_ρ, z), with a prescription for the sign of $p_z = \pm(2E - p_\rho^2 - 2U(\rho, z))^{1/2}$. So, a phase point is moving upward (in the z direction) in the space $(\rho, p_\rho, z)_+$, reaches the boundary of the allowed region determined by the equation $p_z^2 = 0$, and moves downward in the space $(\rho, p_\rho, z)_-$. For the surface of section Σ we take the hyperplane $z = 0$ in phase space, so that the resulting two-dimensional Hill region $D := D_+ \vee D_-$ is defined in the three-dimensional space as follows:

$$D_+ \subseteq (\rho, p_\rho, z = 0)_+ : p_z = +[2(E-U) - p_\rho^2]^{1/2} > 0,$$

$$D_- \subseteq (\rho, p_\rho, z = 0)_- : p_z = -[2(E-U) - p_\rho^2]^{1/2} < 0,$$

with the boundary determined by the equation $p_z^2 = 0$, i.e.

$$p_\rho^2 = 2(E-U) = 2E - (L/\rho)^2 - \tfrac{1}{4}\gamma^2\rho^2 + 2/\rho. \tag{4}$$

Each point in the Hill region $D = D_+ \vee D_-$ thus uniquely determines the initial condition and the corresponding phase orbit. The task of the numerical experiment is now to investigate the mappings $f_{(+,-)} : D_+ \to D_-$, $f_{(-,+)} : D_- \to D_+$, $f_{(+,+)} : D_+ \to D_+$, $f_{(-,-)} : D_- \to D_-$, where $f_{(+,+)} = f_{(+,-)} f_{(-,+)}$ and $f_{(-,-)} = f_{(-,+)} f_{(+,-)}$ are the Poincaré mappings as defined in § 2. Numerically the mapping $f_{(+,+)}$ (or $f_{(-,-)}$) is determined by taking each point from D_+ (or D_-), then integrating the phase orbit until the phase point returns to D_+ (or D_-). The point at which the phase orbit returns to the region D_+ (or D_-) defines the map of the initial point. However, as pointed out in § 2, fixed points, invariant curves and invariant regions of the Poincaré mapping rather than the mapping itself are important. It is therefore convenient to take a point P from D_+ (or D_-) and to calculate a series of the iterated maps $f_{(+,+)}^n(P)$ (or analogously for D_-), where $n = 1, 2, 3, \ldots, N$. (The maximal N which has been used was $N = 1000$.) If all the iterates lie on a curve (= invariant curve of the mapping), then the third integral of motion exists for the given initial condition P. If P is a fixed point of an iterate of the mapping a periodic orbit in phase space is discovered. But if the iterates fill a certain

region densely, then the motion is stochastic, possibly also ergodic, in some region of phase space.

However, in order to study the existence of the third integral, i.e. to investigate the existence of the invariant curves, one can equally well plot the mixed iterates $f_{(+,-)}f_{(-,+)}f_{(+,-)}f_{(-,+)}\ldots f_{(+,-)}$ in the region $p_z^2 > 0$ of the plane $(\rho, p_\rho, z = 0)$ starting, as in our case, from a point P with $p_z > 0$, i.e. $P \in D_+$. That means that we plot each transition of the phase point through the plane $z = 0$ rather than only those moving upward along the z axis. We thus generate both Poincaré mappings $f_{(+,+)}$ and $f_{(-,-)}$ at the same time, and plot the invariant curves of both at the same time. Odd transitions correspond to $f_{(+,+)}$ and even transitions to $f_{(-,-)}$. In this way we lose some information on fixed points of iterates, but nevertheless we are able to determine the stochastic transition energy (or critical energy). The advantage is that the calculations are half as expensive.

Such a calculation has been done firstly for $L = 1$, $\gamma = 1$ and for various energies. The integration of the Hamilton equations was performed using a very rapid and accurate program based on an extrapolation method. (A Cyber 172 machine of the Max-Planck-Institut für Radioastronomie in Bonn was used.) The accuracy of the integration has

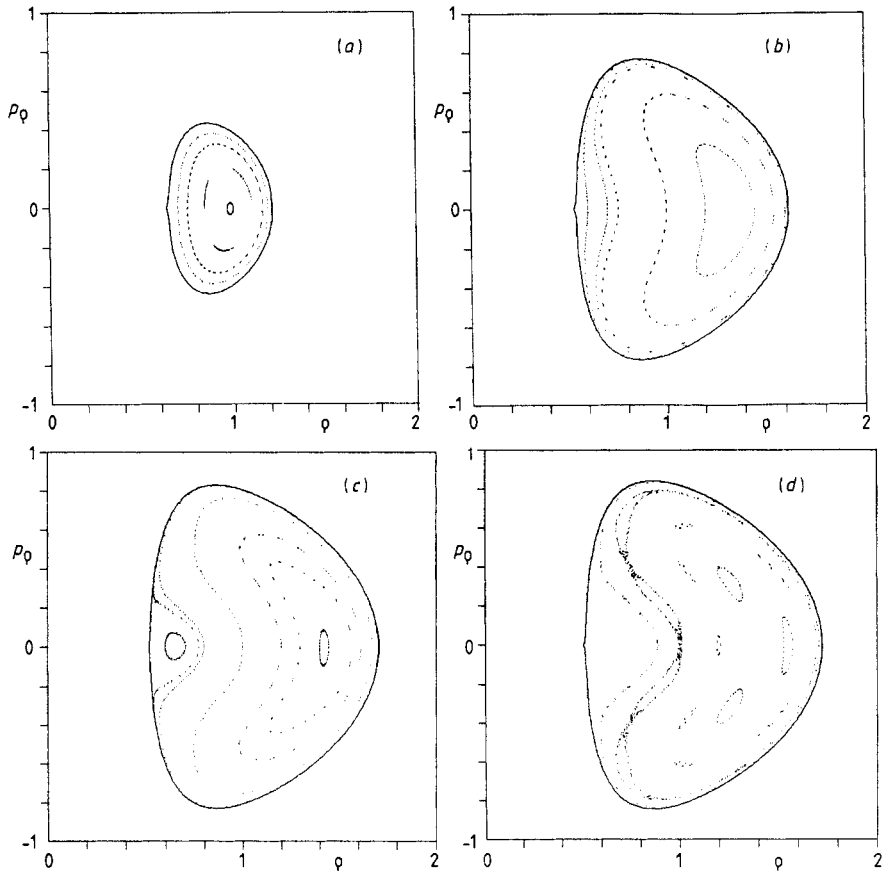

Figure 2. Transition points of the orbits through the Hill region $z = 0$, E = constant for ten different energies (*a*) $E = -0.3$, (*b*) $E = -0.1$, (*c*) $E = -0.05$, (*d*) $E = -0.04$, (*e*) $E = -0.03$, (*f*) $E = -0.01$, (*g*) $E = 0$, (*h*) $E = 0.1$, (*i*) $E = 0.3$, (*j*) $E = 0.5 = E_{esc}$. The full line is the boundary of the allowed region. See § 3.

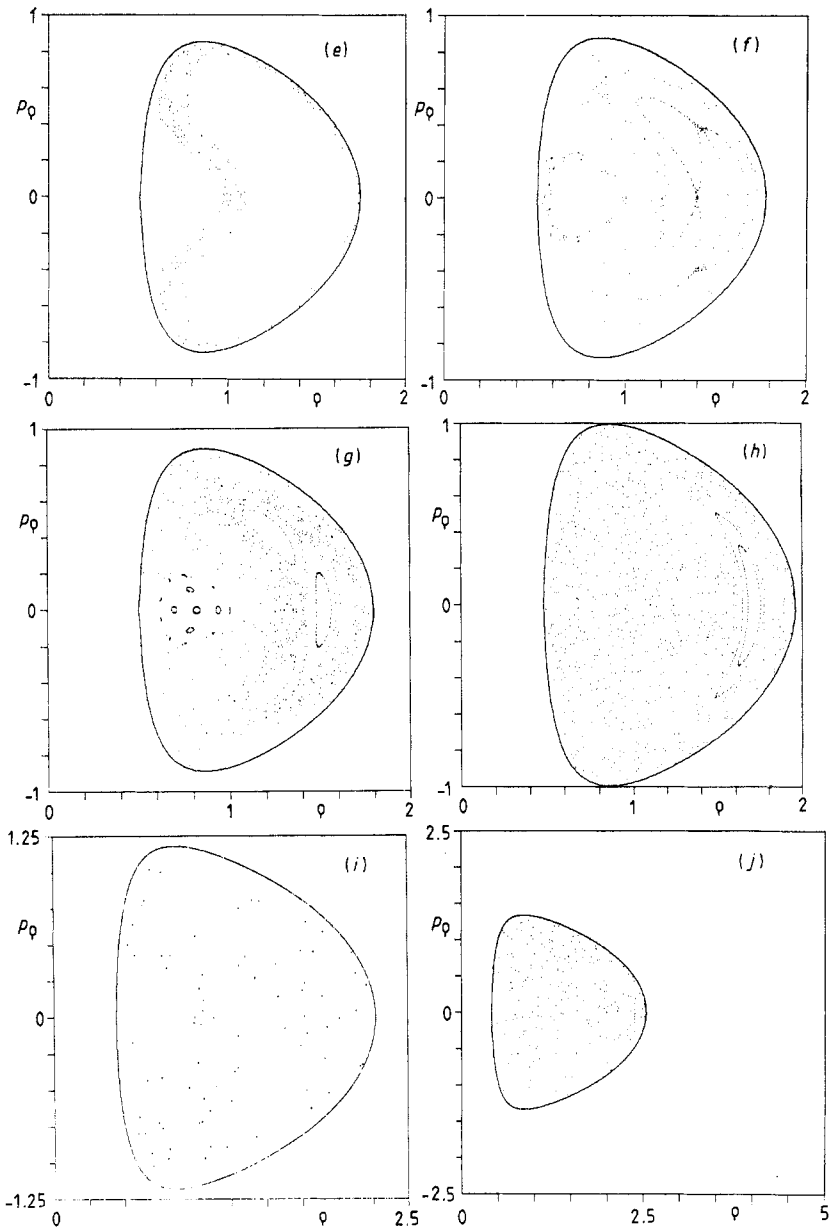

Figure 2. (*continued*).

been tested at every integration step by calculating the current value of the energy E_{num}, which has been compared with the prescribed value E. E_{num} has been seen to increase or decrease by less than 1 part in 10^7 after the 500th iterate has been calculated. Sometimes the accuracy was even better, such as 1 part in 10^{10}, depending on the energy E and the initial conditions.

The results are shown in figures 2(a)–2(j). The magnetic field strength γ and the angular momentum L are set equal to unity, $\gamma = L = 1$. For these values the minimal

energy $E_{\min} = -0.394\,3046$ and the escape energy $E_{esc} = 0.5$. At low energies, such as $E = -0.3$ and $E = -0.1$ in figures 2(a, b) each point of the Hill region D lies on a certain simply connected closed curve formed by the iterates $f_D^n(P)$ with n going up to 500. The outermost curve is the boundary itself, which is always an invariant curve by the Brouwer theorem on a homeomorphism on a compactum (Vinogradov 1979). Similarly, this theorem ensures the existence of at least one fixed point, which in our case is the centrum of the family of closed curves. It corresponds to a strictly periodic orbit in the phase space. One can also see that the curves, e.g. in figure 2(a), are almost periodic orbits, and fill the curve very slowly. For instance, the second innermost curve has almost period three, i.e. a point P on this curve is almost a fixed point of f_D^3. The fact that the whole region D is covered by invariant curves means that a third integral I_3 exists and is isolating for these initial conditions. The curves we see are then the intersection points of an invariant surface $I_3(p, q) = \text{constant}$ with the plane (ρ, p_ρ, $z = 0$). (Such an invariant surface will be discussed later.) At higher energy $E = -0.05$ in figure 2(c) the Hill region is still completely covered by the invariant curves, but a bifurcation has appeared, which produced a new fixed point surrounded by a family of closed curves. At a slightly higher energy $E = -0.04$ in figure 2(d) the whole structure changes more drastically: some of the closed curves (those with an approximate period three for example) bifurcated into three disconnected closed curves belonging to the same orbit! That means that the phase point now periodically jumps from one loop to the next and slowly fills these loops. The neighbouring curve is seen to decay in a set of seven disconnected simple loops. However, a really interesting 'curve' is the next one, which is multiply connected. In fact, it is apparent that it is no longer a curve, since the corners at the intersection phpnts are filled so that their measure is not zero. This is a clear indication that the stability of the corresponding orbit has been considerably weakened and that I_3 for these initial conditions does not exist in a strict sense, but is only effective in preventing the phase point from leaving a certain region (but not a surface) in phase space. Indeed, even after 600 iterations the phase point did not leave the 'curve'. It is interesting to see how this 'curve' proceeds to smear out when going to higher energy $E = -0.03$ in figure 2(e). Here 500 iterates are plotted and we see that the broad belt is essentially densely filled, although it is possible that small islands covered by invariant curves still exist within the belt. The phenomena occurring at the energies $E = -0.04$ and $E = -0.03$ show that we are near a stochastic transition, i.e. that the energy is close to the so-called critical energy E_{crit} (or stochastic transition energy), at which regions in phase space occur that are not covered by the invariant surfaces and the stability of orbits within them is lost. The neutral instability of orbits (Zaslavskii and Chirikov 1972) becomes even stronger as the energy is increased beyond E_{crit}, which eventually implies decay of correlations in phase space so that the motion appears to be completely random. (Observe that the instability in the corners of the intersection points in figure 2(d) has developed at the hyperbolic fixed points of an iterate of f_D.)

The picture at $E = 0$ in figure 2(g) is even more complicated. There are two fixed points, one in the right part (R) and another in the left part (L) of the picture. Both are surrounded by a set of simple closed curves. But as one goes further out these curves bifurcate into a chain of three loops (in the case of R) and in a chain of two loops (in the case of L; here the vertical pair is an invariant curve of $f_{(-,-)}$ while the horizontal pair is invariant with respect to $f_{(+,+)}$. All other invariant curves have been found identical for both mappings.) If one goes still further out, a stochastic region is reached, where the behaviour is chaotic in view of the strong instability of orbits. A very interesting curve is

the envelope of the innermost closed curve around R and of the chain of three loops. This is shown in figure 2(f) for a slightly different energy, $E = -0.01$, but is essentially the same. At even higher energies, e.g. $E = 0.1$, the regions covered by invariant curves rapidly diminish. In figure 2(h) with $E = 0.1$ only one island could be detected. It is filled with invariant curves around a fixed point, and surrounded by a completely stochastic region. Here a *single* orbit of iterates up to 1000 densely covers the whole region, starting from an arbitrary point of the region. At the energy $E = 0.3$ in figure 2(i) no island could be detected and the whole Hill region is found to be a single ergodic component. The same is observed (figure 2(j)) at the escape energy $E = E_{esc} = 0.5$, where the particle cannot yet escape, because the measure of the escape channel in the z direction (see equipotential lines in figure 1) is asymptotically zero, so that the particle cannot find a way out of the potential well. This can happen, however, at energies greater than E_{esc} by an arbitrarily small amount. Such escape orbits will be studied later on.

The conclusion of this section is that the third integral I_3 exists, is isolating and determines the stability of orbits for all energies below the critical energy $E_{crit} = -0.04 \pm 0.005$, and that above this energy it is effective only in a limited region of the energy surface, i.e. for a limited range of initial conditions compatible with the energy. The integral is thus certainly not analytic. The numerical result cannot be an existence proof, but it shows that even if I_2 is only approximate, the available numerical accuracy cannot distinguish between exact and approximate. No rigorous results in this regard are available (Zaslavskii and Chirikov 1972, Whiteman 1977), but it seems very plausible that the invariant curves do *not* cover the Hill region exactly with measure 1, although the measure of the complement is very close to zero. This would imply, if true, that the orbits possess only a certain stability property. The truly invariant curves are then boundaries of very thin stability bands, which cover the whole Hill region. In other words, either the motion of the phase point is confined to the interior of a shell bounded by two exactly invariant surfaces, or it moves on a truly invariant surface. In that case the third integral I_3 must be regarded as an integral of motion which is exact everywhere in phase space with $E < E_{crit}$ up to a set of measure 'close to zero'†. The usage of the words 'I_3 exists', 'integrable', etc should be understood in this spirit. On the other hand, the chaotic motion in a stochastic region of phase space is a consequence of a strong neutral instability (Rabinovich 1978, Zaslavskii and Chirikov 1972, Chirikov 1979), which is probably caused by overlapping and therefore by coupling of nonlinear resonances between different 'modes of oscillation'.

In an early work Gajewski (1970) attempted a stability analysis of the classical orbits in the vicinity of the potential bottom, i.e. for energies close to E_{min}. Near the equilibrium point he developed the potential into a power series and considered the stability of orbits confined to the plane $z = 0$, so that $p_z = 0$. In phase space this motion corresponds to the simple cycling of the phase point on the boundary of the Hill region (see figures 2(a)–2(j)). At sufficiently low energies this is of course a simple harmonic motion. He further asked whether small oscillations in the z direction are stable for this

† How close to zero? We emphasise again that the available numerical accuracy is not high enough to resolve the width of invariant shells and thus cannot give a quantitative answer. The possibility that the measure is exactly zero, i.e. that the invariant surfaces are everywhere dense on the energy surface, cannot be excluded as yet. Our conjecture that this measure vanishes only approximately is based on results of the KAM theory (Arnold and Avez 1968). On the other hand, for energies above the critical energy it has been shown by Henon and Heiles (1964) that the relative volume of the stochastic region increases linearly. But the width of the invariant shells covering the laminar islands could not be resolved as well.

type of motion, which is described by the invariant curves within a thin belt at the boundary of the Hill region. The small oscillations in the z direction are again essentially harmonic, but the frequency depends on the instantaneous value of the ρ coordinate, so that the z oscillator is modulated by the periodic changes of ρ. This is then a simple parametric resonance (Arnold and Avez 1968), governed by an equation for the z oscillations which is equivalent to the famous pendulum equation with harmonically varying frequency, i.e. the Mathieu equation. He therefore suggested that the resonant orbits, i.e. such that the frequencies of both harmonic oscillators are rationally connected, are unstable. However, this analysis is oversimplified for two reasons: firstly, the motion of the ρ oscillator cannot be kept fixed when the amplitude of the z oscillations increases due to the parametric excitation, since this would mean that the total energy of both oscillators is not constant. Secondly, his analysis is in fact linear, in that he assumes that the frequency of the z oscillator does *not* depend on the amplitude of the z oscillations. Because the frequency in fact *does depend* upon the amplitude (the so-called non-isochronicity, implied by the nonlinearity of the system (cf Zaslavskii and Chirikov 1972)) a resonant orbit will become non-resonant when the amplitude is slightly increased. This is in fact the way in which nonlinearity implies stability, although the system appears to be unstable when analysed to the lowest, linear approximation. The actual reason for an instability of a nonlinear system is the overlapping or merging of resonances, as has been pointed out by Zaslavskii and Chirikov.

4. The dependence of the critical energy on the magnetic field strength

Similar calculations to those described in § 3 have been performed for $L = 1$ and various values of $\gamma = 0.1, 0.5, 2, 5, 10, 50$. The value of the critical energy $E_{crit} = E_{crit}(\gamma, L = 1)$ has been determined for this discrete set of points. In figure 3 we plot the differences $E_{esc}(\gamma, 1) - E_{crit}(\gamma, 1)$ and $E_{crit}(\gamma, 1) - E_{min}(\gamma, 1)$ as functions of the magnetic field

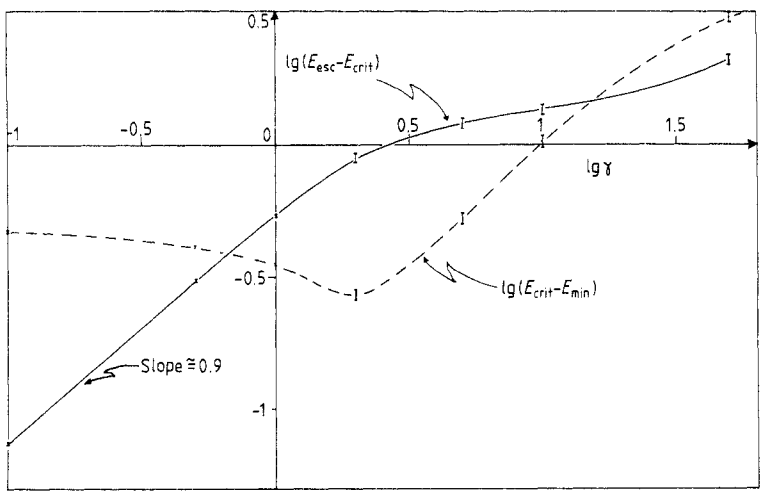

Figure 3. A plot of the differences $\lg(E_{esc} - E_{crit})$ (full line) and $\lg(E_{crit} - E_{min})$ (dotted line) versus $\lg \gamma$. Note that the critical energy E_{crit} approaches the escape energy E_{esc} as a power with an exponent ≈ 0.9 when the magnetic field strength goes to zero.

strength. The critical energy lies always between E_{esc} and E_{min}. In the Zeeman region, where γ is small and the Hamiltonian nearly integrable, as well as in the Landau region, where γ is large and the system is again almost integrable, the critical energy approaches the escape energy. For $\gamma \to 0$ it obeys a power law with an exponent ≈ 0.9. On the other hand, in the intermediate region ($\gamma \approx 1$) the critical energy is lowest and comes close to the minimal energy. This is clearly seen in figure 4 where the relative critical energy $\mu(\gamma) := (E_{crit} - E_{min})/(E_{esc} - E_{min})$ is plotted. Its minimum value $\mu_{min} = 0.22$ is reached at $\gamma_{min} \approx 2.7$, while it approaches unity in both limiting cases. For all energies $E > E_{crit}$ lying in the shaded region above $\mu(\gamma)$, the third integral I_3 does not exist, or it exists in only limited regions of the energy surface in phase space. Below the critical curve we have the regular region, where I_3 exists for all initial conditions compatible with the given energy.

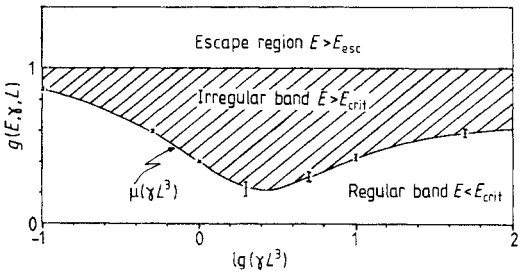

Figure 4. A plot of the relative energy $g(E, \gamma, L) := (E - E_{min})/(E_{esc} - E_{min})$ versus $\lg(\gamma L^3)$. The critical relative energy $g(E_{crit}, \gamma, L) = \mu(\gamma L^3)$ approaches unity in the limits $\gamma \to 0$ and $\gamma \to \infty$. In the regular band the third integral exists, while in the irregular band it exists at most for a limited range of initial conditions compatible with the energy. The minimum of μ equals ≈ 0.22 for $\gamma L^3 = 2.7$.

5. The dependence of the critical energy on angular momentum

We now show that the critical energy is known for each $L \neq 0$ if it is known at some arbitrary $L \neq 0$, say, as in our particular case, $L = 1$. The reason is a simple invariance of the Hamiltonian H_r from equation (2) under a certain rescaling of the variables. To show this we write $H_r = H_r(\rho, p_\rho, z, p_z; \gamma, L)$. Then the following invariance can easily be verified:

$$H_r(\rho, p_\rho, z, p_z; \gamma, L) = L^{-2} H_r(\rho/L^2, p_\rho L, z/L^2, p_z L; \gamma L^3, 1), \tag{5}$$

which simply means that the coordinates have been rescaled by a factor L^{-2}, while time has been rescaled by a factor L^{-3}, and the energy by L^{-2} together with γ being rescaled by L^3. We have thus

$$\begin{aligned} E_{min}(\gamma, L) &= L^{-2} E_{min}(\gamma L^3, 1), \\ E_{esc}(\gamma, L) &= L^{-2} E_{esc}(\gamma L^3, 1) = \tfrac{1}{2}\gamma |L|, \\ E_{crit}(\gamma, L) &= L^{-2} E_{crit}(\gamma L^3, 1). \end{aligned} \tag{6}$$

We have, therefore, the immediate result that the relative energy

$$g(E, \gamma, L) := (E - E_{min}(\gamma, L))/(E_{esc}(\gamma, L) - E_{min}(\gamma, L))$$

obeys the equations

$$g(E, \gamma, L) = (E - E_{\min}(\gamma L^3, 1))/(E_{\text{esc}}(\gamma L^3, 1) - E_{\min}(\gamma L^3, 1)),$$
$$g(E_{\text{crit}}, \gamma, L) = \mu(\gamma L^3), \tag{7}$$

where $\mu(x)$ is plotted in figure 4. As a consequence, the minimal value of $g(E_{\text{crit}}, \gamma, L)$ is always equal to $\mu_{\min} \cong 0.22$ and is reached at $\gamma_{\min} \cong 2.7/L^3$. This means that for higher angular momentum L, the intermediate region of strong-field mixing (between the Coulomb and the magnetic field) shifts to lower field strengths. The value of the minimal energy $E_{\min}$ can be given explicitly as

$$E_{\min}(\gamma, L) = (2 - 3\lambda_0)/2L^2\lambda_0^2, \qquad \lambda_0 := \lambda(\gamma L^3/2), \tag{8}$$

where the function $\lambda(x)$ is defined as the positive root of the equation†

$$x^2\lambda^4 = 1 - \lambda. \tag{9}$$

Obviously $\lambda \in [0, 1]$. A plot of the function $\lambda(x)$ is given in figure 5.

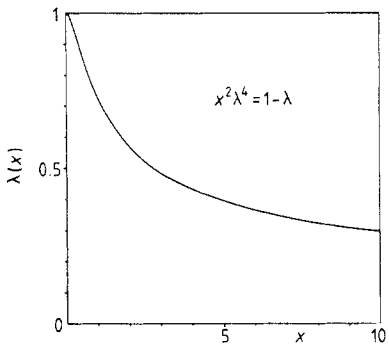

Figure 5. The positive root λ of the equation $x^2\lambda^4 = 1 - \lambda$ as a function of x. For small x one has $\lambda \cong 1 - x^2$ and for $x \gg 1$, $\lambda \cong x^{-1/2}$.

For small x we have $\lambda(x) \cong 1 - x^2$, while for $x \gg 1$ one has $\lambda(x) \cong 1/\sqrt{x}$. Therefore

$$E_{\min} \underset{\gamma \ll 1}{=} -\tfrac{1}{2}L^{-2}(1 - \tfrac{1}{4}\gamma^2 L^6 + O(\gamma^4 L^{12})), \tag{10}$$

while

$$E_{\text{esc}} - E_{\min} \xrightarrow[\gamma \to \infty]{} \tfrac{3}{2}(\gamma L^3/2)^{1/2}. \tag{11}$$

Finally, it should be noted that Gajewski (1970) eliminated the field dependence of the Hamiltonian by an appropriate stretching of variables (rescaling of time and coordinates), and considered the dependence on the angular momentum L instead. Unfortunately, as is clear, one cannot eliminate the dependence on both parameters.

† Observe the interesting fact that the Hamiltonian (1) can be brought to a form with a 'convex linear mixing' of the magnetic and the Coulomb potential by rescaling the momenta $p' = \lambda p$ and coordinates $q' = q/\lambda$ with $H' = \lambda^2 H$, the parameter λ obeying precisely the condition (9), namely $\lambda = \lambda(\gamma)$. Under this transformation the new Hamiltonian reads $H' = p'^2/2 + (1 - \lambda)\rho'^2/8 - \lambda/r'$, i.e. for $\lambda = 0$ we have no Coulomb interaction, while for $\lambda = 1$ we have no magnetic field.

6. An invariant surface defined by the third integral

Having obtained the range of energies $E < E_{crit}$ for which the third integral exists, we would like to get more insight into the nature of this integral. Numerically this is possible e.g. when we study other Poincaré mappings defined by the Hamilton system. The aim is to obtain intersection curves of an invariant surface $I_3(p, q) =$ constant with different projection planes. This has been done for the case $\gamma = L = 1$ and $E = -0.1$, for an orbit defined by the initial conditions $\rho = 1$, $p_\rho = z = 0$ and $p_z = [2(E - U)]^{1/2}$. In figure 6 the intersection curve of this surface with the plane $p_\rho = 0$ is shown. The curve

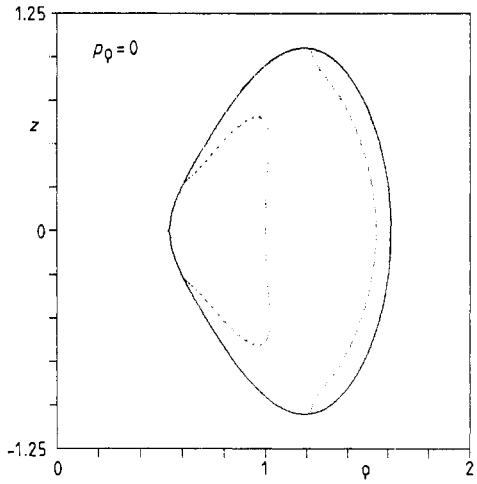

Figure 6. The intersection curve of the invariant surface of § 6 with the plane $p_\rho = 0$ and $E =$ constant $= -0.1$. The full line is the boundary of the allowed region.

consists of two disconnected branches and the phase point can jump from one branch to another. The topology of the invariant surface is revealed in figures 7(*a*)–7(*h*). Here the intersection curves with the planes $z = 0, 0.1, 0.2, 0.25, 0.3, 0.4, 0.6, 0.8$ are plotted. The full lines (C_+ curves) correspond to the upward motion ($p_z > 0$) of the phase point, while the dotted lines (C_- curves) correspond to the downward motion ($p_z < 0$). We see that C_+ and C_- are conjugate with respect to the reflection $p_\rho \to -p_\rho$ and are identical in (ρ, p_ρ) coordinates when $z = 0$. It has been found that the curves C_+ and C_- are also conjugate with respect to the reflection $z \to -z$, so that the surface is invariant under $(z, p_z) \to (-z, -p_z)$. We see that the phase point is moving upward on a cylinder (defined by C_+ curves), reaches the boundary when $p_z = 0$ and moves downward on a different cylinder (defined by C_- curves). The motion is obviously quasiperiodic on the surface whose geometrical symmetries can be summarised as follows: $I_3(\rho, p_\rho, z, p_z) = I_3(\rho, p_\rho, -z, -p_z) = I_3(\rho, -p_\rho, z, -p_z)$ and the special case $I_3(\rho, p_\rho, 0, p_z) = I_3(\rho, p_\rho, 0, -p_z) = I_3(\rho, -p_\rho, 0, p_z)$. The topology of this specific invariant surface is in fact of the simplest kind, i.e. the surface is an invariant torus. The reason is that at $E = -0.1$ the system is not far from the case of two weakly coupled harmonic oscillators in the vicinity of the bottom of the potential well $E_{min} = -0.394\,3046$. However, this type of the invariant surface is expected to be the generic case for all energies below the first bifurcation leasing to the appearance of a second fixed point (see § 3 and

figure 2(*c*)). Note that most of the bifurcations observed in figures 2(*a*)–2(*j*) are *not* generic for area preserving maps (see Greene *et al* 1981 and references therein).

7. The escape orbits

For energies higher than the escape energy the potential lines open and the particle can escape to infinity along the z axis (see figure 1). A phase orbit leaving the plane $z = 0$ will possibly never return to this plane, so that the plane $p_\rho = 0$ is more suitable for studying the escape orbits. Such an orbit is shown in figure 8(*a*), where $E = 0.6$, while $\gamma = L = 1$ ($E_{esc} = 0.5$). The initial conditions were $\rho = 2.68$, $p_\rho = 0$, $z = 0$ and $p_z = [2(E - U)]^{1/2}$. The particle moves up and down while spiralling around the z axis and reflecting at the equipotential line $E = 0.6$, until it finally finds the escape channel and

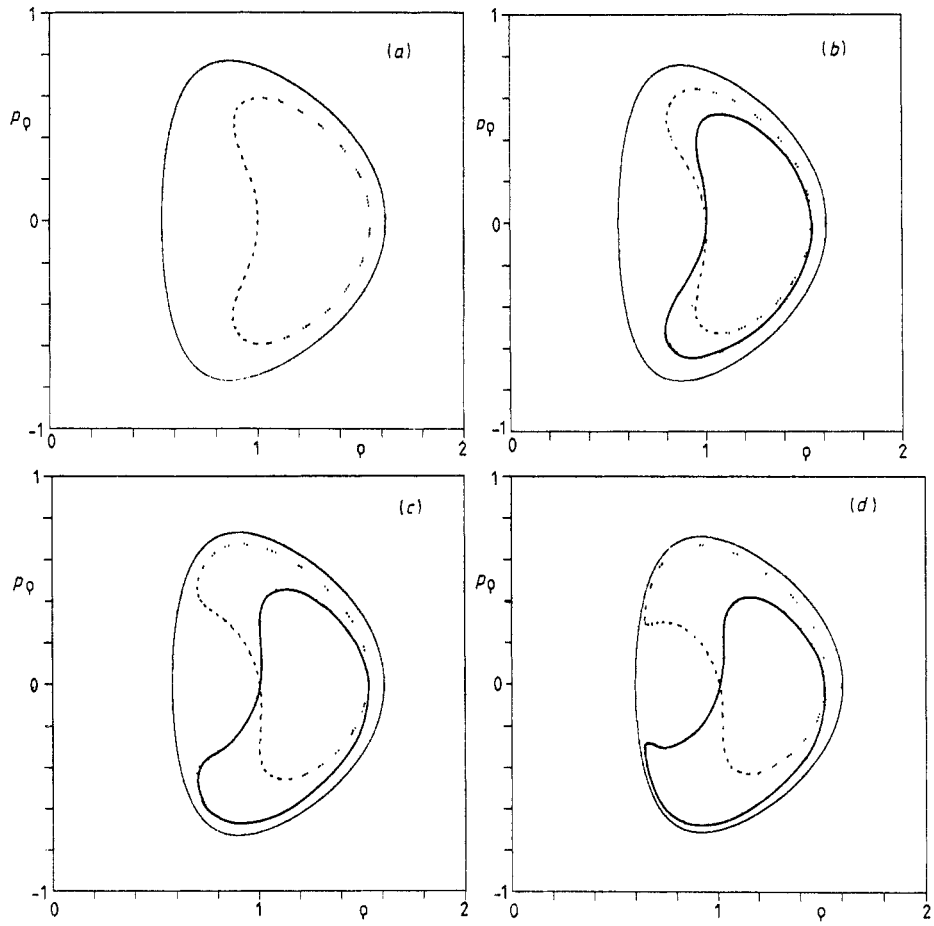

Figure 7. The intersection curves of the orbit defined by the initial conditions $\rho = 1$, $p_\rho = z = 0$ and $p_z = [2(E - U)]^{1/2}$ with the planes (*a*) $z = 0$, (*b*) 0.1, (*c*) 0.2, (*d*) 0.25, (*e*) 0.3, (*f*) 0.4, (*g*) 0.6, (*h*) 0.8. Here $\gamma = L = 1$ and $E = -0.1$. The full lines within the allowed region correspond to the upward motion ($p_z > 0$), whereas the dotted lines correspond to the downward motion ($p_z < 0$) of the phase point.

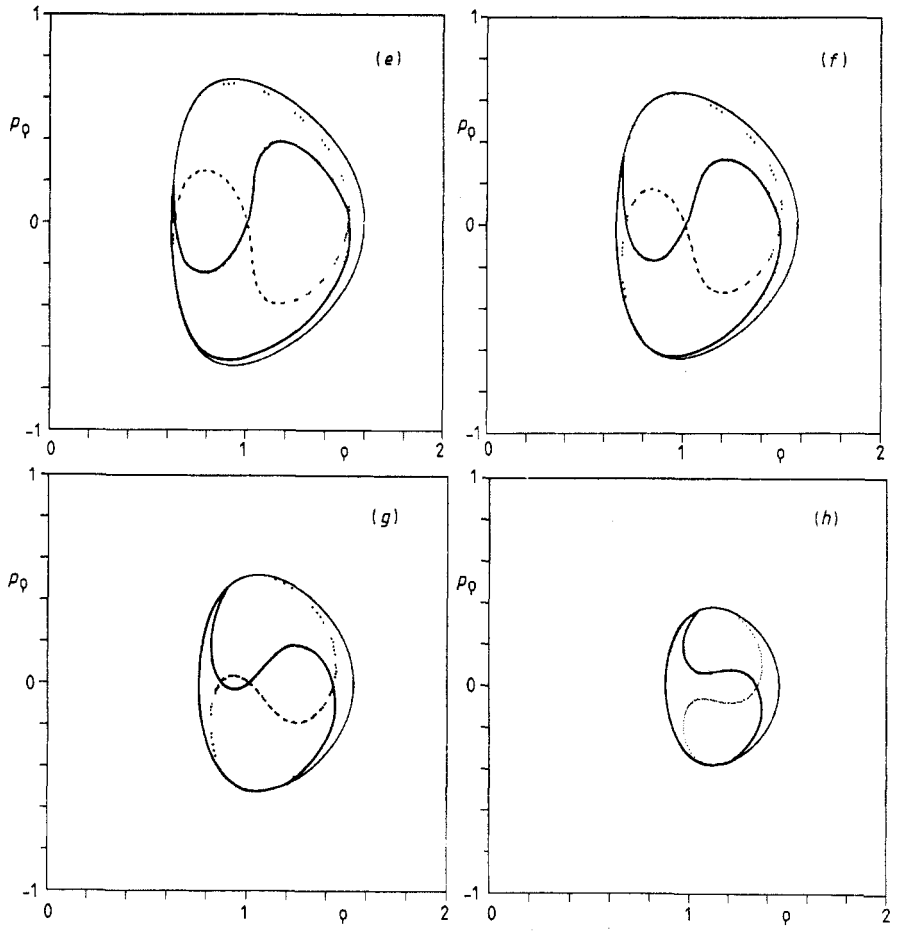

Figure 7. (*continued*).

goes to $z = -\infty$. It can be seen that the motion not far from the plane $z = 0$, say $|z| \geqslant 3$, is adiabatic, i.e. the motion becomes partially ordered, and an adiabatic invariant is effective. The value of the adiabatic invariant can change abruptly in the stochastic region near the plane $z = 0$. Here the Coulomb potential and the magnetic potential are of comparable strength, while further out, say for $|z| \geqslant 3$, the Coulomb interaction becomes asymptotically negligible so that $\oint p_\rho \, d\rho$ is an adiabatic invariant. In view of the stochastic motion near the plane $z = 0$ the particle can reach any value of the adiabatic invariant so as to escape. In the case of figure 8(*a*) three reflections were necessary to find the escape channel. This is also illustrated in figure 8(*b*) where the projection (ρ, p_ρ) of the point (ρ, p_ρ, z) at each integration step is plotted with a small rectangle for $z > 0$ and a small triangle for $z < 0$. This type of escape orbit has been found typical in the sense that no initial conditions for any $E > E_{esc}$ could be found for which the particle would remain in a limited region of phase space. In other words: the stochastic behaviour near the plane $z = 0$ of strong mixing of potentials ensures that the energy condition $E > E_{esc}$ is also a sufficient condition for escape.

It seems to be a general rule that the critical energy, i.e. the stochastic transition energy, of a non-integrable Hamilton system always lies either below the escape energy

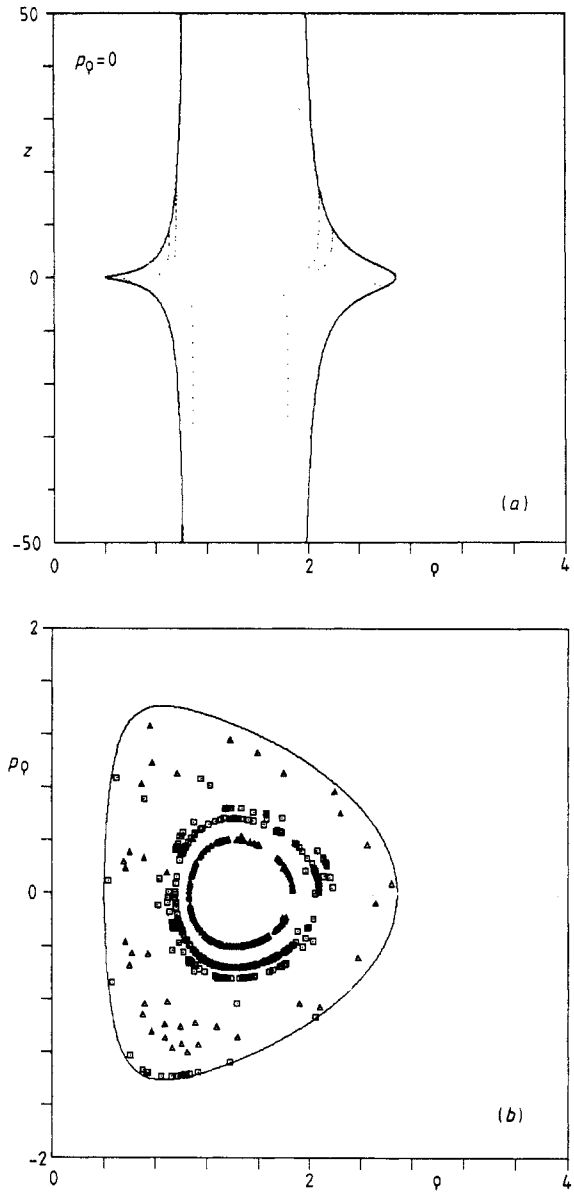

Figure 8. An escape orbit, $E = 0.6$, $\gamma = 1$, $L = 1$, plotted (a) in the plane $p_\rho = 0$ and projected (b) to the plane $z = 0$. See § 7. ⊡ $z > 0$, △ $z < 0$.

if the potential well is a single well, or below the transition energy (corresponding to a separatrix in phase space), at which the phase point can enter an adjacent potential well (when the particle moves in a double potential well). This observation is supported also by the numerical works by Henon and Heiles (1964) as well as by Ali and Somorjai (1980), who studied a double potential well. Indeed, this is what one would expect on physical grounds: a particle whose energy is near the escape energy is almost free, and in the course of its (still finite) motion passes through regions where the influence of the

potential is very weak. As a consequence, the motion is very sensitive to any small perturbations which are nevertheless comparable to the potential (in the remote regions). In other words, the motion of a system whose energy is close to the escape energy (or transition energy in the case of a double well) is unstable. (One speaks of the so-called neutral instability, since due to Liouville's theorem the phase space volume is conserved, so that a mixing rather than unlimited divergence of orbits occurs.) In this regard one can consider the analogy with Sinai's 'billiard theorem' (Arnold and Avez 1968). There it has been shown that the motion of a point particle in a box with convex obstacles and/or concave walls is unstable and that it is in fact mixing (which implies ergodicity). The analogy is now in the observation that the equipotential surfaces in configuration space open when the escape (or transition) energy is reached. They, being the boundaries of the allowed region (=: box), must therefore become concave at least in some region. In spite of the fact that the walls are not rigid, since in the vicinity of the wall the particle is repelled by an approximately constant force pointing inwards and perpendicularly to the equipotential surface, the reflection obeys the law 'angle of incidence = angle of reflection' in the sense that its parabolic orbit is symmetric with respect to the point of the closest approach. One expects a qualitatively similar influence of the boundaries of the box on the motion of the system as a whole; the system should be unstable. A generalisation of the Sinai theorem to the case of a box with soft concave walls is thus of great interest. A rigorous proof would explain the 'rule' observed in numerical experiments.

However, matters are not as simple as they seem. Clearly, such a rough criterion overestimates the role of the boundaries and underestimates the interactions with the potential in the interior of a box. A precise formulation of the criterion is more involved. This is shown by table 1 where the numerically determined critical energy E_{crit} is compared with the energy E_{geom} at which the equipotential line $U(\rho, z) = E_{geom}$ = constant becomes concave in some region (i.e. its curvature becomes negative). E_{geom} is neither the upper nor the lower bound for the critical energy, but its value is not far from E_{crit}.

Table 1. Comparison of the critical energy E_{crit} with the energy E_{geom} at which the equipotential line is concave for the first time as the energy is increasing. (The value of the angular momentum L is equal to unity, $L = 1$.)

γ	E_{geom}	E_{crit}
0.1	−0.1531	−0.025 ± 5
0.5	−0.0942	−0.055 ± 5
1	+0.0413	−0.040 ± 5
2	+0.3895	+0.10 ± 5
5	+1.611	+1.30 ± 5
10	+3.810	+3.65 ± 5
50	+22.597	+22.9 ± 1

8. A summary of the classical case

We conclude (see figure 4) that for energies E smaller than the critical energy E_{crit} the third integral exists and the Hamilton system is (nearly) integrable. When the energy E

lies in the irregular band, i.e. when $\mu(\gamma L^3) \leq g(E, \gamma, L) \leq 1$, the system is stochastic and I_3 exists at most in small islands of the initial conditions, whose measure goes to zero as the energy approaches the escape energy. Above the escape energy, i.e. when $g(E, \gamma, L) > 1$ or $E > E_{esc} = \frac{1}{2}\gamma|L|$, the particle can escape to infinity $|z| = \infty$, and its motion again becomes partially ordered in the sense that the adiabatic invariant $\oint p_\rho \, d\rho$ is effective, becoming asymptotically an exact constant of motion as $|z| \to \infty$. The motion is, however, still stochastic near the plane $z = 0$, where the Coulomb and the magnetic potential can be of comparable strength. The energy condition $E > E_{esc}$ is a sufficient condition for escape.

Figure 4 shows that the width of the irregular band decreases rapidly as one approaches the limiting cases $\gamma \to 0$ or $\gamma \to \infty$, so that the Hamiltonian is then nearly integrable for almost all energies. The maximal width (with respect to varying γ and L) of the irregular band equals 0.78 and is reached for $\gamma_{min} = 2.7/L^3$.

In the limit $L \to 0$ we have $E_{min}(\gamma, L) \to -\infty$, $E_{esc} \to 0$, while $E_{esc}(\gamma, L) - E_{crit}(\gamma, L) = L^{-2}(E_{esc}(\gamma L^3, 1) - E_{crit}(\gamma L^3, 1)) \propto L^{-2}(\gamma L^3)^{0.9} \to 0$. Hence in the limit $L \to 0$ the critical energy comes arbitrarily close to the escape energy uniformly for all finite γ, and the Hamiltonian is then integrable for all energies below the escape energy $E_{esc} = 0$.

9. Relation to the quantum mechanical problem

The analogy between classical and quantum mechanics when formulated as Lie algebras of Poisson brackets is striking, but cannot be raised to an isomorphism (Abraham and Marsden 1978, Kundt 1966). This presents undoubtedly serious limits to a straightforward parallelism between the classical and quantum mechanical properties of a Hamilton system.

Our case does not seem to suffer from the non-existence of the general homomorphism. Our conjecture is that a quantum mechanical counterpart of the third integral of motion I_3 exists for $E < E_{crit}$. It is precisely the dynamical symmetry generated by this quantum mechanical constant of motion which has been detected in the numerical experiment by Zimmerman *et al* (1980). They studied the energy spectrum of the Hamiltonian (2) with $L = 0$, and γ in the range between 4.26×10^{-5} and 8.52×10^{-3} (i.e. the magnetic field strength $10\text{T} \leq B \leq 10^3\text{T}$). They inspected the energy levels below the zero-field ionisation limit $E = E_{esc} = E_{crit} = 0$ which lie in the classical regular band. The observed crossings and/or close anti-crossings are therefore in complete agreement with the existence of the third integral I_3 and support the conjecture above. Not in agreement is their observation that the separation of the anti-crossings rapidly diminishes as the energy of the levels increases. From the classical behaviour of the Hamiltonian one would expect that the dynamical symmetry is most effective at low energies, whereas Zimmerman *et al* conclude the opposite. The reason for this discrepancy might be explained when more is known about the approximate dynamical symmetry.

Of course, a final confirmation of the conjecture can be supplied only when the third integral of motion I_3 and the corresponding quantum mechanical observable (commuting with the Hamiltonian) are explicitly constructed. As mentioned in the Introduction, algorithms for the construction of formal integrals of motion in classical mechanics are known, but can be so complicated that a computer must be used to do all the algebraic manipulations (Gustavson 1966). In the case of the Henon–Heiles potential (1964), the invariant surfaces defined by the formal integral of motion agree

with the numerical calculations for all energies below the critical energy. We therefore propose to use such an algorithm in order to construct a formal integral of motion which is close to I_3 in the regular band (figure 4). The same algorithm can, we hope, be translated into the language of quantum mechanics, so that a construction of the corresponding quantum mechanical constant of motion could be done along with the classical one. The accuracy of the formal result can be tested by comparing the invariant surfaces generated by the formal integral with those calculated in this work. Once we have constructed the formal constant of motion corresponding to I_3 we can use it to approximately separate the Schrödinger equation. In this way we hope to obtain more accurate values of the energy eigenvalues, as has been suggested by Zimmerman *et al* (1980).

However, from our classical calculations it is clear that this approach can be successful only for a limited range of energies, namely only for levels below the critical energy. It is expected that above the critical energy such a method fails, since the classical Hamiltonian is stochastic. It should therefore be extremely interesting to study the energy spectrum for the levels in the vicinity of the critical energy in order to see whether the spectrum changes qualitatively at the transition between the regular and irregular bands. For this purpose more calculations like that by Zimmerman *et al* should be performed.

A reason for the usefulness of the classical calculations of the present work is not only a determining of the conditions for the existence of the constant of motion (note that we have determined the critical energy for a large range of the magnetic field strength and for all values of the angular momentum L). An investigation of the correspondence of the classical and quantum mechanical non-integrable Hamilton systems is of general interest. Although a lot of work has been done in this respect (Percival 1979, Gutzwiller 1978, Berry 1978, 1980, 1981, 1982), we still lack a clear understanding of the subject. In particular, the problem of the hydrogen atom in a magnetic field could serve as a test object of the ideas by Percival. He studied the quantisation of the Henon–Heiles potential and proposed to distinguish between the regular energy levels (with energies lying in the regular band, i.e. below the critical energy), and the irregular levels (corresponding to the irregular band). The former have been found to be stable under small perturbations of the Hamiltonian, while the latter are unstable and in contrast to the regular levels randomly distributed. There is, however, from what we know about the hydrogen atom in a magnetic field, no clear evidence for such a clean classification of the energy levels. A recent work by Clark and Taylor (1980) seems to be consistent with the existence of the irregular levels above the critical energy.

10. A note on the correspondence diagram

Since angular momentum and parity together with the energy are not the only existing symmetries of the Hamiltonian (1), one cannot simply use the Neumann-Wigner non-crossing rule for the energy levels (of given parity and given angular momentum) as functions of the magnetic field strength. Due to the third symmetry, crossings and/or close anti-crossings (with separation possibly less than the natural line width) are allowed, depending on whether the dynamical symmetry can be considered exact or approximate. Therefore it is clear that even the question of the correspondence diagram relating the levels in the Zeeman and Landau regions cannot be answered at

present. Many different proposals have been made in this respect (Simola and Virtamo 1978, Garstang 1977, Rau and Spruch 1976, Robnik 1980a, b). In the latter work I stated a theorem on the nodal structure of the wavefunctions of a pure quantum mechanical state, and claimed that the number of nodal cells defined by the nodal surfaces in configuration space is a conserved quantity (adiabatic invariant) and can be used to establish the correspondence diagram. The proof was based on a lemma that the volume of a nodal cell is uniformly bounded from below when the energy is uniformly bounded from above, so that a newly formed nodal cell cannot have arbitrarily small volume. The lemma thus prohibits the disappearance of an $(N-1)$-dimensional boundary between two nodal cells in N-dimensional configuration space. The theorem is thus valid in one dimension, $N=1$. In a many-dimensional configuration space two nodal cells can touch in a surface of $N-2, N-3, \ldots, 1, 0$ dimensions, whose diappearance is *not* forbidden by the lemma, so that a new, larger nodal cell can be formed by merging of two cells along an $(N-2)$, $(N-3)$, . . .-dimensional boundary. The proof, therefore, contained a gap. While the lemma (Robnik 1980b) is correct, the theorem must be considered as false for all N except $N=1$ and the correspondence diagram as a mere conjecture like that by Garstang (1977) which was based on arguments by Rau and Spruch (1976). However, it might appear that the number of nodal cells *generically* (i.e. in almost all cases) *is* a conserved quantity, e.g. when the spectrum is non-degenerate (Albert 1973, Uhlenbeck 1976).

11. Conclusions

We have seen that for the hydrogen atom in a magnetic field as a classical Hamilton system there exists a critical energy E_{crit} for each value of the angular momentum and magnetic field strength, which lies above the minimum energy $E_{\min}$ of the potential well and below the escape energy E_{esc}. It approaches the escape energy in the limits of vanishing and very large magnetic field strength, while it is lowest in the intermediate region where $\gamma \cong 1$, i.e. $B \cong B_0 = 2.35 \times 10^9$ G. For energies E between $E_{\min}$ and E_{crit}, the third integral exists and is isolating for all initial conditions compatible with the energy surface E = constant (regular band). For energies E between the critical energy E_{crit} and the escape energy E_{esc} regions of initial conditions exist in which the system is unstable and behaves stochastically. As the energy E approaches the escape energy E_{esc}, the system becomes completely stochastic.

The existence of the third integral is in agreement with the numerical calculations of the quantum mechanical energy levels made by Zimmerman *et al* (1980), who concluded that an approximate dynamical symmetry of the Hamiltonian must exist. They assumed that the symmetry is more effective at higher energies, whereas the present classical calculations show the opposite. To clarify this discrepancy it is suggested to perform Zimmerman's calculations also for levels above the critical energy, i.e. in the irregular band. (Unfortunately, their calculations performed so far refer to the levels of even parity and zero angular momentum $L=0$, in which case $E_{\text{crit}} = E_{\text{esc}} = 0$, so that all levels inspected in their work lie in the classical regular band, i.e. below the critical energy.)

Their suggestion to use this dynamical symmetry in order to approximately separate the Schrödinger equation and to obtain more accurate values of the energy levels should be followed along these lines: (i) construct the formal integral of motion using an algorithm like that by Gustavson (1966); this is not a trivial procedure and one has to

use a computer to do all the algebraic manipulations; (ii) compare the invariant surfaces defined by this formal integral of motion with those obtained in this work; this shows the accuracy of the formal result; (iii) the formal integral is to be translated into its quantum mechanical counterpart; (iv) finally, one solves the Schrödinger equation.

However, this procedure cannot be successful where the third integral does not exist, i.e. in the irregular band $E > E_{crit}$, and cannot yield the complete energy spectrum. In the irregular band one cannot abandon the usage of either quasiclassical methods, like that by Gutzwiller (1980), or the numerical methods. Of course, both approaches are important. In particular, it would be interesting to see what is the qualitative difference (if any) between the spectra in the regular and irregular bands. This question is of general interest in the quantisation of non-integrable systems.

Concerning the study of general properties of classical non-integrable Hamilton systems, two problems are of central importance on which more work should be done: (i) the investigation of the precise nature of the third integral; is it exact or approximate?; are the invariant surfaces everywhere dense on an energy surface $E =$ constant $< E_{crit}$, or not? (ii) is it possible to generalise Sinai's billiard theorem to the case of a box with soft and concave boundaries; this would explain the observed 'rule', that the stochasticity sets in below the escape (or transition) energy, i.e. $E_{crit} < E_{esc}$.

From the general point of view, the problems indicated are important because they are, in fact, bridges between classical mechanics, quantum mechanics and statistical mechanics. We may hope to understand their interrelations in greater depth when solving such problems.

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