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LETTER TO THE EDITOR

Analytic simulation of the Poincaré surface of sections for the diamagnetic Kepler problem

H Hasegawa, A Harada and Y Okazaki

Department of Physics, Kyoto University, Kyoto 606, Japan

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Abstract. The Poincaré surface-of-section analysis which we previously reported on the diamagnetic Kepler problem (classical hydrogen atom in a uniform magnetic field) in a transition region from regular to chaotic motions is simulated by an analytic means, by taking intersections of the energy integral and the approximate integral Λ of Solovev to obtain sections of the two separate regions of the motion that exist in the limit of a weak magnetic field ($B \to 0$). The origin of the unique hyperbolic point and the separatrix around which the onset of chaos takes place are thus identified. The invariant tori arising near the full chaos are shown to be simulated by this method but with modified parameter values in the expression Λ.

The experimental indication by Zimmerman *et al* (1980) and the theoretical consideration by Clark and Taylor (1980) about the existence of an approximate third integral in the problem of non-integrable Hamiltonian dynamics of hydrogen in a uniform magnetic field stimulated a number of further investigations of the quantum mechanical energy (or, optical) spectra of diamagnetic Rydberg atoms in search of a possible regularity (Castro *et al* 1980, Delande and Gay 1981, Delande *et al* 1982, Robnik 1981, Clark 1981, Solovev 1981, Herrick 1982, Sumetskii 1982, Delos *et al* 1983).

The first concrete presentation of the third integral was admittedly due to Solovev (1981, 1982), who obtained the form

$$\Lambda = 4(A_x^2 + A_y^2) - A_z^2 \tag{1}$$

where $\boldsymbol{A}$ is the Runge–Lenz vector given by

$$\boldsymbol{A} = \boldsymbol{p} \times (\boldsymbol{r} \times \boldsymbol{p}) - \boldsymbol{r}/r. \tag{2}$$

His derivation was based on the method of perturbation average in classical mechanics (Arnold 1979). By putting the form Λ in (1) into a scheme of semiclassical quantisation of the motion of the polar angle θ in the usual polar coordinate system, Solovev found that in the limit of a weak magnetic field there exist two separate regions of the Kepler motions. One of these corresponds to $\Lambda > 0$ of a rotational nature and the other to $\Lambda < 0$ of a librational nature, reflecting a neutation and an oscillation, respectively, of the Runge–Lenz vector (Delande *et al* 1982). This feature was confirmed by a subsequent quantal formulation by Herrick (1982) and a more elaborate classical analysis by Delos *et al* (1983).

The purpose of this letter is to show that the very existence of the separate motions mentioned above, if considered as the unperturbed motion on which the magnetic field

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acts as perturbation, gives rise to *chaos* inherent in such non-integrable Hamiltonian dynamics. This will be seen from an analytic construction of the Poincaré surface of section by using Solovev's approximate integral and comparing it with our previous result, in which we exhibited a transition of the solution of the equations of motion from its regular behaviour to a chaotic one (Harada and Hasegawa 1983). We will argue using numerical evidence that a more general form for Λ than (1), i.e.

$$k^2\Lambda = (1-k^2)(A_x^2 + A_y^2) - k^2 A_z^2 \tag{3}$$

($k^2 = \frac{1}{5}$ yields Solovev's form (2)), may be of use for the approximate integral relevant to the strong mixing regime where the dynamics is almost chaotic.

The full Hamiltonian for the Kepler motion in a uniform magnetic field B is given in the cylindrical coordinate system ($\rho z \phi$; $p_\rho p_z p_\phi$) by

$$\begin{aligned} H &= \tfrac{1}{2}(p_\rho^2 + p_z^2) + \tfrac{1}{2}m^2\rho^{-2} + \tfrac{1}{2}mB + \tfrac{1}{8}B^2\rho^2 - (\rho^2 + z^2)^{-1/2} \\ &= \tfrac{1}{2}(p_\rho^2 + p_z^2) + \tfrac{1}{2}\rho^{-2}(m + \tfrac{1}{2}B\rho^2)^2 - (\rho^2 + z^2)^{-1/2} \end{aligned} \tag{4}$$

where m denotes the value of the momentum p_ϕ (angular momentum z-component $\parallel \boldsymbol{B}$) conjugate to the cyclic variable ϕ so that

$$\rho^2\dot{\phi} = p_\phi + \tfrac{1}{2}B\rho^2 = m + \tfrac{1}{2}B\rho^2, \tag{5}$$

and the unit of B is assumed such that the cyclotron energy $\hbar\omega_c$ is measured in R_y (twice Robnick's number (Robnick 1981)). Thus, the system represented in the Hamiltonian (4) is of two degrees of freedom, and hence every trajectory of the associated equations of motion with a constant energy E lies in a three-dimensional hypersurface of the four-dimensional phase space (ρ, p_ρ, z, p_z), which must be filled with a number of two-dimensional tori (so-called invariant, or KAM tori), provided the system is an integrable one. For example, in the absence of the magnetic field i.e. $B = 0$, the Hamiltonian (4) is separable (the corresponding Hamilton–Jacobi equation is decomposed into two independent ones) in terms of the polar coordinate system, and hence it is integrable.

Reinhardt and Farrelly (1982) stressed the conceptual difference between the *separability* and the *integrability* of Hamiltonian systems, saying that the latter concept includes a much wider class of systems than the former. Thus, the existence of an approximate integral at least in a restricted range of relevant parameters (here, the energy parameter E or the field strength B) implies that the system belongs to an integrable one in the same range, although the Hamiltonian is non-separable. The test of such an approximate integrability for Hamiltonians of two degrees of freedom by means of the Poincaré surface-of-section analysis was initiated by Hénon and Heiles (1964), but the application of it to the diamagnetic Kepler problem (4) has been made only recently (Robnik 1981, Reinhardt and Farrelly 1982, Harada and Hasegawa 1983). Robnik's result did not contain the special case $m = 0$; the case is easier than $m \neq 0$ from a conceptual point of view but harder from the computer–technical one, and the Reinhardt–Farrelly result was this $m = 0$ case in the parabolic coordinate representation that differs from the surface of section chosen by Robnik and also by us.

Our results of computer experiments are shown in figure 1. The series 1*a*, *b*, *c*... represents the Poincaré map taken on the surface of section $z = 0$ of the $p_\rho - \rho$ plane provided by the previous numerical integration of the equations of motion with H in

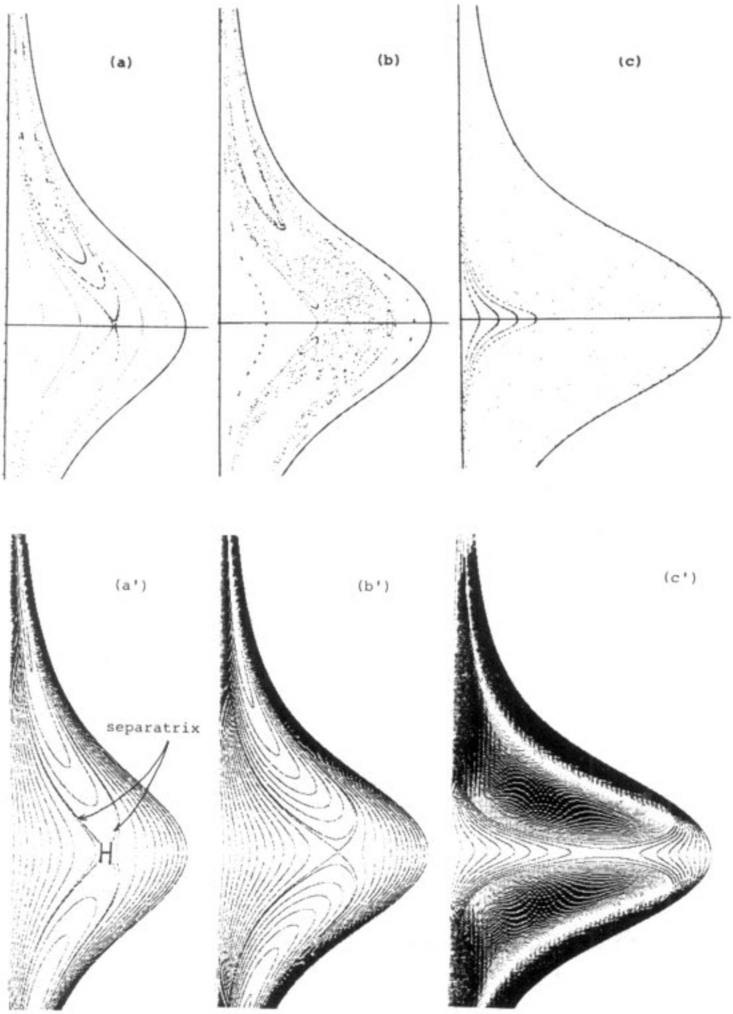

Figure 1. The Poincaré surface of section of $z=0$, $p_\rho-\rho$ plane in the cylindrical coordinate system for the diamagnetic Kepler motions: (a), (b), (c), are those computed by integrating the equations of motion, and $(a)'$, $(b)'$, $(c)'$ are those simulated analytically as indicated in the text. (a)–(a') $m=0$, $B=2$, $E=-1$; $k^2=\frac{1}{5}$ for the simulation (b)–(b') $m=0$, $B=2$, $E=-0.7$; $k^2=0.25$ (c)–(c') $m=0$, $B=2$, $E=-0.3$; $k^2=0.8$.

(4), where the values of m and B are fixed and the energy E is varied:

$$m=0, \qquad B=2 \qquad (\gamma=2 \text{ cf Harada and Hasegawa 1983}) \tag{6}$$

$$(a)\ E=-1, \qquad (b)\ E=-0.7, \qquad (c)\ E=-0.3 \text{ (in atomic units)}. \tag{7}$$

The magnetic field strength indicated in (6) is unrealistically large ($B=4.7\times10^5$ T), but, as we have noted before (Harada and Hasegawa 1983, Hasegawa *et al* 1983), there exists an exact scaling relation between the two constants of motion and the magnetic field strength: Let X be a measurable quantity of the hydrogen atom (e.g. a spectral intensity) that may depend on E, m and B. Then

$$X(E;m;B)=X(B^{-2/3}E, B^{1/3}m;1). \tag{8}$$

In particular for $m=0$, the function X of E and B must be a single-variable function $X(B^{-2/3}E)$. Therefore, the value of X for $B=1$T (e.g. in figure 1 referring to (7)) can be seen from X for $B=10^6$T by reducing the energy E by a factor of $(10^6)^{-2/3}=10^{-4}$. This means that the situation in figure 1 actually corresponds to the principal quantum number n of the order of 100 for $B=1$T (or, $n\sim 60$ for $B=4$T), that is in the range of energy where the optical spectrum behaves irregularly far beyond the quadratic Zeeman regime (Clark and Taylor 1980).

We have computed analytic simulation curves on the $z=0$ surface of section by taking each intersection of the energy integral $H=E$ and the approximate integral Λ in (1) (or, more generally in (3) with k^2 different from Solovev's value $\frac{1}{5}$) with Λ being changed, which are exhibited in the series $1a'b'c'\ldots$ in comparison with $1abc\ldots$. A typical comparison in the literature is the simulation of the Poincaré map for the Hénon–Heiles system by Gustavson using the transformation to a normal form (Gustavson 1966). We note that Gustavson's method is not directly applicable to the Kepler problem because of the non-polynomial potential and also because of the special degeneracy of the period for the unperturbed motion (1 : 1 rational winding number). Our result may, however, be looked upon as the lowest order transform of Gustavson, since the approximate invariant is a quartic function of the momentum variable as can be seen from (2). It is important to note that this simplest way of constructing the surface of section can simulate the essence of the Poincaré map for the diamagnetic Kepler motion deduced from the direct integrations; the unique hyperbolic point H and a pair of separatrix lines through it that separate the two regions of the map. It is not obvious in our problem that chaos arises in increasing the parameter E or B associated with this separatrix in view of the usual homoclinicity argument (another hyperbolic point $\bar{\mathrm{H}}$ counter to H cannot be located in the present analysis—it could be the mirror image of H on the fictitious negative ρ-axis due to the formal symmetry of the Hamiltonian (4)).

Undoubtedly, however, the onset of chaos takes place around the separatrix by inspection in figure 1(b), and one sees that the chaotic motions are those trajectories which wander in both regions. Thus, the existence of Solovev's two regions of the diamagnetic Kepler motion valid precisely for the limit $B\to 0$ but intermixing between them for non-zero B actually produces chaos. A precise correspondence of the separate regions in phase space, outside and inside of the Solovev cone, to those mapped onto the $z=0$ surface of section deduced by numerical integrations has been confirmed analytically, a detail of which will be given below.

Our procedure to deduce the intersection formula for drawing figure $1a'b'c'$ is as follows: for the concept of 'approximate integral' beyond the perturbation regime, the form (3) will be used with an unspecified k^2, and besides the Lenz vector $\boldsymbol{A}$ will be modified such that

$$\boldsymbol{A}\equiv \boldsymbol{v}\times(\boldsymbol{r}\times\boldsymbol{v})-\boldsymbol{r}/r, \qquad \boldsymbol{v}=\boldsymbol{p}+\tfrac{1}{2}\boldsymbol{B}\times\boldsymbol{r}. \tag{2'}$$

This is for convenience, because together with the similar modification of the angular momentum, $\boldsymbol{L}\equiv\boldsymbol{r}\times\boldsymbol{v}$, an exact identity holds:

$$\boldsymbol{A}^2=1+2E\boldsymbol{L}^2 \qquad \begin{pmatrix} E \text{ is the total energy, the} \\ \text{magnetic part inclusive} \end{pmatrix} \tag{9}$$

The coefficient value k^2 in (3) should be determined so that the secular part of Λ is eliminated: following the method of average, we take

$$\langle \mathrm{d}\Lambda/\mathrm{d}t\rangle=0 \qquad \text{or} \qquad 1-k^2=\langle A_z\,\mathrm{d}A_z/\mathrm{d}t\rangle/\langle \boldsymbol{A}\cdot\mathrm{d}\boldsymbol{A}/\mathrm{d}t\rangle, \tag{10}$$

where the average is taken over a (quasi) periodic orbit whenever it is defined. For example, it can be proved that if the average is taken over a Kepler ellipse then Solovev's value $k^2=\frac{1}{5}$ is deduced if terms $O(B^3)$ are discarded. Let the form (3) be expressed in terms of the cylindrical coordinates on the $z=0$ surface of section by using $\boldsymbol{L}^2=\rho^2p_z^2+\rho^4\dot{\phi}^2$ and $A_z^2=\rho^2p_\rho^2p_z^2$. By eliminating p_z^2 from the energy integral, together with the relation (9), we get a quartic equation for p_ρ as follows:

$$ap_\rho^4+\{1+a[\rho^2\dot{\phi}^2-2(E+\rho^{-1})]\}p_\rho^2+b\rho^{-2}+\rho^2\dot{\phi}^2-2(E+\rho^{-1})=0 \tag{11}$$

where $\dot{\phi}^2$ is given from (5) and

$$a=[-2E(1-k^2)]^{-1}, \qquad b=[-2E(1-k^2)]^{-1}[1-k^2(1+\Lambda)]-\langle\rho^4\dot{\phi}^2\rangle. \tag{12}$$

We needed an unavoidable averaging for the expression b in (12) that makes b a constant parameter: it is necessary because $p_z=0$ must result automatically at a specific value of $b(=0)$ that yields the outer-most contour of each map corresponding to the maximal allowed Λ. In the limit $B\to 0$, $\rho^4\dot{\phi}^2\to m^2$ so that a root of the quartic equation (11) for p_ρ yields an exact map of the Solovev cone, inside and outside of it, onto the structure of the $z=0$ surface of section. The intersection formula (11) in this situation $(k^2=\frac{1}{5})$ reduces to

$$(ap_\rho^4+\tfrac{9}{4}p_\rho^2+\tfrac{5}{4}a^{-1})\rho^2-2(ap_\rho^2+1)\rho+\tfrac{1}{5}a(4-\Lambda)=0. \tag{13}$$

This quadratic equation for ρ has the discriminant

$$D=\tfrac{1}{5}a^2(1+\Lambda)[p_\rho^2+\tfrac{5}{4}\Lambda a^{-1}(1+\Lambda)^{-1}](p_\rho^2+a^{-1}), \tag{14}$$

from which it can be seen that

(i) $0<\Lambda<4$; $D>0$ two different real roots of ρ, which corresponds to outside of the cone.

(ii) $-1<\Lambda<0$; $D\gtrless 0$ for $p_\rho^2\gtrless -\frac{5}{4}\Lambda a^{-1}(1+\Lambda)^{-1}$ two different real roots of ρ separated by a zone, which correspond to two insides of the cone.

(iii) $\Lambda=0$; $D=0$ two separatrix lines meet at the point $\rho=\frac{4}{5}a$ (the hyperbolic point). These are illustrated in figure 2.

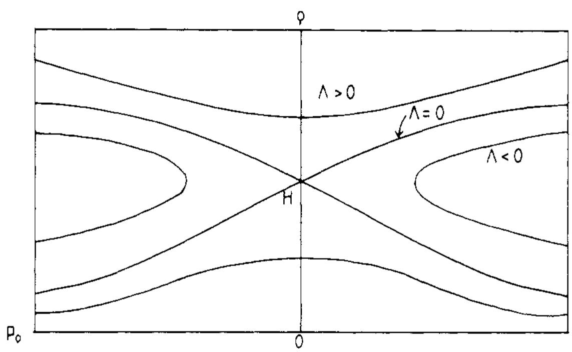

Figure 2. Exact geometrical correspondence of Solovev's hyperbola $4(A_x^2+A_y^2)-A_z^2=\Lambda$ onto the surface of section given in figure 1 for $B\to 0$ (schematic), explained in the text.

The most significant point of our results in figure 1 is that invariant tori still remain even in the almost chaotic regime (1*c*), which are located near the outer-most contour. This contour corresponds to the limit of the Poincaré mapping series for $\Lambda\to\Lambda_{\max}$ ($b\to 0$ as stated above), so that the existence of the undestroyed tori there implies the discrete quantal spectra specified by the quantum number $\Lambda \sim \Lambda_{max}$ (the flattest situation of the A-vector): Thus, this will yield a qualitative understanding of the resonance phenomena (quasi-Landau resonance) discussed by Fano (1983), although more is to be done for the complete solution. Finally, we note that a numerical indication has been obtained about the behaviour of k^2 in (3) and (10): k^2 increases at the transition region to chaos so that

$$k^2(E, B) = k^2(B^{-2/3}E) \xrightarrow{E\to 0, \text{ or } B\to\infty} 1.$$

This is shown in figure 1(c) where the numerically deduced group of tori located along the ρ axis left to the chaotic area are more steeply shaped than predicted by the formula (11) with Solovev's value $k^2 = \frac{1}{5}$ but are satisfactorily simulated by the same formula with $k^2 = 0.8$ (figure 1(c)′). The assumption of the approximate constancy of Λ of the form (3) with $k^2 \simeq 1$, i.e. the constancy of A_z^2, is compatible with the proposal of the symmetry made by Clark (1981), according to which $\Sigma \equiv A_z|A_z|^{-1}$ commutes approximately with the diamagnetic Kepler Hamiltonian.

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