NOTE

Etude No. 3: Classical Exact Solutions for the Zeeman Effect of Hydrogen Atom

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ABSTRUCT

The Lorentz equation of motion for an electron in hydrogen atom is solved analytically,exactly. It is found that the features of the Zeeman effect, i. e., line-numbers of the splitting,magnetic field dependence (linear or quadratic, for example), are all depends on the magnetic field strength-itself. This may suggest that some intermediate process should be deemed between classical and quantum mechanical models.

CONTENTS :

§ 1 Introduction

It was about a century ago, when Zeeman observed the magnetic field effects on the spectrum of emitted light. Later, H. A. Lorentz pointed out, that this "Zeeman Effect" can be explained by employing the Lorentz's equation of motion for the electrons on a harmonic motion [1]. This is called the Simple Zeeman effect, or the Lorentz's Triplet. The calculation is so simple and the problem appeared to be settled quite well.

However, the experiments went on with more surprising fashion. Firstly, the structure of the spectrum turned out to be more complicated than doublet and/or triplet. It appeared with quartet, sextet, for example, in some cases. Secondly, the unexpected magnetic field strength dependence showed up.

The quantum-mechnicians, of course, came in on the subject [2]. They started with the excact and well accepted grand Hamiltonians with the magnetic vector potential. They regarded that the core of the problem is how to quantize the angular momentum of the electrons in the atom. They succeeded in for explaining the almost all the phenomena, needless to say about "Simple Zeemann Effect". They extended their works over the complicated electron configurations under strong magnetic field.

Their efforts fanned out to many directions with great success. They classified the phenomena into three categories, depending on the magnetic field strengths ; i. e. (1) the linear (or simple) Zeeman, (2)the quadratic (or diamagnetic second order) Zeeman, (3) the Paschen-Back effect, and the Landau level effect [3].

However, as is well known, the quantum mechanics does not take care of the change of the space cordinate of a particle upon the time. It handles just the energy difference (or change) of the expectation value of the system by employing the space-time probability density of the particles. By so doing, they lost the contact with the classical mechanics. No one even thought that he was loosing something important. Finally Chaos came up to the surface in the classical mechnics, and peoples realized that in the regime of the 2), in the quadratic Zeeman, there exist the chaos phenomena [4].

Actually, it was hard to anticipate Chaos in the theory of the second order Zeeman effect from the beginning. However, lucky enough, there were optical data with high magnetic intensity. They analized the data by starting from the classical Lorentz's equation. Therefore it is vividly shown what is taking place on the classical orbit of the electron in the atom. It is found there are serious relations between the second order Zeeman effect and the chaos theory. People named the phenomena as DKP (diamagnetic Kepler problem) [5, 6, 7, 8, 9].

Such is the rough sketch of the history of the Zeeman effect. It may appear to the specialists' eyes of the Zeeman effect that the progress of this field is very systematical and logical. However, to the "Side line watcheres' point of view", the progress appears to be very temperamental and happy-go-lucky fashion.

The purpose of this work is to extend the way of solving the classical Lorentz's equation of motion to the farthest end. Another words, author tries to solve the classical equation of motion by the strictly mathematical fashion. This is in hope that we will be able to find the physical vision on the magnetic dependence of the energy separation of the orbital electron. To the author's opinion, it appears that no rigorous reason is to be seen to switch the vector coupling model from the simple zeeman effect to the Pachen-Bach effect etc.

§ 2 Exact Solution of the Algebraic Lorentz Differential Operator Equation

Lorentz showed the most classical equation of motion for the electron in the atom (which represents the 1s-electron in hydrogen orbit) in his lecture note (1). Let's start from this equation, since this is the most typical classical dynamical equation for the particle, and the physical image is crystal clear, i. e.,

$$m(d^2\xi/dt^2) = -f\xi + (e/c)Hz(d\eta/dt) \qquad (1)$$

$$m(d^2\eta/dt^2) = -f\eta - (e/c)Hz(d\xi/dt), \qquad (2)$$

$$m(d^2\zeta/dt^2) = -f\zeta \qquad (3)$$

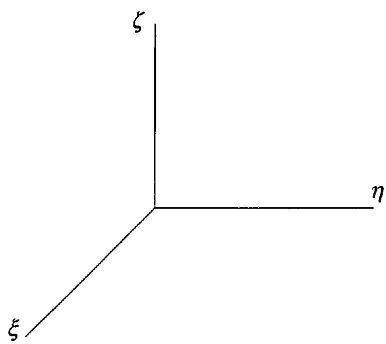

Fig. 1 The Cartesian coordinates (ξ, η, ζ) for equation of motion of an electron in Hydrogen atom : The origin of the coordinates is at the center of the nucleus of the atom.

where the axes ξ, η, ζ correspond to the x, y z axes as shown in Fig.1.

Let's replace d/dt by D, then the above equations of motion of an electron become following simultaneous algebraic equations for D ;

$$mD^2\xi = -f\xi + (e/c)HzD\eta \tag{4}$$
$$mD^2\eta = -f\eta - (e/c)HzD\xi \tag{5}$$
$$mD^2\zeta = -f\zeta. \tag{6}$$

Operating D from the left side of the equations (4) and (5), we obtain the following equations (7) and (8) :

$$mD^3\xi = -f\,D\xi + (e/c)HzD^2\eta \tag{7}$$
$$mD^3\eta = -f\,D\eta - (e/c)HzD^2\xi. \tag{8}$$

We put the left side of the equation (5), $mD^2\eta$, into the 2nd term of the right side of the equation (7), then after some manipulation, we get the following equation ;

$$mD^3\xi = -D\xi\{f + (1/m)(eHz/c)^2\} + (eHz/c)(-f/m)\eta \tag{9}$$

Similarly, by the combination of the equations (4) and (8), we get the following ;

$$mD^3\eta = -D\eta\{f + (1/m)(eHz/c)^2\} - (eHz/c)(-f/m)\xi. \tag{10}$$

We realize that these are the coupled non-linear differential equations, and therefore, there is high posibility that chaos will take place under some conditions. However, before we jump onto a computor for the numerical calculations, we should try to obtain the analytical results. Analytical result is, sometimes, much better than the numerical calculation for looking over the prospect of the phenomena.

Looking for the way to get the separation of variables, ξ and η, we subtract eq. (10) from eq. (9) and we have,

$$\mathrm{m}D^3(\xi-\eta) = -D(\xi-\eta)\{f+(1/m)(eHz/c)^2\} \\ +(eHz/c)(-f/m)(\xi+\eta) \qquad (11)$$

Similarly,by adding equations (9) and (10), we obtain more or less twin like equation (12), as following ;

$$\mathrm{m}D^3(\xi+\eta) = -D(\xi+\eta)\{f+(1/m)(eHz/c)^2\} \\ +(eHz/c)(-f/m)(\eta-\xi) \qquad (12)$$

From equation (11), we rewrite the variable $(\xi+\eta)$ as follows,

$$\xi+\eta = (c/eHz)(-m/f)\{mD^3(\xi-\eta) \\ +D(\xi-\eta)\{f+(1/m)(eHz/c)^2\} \qquad (13)$$

By putting the variable $\xi+\eta$ into eq. (12), and paying attension to the sign difference between $\xi-\eta$ and $\eta-\xi$, we finally obtain the Lorentz equation of motion for the variable $(\xi-\eta)$ as follows ;

$$\langle\!\langle [mD^3+\{f+(1/m)(eHz/c)^2\}D]^2 \\ -(eHz/c)^2(-f/m)^2\rangle\!\rangle(\xi-\eta) = 0 \qquad (14)$$

A factorization of eq. (14) can be easily performed, and the result is shown as follows ;

$$[D^3+\{f/m+(eHz/mc)^2\}D-(eHz/mc)(f/m)](\xi-\eta)=0 \tag{15}$$
$$[D^3+\{f/m+(eHz/mc)^2\}D+(eHz/mc)(f/m)](\xi-\eta)=0 \tag{16}$$

As for the variable $(\xi+\eta)$, it ends up with a pair of the allmost similar equations ; a pure imaginary factor (i) is multiplied upon the last term in eqs. (15) and (16).

$$[D^3+\{f/m+(eHz/mc)^2\}D-i(eHz/mc)(f/m)](\xi+\eta)=0 \tag{17}$$
$$[D^3+\{f/m+(eHz/mc)^2\}D+i(eHz/mc)(f/m)](\xi+\eta)=0 \tag{18}$$

Those above equations are all analytical equation of the 3rd order of D, and it should be factorized for a linear equation of D where they have a root. We notice that all the coefficient factors in equations, (15), (16), (17), and (18), are identical. Therefore, we replace the factor-terms by following simple letters, p and q ;

$$\{f/m+(eHz/mc)^2\}=-3p \tag{19}$$
$$(eHz/mc)(f/m)=-2q \tag{20}$$

Then the equations of motion, (15), (16), (17), and (18), can be writen simply as follows ;

$$\{D^3-3pD-2(\pm q)\}(\xi-\eta)=0 \qquad (21)\ \text{[for eqs. 15, 16]}$$
$$\{D^3-3pD-2i(\pm q)\}(\xi+\eta)=0. \qquad (22)\ \text{[for eqs. 17, 18]}$$

We can apply the Cardan's solution for the cubic equation, i. e. for eqs. (21) and (22). We see that there are 4 cases for the solution, corresponding to each (±) sign in eq. (21) and eq. (22). Let's start from the first case ;

$$\text{[Case 1]} \quad \{D^3 - 3pD - 2(+q)\}(\xi - \eta) = 0 \tag{23}$$

We want to factorize the cubic equation for D. The each "root" for this equation, α_1, β_1, γ_1 can be writen down by employing the discriminant, d_1, as following ;

$$d_1 = q^2 - p^3, \text{ and } \omega = (-1 + 3i)/2, \quad \omega^2 = (-1 - 3i)/2 \tag{24}$$

We obtain the following results ;

$$\alpha_1 = \{q + (d_1)^{1/2}\}^{1/3} + \{q - (d_1)^{1/2}\}^{1/3} \tag{25}$$
$$\beta_1 = \omega\{q + (d_1)^{1/2}\}^{1/3} + \omega^2\{q - (d_1)^{1/2}\}^{1/3} \tag{26}$$
$$\gamma_1 = \omega^2\{q + (d_1)^{1/2}\}^{1/3} + \omega\{q - (d_1)^{1/2}\}^{1/3} \tag{27}$$

It must be instructive to point out, that α_1, β_1, and γ_1 are the root for the cubic equation for the derivative operator for time (t). Therefore, these three factorized terms can be writen as a product as following ;

$$\{(D - \alpha_1)(D - \beta_1)(D - \gamma_1)\}(\xi - \eta) = 0 \tag{28}$$

Therefore, the complementry function, or the general solution for this case is,

$$(\xi - \eta) = C_{11}\exp(+\alpha_1 t) + C_{12}\exp(+\beta_1 t) + C_{13}\exp(+\gamma_1 t) \tag{29}$$

【Case 2】 $\{D^3 - 3pD - 2(-q)\}(\xi - \eta) = 0$

From the definition for d, the discriminant for the case 2 is the same as for the case 1. i. e.,

$$d_2 = (-q)^2 - p^3 = d_1 \tag{30}$$

However, "the roots" are different. They are,

$$\alpha_2 = \{(-q) + (d_1)^{1/2}\}^{1/3} + \{(-q) - (d_1)^{1/2}\}^{1/3} \tag{31}$$

$$\beta_2 = \omega\{(-q) + (d_1)^{1/2}\}^{1/3} + \omega^2\{(-q) - (d_1)^{1/2}\}^{1/3} \tag{32}$$

$$\gamma_2 = \omega^2(-q) + (d_1)^{1/2}\}^{1/3} + \omega\{(-q) - (d_1)^{1/2}\}^{1/3} \tag{33}$$

The general solution for this case is, like case 1,

$$(\xi - \eta) = C_{21}\exp(+\alpha_2 t) + C_{22}\exp(+\beta_2 t) + C_{23}\exp(+\gamma_2 t) \tag{34}$$

【Case 3】 $\{D^3 - 3pD - 2(+iq)\}(\xi + \eta) = 0$ (35)

The discriminant for this case is, by the definition, as follows,

$$d_3 = (iq)^2 - p^3 = (-)q^2 - p^3 \tag{36}$$

The roots for this case are,

$$\alpha_3 = \{(iq) + (d_3)^{1/2}\}^{1/3} + \{(iq) - (d_3)^{1/2}\}^{1/3} \tag{37}$$

$$\beta_3 = \omega\{(iq) + (d_3)^{1/2}\}^{1/3} + \omega^2\{(iq) - (d_3)^{1/2}\}^{1/3} \tag{38}$$

$$\gamma_3 = \omega^2\{(iq) + (d_3)^{1/2}\}^{1/3} + \omega\{(iq) - (d_3)^{1/2}\}^{1/3} \tag{39}$$

The general solution for this case is,

$$(\xi + \eta) = C_{31}\exp(+\alpha_3 t) + C_{32}\exp(+\beta_3 t) + C_{33}\exp(+\gamma_3 t) \tag{40}$$

It should be noticed that the root for this case can be complex number. This will be easily seen, if we assume $d_3 = 0$. In this case, $\alpha_3 = 2(iq)^{1/3}$, and therefore, $\alpha_3 = (-i)(2q)^{1/3}$. Then the solution is

$$(\xi + \eta) = C_{31}\exp(-i\,\upsilon\, t),\text{ plus etc.} \tag{41}$$

Of course, these terms represent the harmonic motion of the electron. More arguments will be given in the later section.

$$\text{【Case 4】}\ \{D^3 - 3pD - 2(-iq)\}(\xi + \eta) = 0 \tag{42}$$

The discriminant for this case is the same as case 3. Since,

$$d_4 = (-iq)^2 - p^3 = d_3, \tag{43}$$

However, the value of the roots are different.

$$\alpha_4 = \{(-iq) + (d_3)^{1/2}\}^{1/3} + \{(-iq) - (d_3)^{1/2}\}^{1/3} \tag{44}$$

$$\beta_4 = \omega\{(-iq) + (d_3)^{1/2}\}^{1/3} + \omega^2\{(-iq) - (d_3)^{1/2}\}^{1/3} \tag{45}$$

$$\gamma_4 = \omega^2\{(-iq) + (d_3)^{1/2}\}^{1/3} + \omega\{(-iq) - (d_3)^{1/2}\}^{1/3} \tag{46}$$

The general solution for this case is,

$$(\xi + \eta) = C_{41}\exp(+\alpha_4 t) + C_{42}\exp(+\beta_4 t) + C_{43}\exp(+\gamma_4 t) \tag{47}$$

Again, in eq. (47), it is easy to forsee that the root for this case can be a complex number. Supose $d_3 = 0$, then $\alpha_4 = 2(-iq)^{1/3} = (2q)^{1/3}(+i)$. This will end up with a harmonic oscilation term,

$$(\xi + \eta) = C_{41}\exp(i\,\upsilon\,t), \text{ plus etc.} \tag{48}$$

As a concluding remark for this section (§ 2) we can say as following ;

By combining the general solutions, (29) and (40), with (34) and (48), we can perfectly separate ξ and η. This is in turn we can perfectly determine the orbit of the moving electron in the atomic orbit. Needless to say, this is because we are handling the classical dynamics. However, the nice thing about the classical dynamics is we are completely free from the ambiguous choice for the vector model, which depends upon the magnetic field strength to the angular momentum. Another words, readers may agree to say that the complicated Zeeman effect phenomena is inherited from the motion of the orbital electron itself. The author refrain from arguing the chaos phenomena under the strong magnetic field. This is simply because we do not have enough time to discuss here.

§ 3 Magnetic Field Dependence of the Energy Separation

It is well known that the number of the real root for the cubic equation depends on the sign of the discriminant ; d_1 or d_3. Actually, as we have seen in the basic eq. (14), we are handling the 6th order algebraic equations. Therefore, we will have 6 real roots for the maximum case.

There are only two types for the discriminant.

$d_1 = q^2 - p^3$: for the case 1, and case 2, i. e., for $(\xi - \eta)$.
$d_3 = -q^2 - p^3$: for the case 3, and case 4, i. e., for $(\xi + \eta)$

Let's write down the discriminants explicitly ;

$$d_1 = q^2 - p^3 = \{(-eHz/2mc)(f/m)\}^2 - (-1/3)^3\{(f/m) + (eHz/mc)^2\}^3 \tag{49}$$

$$d_3 = -q^2 - p^3 = (-1)\{(-eHz/2mc)(f/m)\}^2 - (-1/3)^3\{(f/m) + (eHz/mc)^2\}^3 \tag{50}$$

and let's proceed our discussion stepwise :

[Step 1]

Any cubic function has at least one real number root. The rest of the two roots are governed by the sign of the discriminant.

(1) $d_i > 0$, we have 2 complex conjugate roots. [1 real, 2 complex, in all]
(2) $d_i = 0$, we have just 1 identical real number root. [2 real, in all]
(3) $d_i < 0$, we have 2 different real number roots. [3 real, in all]

It must be stressed here, that the above discriminants, d_1 or d_3, depend on Hz itself. Therefore, it is surprising to find that the splitting line number for the magnetic effect is the results of the interaction of the orbital electron and the magnetic field itself. It is not because of the number of energy levels within atom. Therefore it appears very artificial, to the author eyes, to change the employing vector model from simple-Zeeman case to Paschen-Bach effect.

[Step 2]

It should be noticed that when Hz = 0, then d_1 and d_3 become positive ; (>). Therefore, we get only one real number root for each variable ; ξ and η.

Since, $d_1 = d_3 = +(f/3m)^3$, the roots for each case are as following ;

【Case 1】 $\alpha_1 = 0$ (51)

$\beta_1 = \omega\,(f/3m)^{1/2} - \omega^2\,(f/3m)^{1/2}$ (52)

$\gamma_1 = \omega^2\,(f/3m)^{1/2} - \omega\,(f/3m)^{1/2}$ (53)

$(\xi - \eta) = C_{11} + C_{12}\exp(\beta_1 t) + C_{13}\exp(\gamma_1 t)$ (54)

【Case 2】 $\alpha_2 = 0,\quad \beta_2 = \beta_1,\quad \gamma_2 = \gamma_1$ (55)

$(\xi - \eta) = C_{21} + C_{22}\exp(\beta_1 t) + C_{23}\exp(\gamma_1 t)$ (56)

【Case 3】 $\alpha_3 = 0,\quad \beta_3 = \beta_1,\quad \gamma_3 = \gamma_1$ (57)

$(\xi + \eta) = C_{31} + C_{32}\exp(\beta_1 t) + C_{33}\exp(\gamma_1 t)$ (58)

【Case 4】 $\alpha_4 = 0,\quad \beta_4 = \beta_1,\quad \gamma_4 = \gamma_1$ (59)

$(\xi + \eta) = C_{41} + C_{42}\exp(\beta_1 t) + C_4 3\exp(\gamma_1 t)$ (60)

As the results, we get the following simultaneous equations ;

$$(\xi - \eta) = C_{11} + C_{12}\exp(\beta_1 t) + C_{13}\exp(\gamma_1 t) \quad (61)$$

$$(\xi + \eta) = C_{31} + C_{32}\exp(\beta_1 t) + C_{33}\exp(\gamma_1 t) \quad (62)$$

Therefore, the solution is reduced from the above eqs. (61) and (62),

$$\xi = 1/2\{(C_{11} + C_{31}) + (C_{12} + C_{32})\exp(\beta_1 t) + (C_{13} + C_{33})\exp(\gamma_1 t)\} \quad (63)$$

$$\eta = 1/2\{(C_{31} - C_{11}) + (C_{32} - C_{12})\exp(\beta_1 t) + (C_{33} - C_{13})\exp(\gamma_1 t)\} \quad (64)$$

As we understand from eqs. (52) and (53), since β_1 and γ_1 are complex imaginary number, then we get the simple harmonic solutions.

[Step 3]

When Hz is not zero, i. e. Hz $\neq$ 0, we have three choices for each value of d_1, d_2, d_3, and d_4. As we have defined the variables p and q by eqs. (19) and (20), we have always the discriminant di (i = 1, 2, 3, 4) like eq. (49) or eq. (50). Therefore, we have to examine d, case after case ;

【Case 1, and Case 2】

The equation of motion for these cases is as shown below ;

$$\{D^3 - 3pD - (\pm q)\}(\xi - \eta) = 0, \quad (21)$$

and the discriminants, d, for these cases become identical, i. e.,

$$\begin{aligned} d = d_1 = d_2 &= (\pm q)^2 - p^3. \\ &= \{(-1/2)(\pm eHz/mc)(f/m)\}^2 - (-1/3)^3\{(f/m)+(eHz/mc)^2\}^3 \quad (65) \end{aligned}$$

The root formula for α_1, α_2, becomes,

$$\begin{aligned} \alpha_{1,2} &= \{\pm q + (d)^{1/2}\}^{1/3} + \{\pm q - (d)^{1/2}\}^{1/3} \\ &= \{(\pm eHz/2mc)(f/m) + (d)^{1/2}\}^{1/3} + \{(\pm Hz/2mc)(f/m) \end{aligned}$$

$$-(d)^{1/2}\}^{1/3} \quad (66)$$

[We will get to other roots, $\beta_{1,2}$ and $\gamma_{1,2}$, shortly].

As we stated in [Step 1], we have 3-choices for each discriminant d, i. e. ;

(1) $d > 0$, 1 real and 2 complex conjugate numbers in all.
(2) $d = 0$, 2 real number roots in all.
(3) $d < 0$, 3 real number roots in all.

Let's concentrate our effort to the cases (2), where $d = 0$, for the moment. This is the simplest case within the above three, and we get the following real number roots,

$$\alpha_1 = q^{1/3} + q^{1/3} = 2q^{1/3} \qquad \text{(cf.eq.66)}$$
$$= 2\{(-eHz/2mc)(f/m)\}^{1/3}$$
$$\alpha_2 = 2\{(+eHz/2mc)(f/m)\}^{1/3} = -\alpha_1$$

For other roots, β and γ, we have,

$$\beta_1 = (\omega + \omega^2)q^{1/3} = \{(-1+3i)/2 + (-1-3i)/2\}q^{1/3} = -1q^{1/3}$$
$$\gamma_1 = \beta_1$$
$$\beta_2 = (\omega + \omega^2)(-q)^{1/3} = +q^{1/3} = -\beta_1$$
$$\gamma_2 = \beta_2$$

【 Case 3, and Case 4】

In this case, equation of motion are shown in eqs. (35), and (42). The discriminants for these cases are shown in (36) and (43),

$$\alpha = d_3 = d_4 = (\pm iq)^2 - p^3$$
$$\alpha_3 = 2(iq)^{1/3} = 2(-i)q^{1/3}$$
$$\alpha_4 = 2(-iq)^{1/3} = 2(i)q^{1/3} = -\alpha_3$$
$$\beta_3 = (\omega + \omega^2)(iq)^{1/3} = (-i)(\omega + \omega^2)q^{1/3} = (i)q^{1/3}$$
$$\beta_4 = -\beta_3$$
$$\gamma_3 = (\omega^2 + \omega)(iq)^{1/3} = \beta_3$$
$$\gamma_4 = (\omega^2 + \omega)(-iq)^{1/3} = (-1)(i)q^{1/3} = -\beta_3$$

Now the variable q is defined by the eq. (20), as following,

$$-2q = (eHz/mc)(f/m). \tag{20}$$

All the roots for the 〚Case 1, and Case 2〛 and 〚Case 3, and Cas 4〛 in [Step

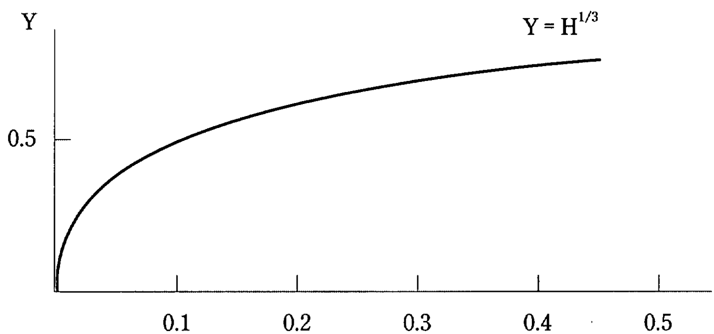

Fig. 2 The magnetic field dependence of the Zeeman effect : the orientation of the magenetic field is perpendicular to the orbiatal plane of an electron in hydrogen atom.

3], i. e., when d = 0, we have the same magnetic field (H) dependence for the root. Therefore, writing down the form explicitly, we get as the conclusion ;

$(\alpha,\ \beta,\ \gamma)$ is proportional to $[H^{1/3}]$.

In Fig. 2, we show the function of, $Y \sim H^{1/3}$.

§ 4 Applications

In Fig.3, we can see the "Zeeman effect" of the light which is emitted from a "Black Spot" on the sun [10]. The distribution of the magnetic field on the surface is unknown. However, the strength of the splitting of the light shows a curved structure. This structure appears to be very similar to the curve shown in Fig.2, i. e., 1/3 power to H. To the author's knowledg, it appears there is no experimental results nor explanation that handled this 1/3rd dependence on H.

It must be easier for this case of classical treatment for the Zeeman effect, than the quantum mechnical method, to get to chaos. This is because we are handling the classical equation of motion,and it should be connected to the chaos, more or less directly.

Conclusions

It is shown that the classical equations of motion for an electron in hydrogen atom can be solved analytically. To the author's knowledfge, this is the first time that solved the non-linear simultaneous equations, analytically.

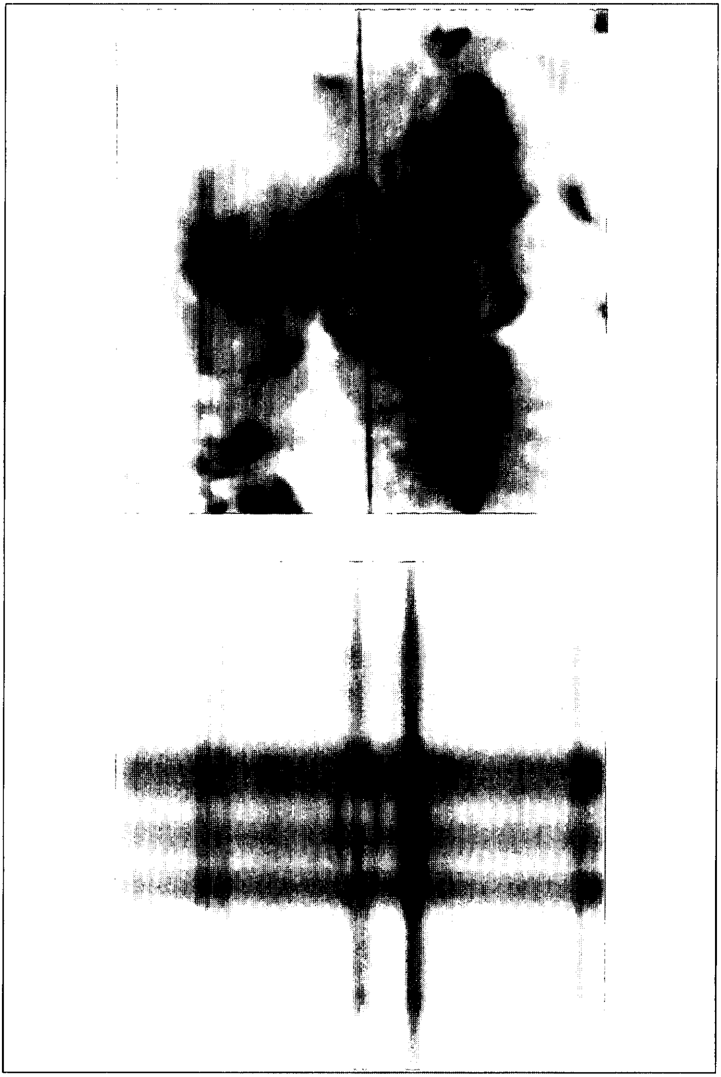

Fig. 3 Zeeman effect for the light which is emitted near the Black-Spot upon the sun surface. Note that the shape of the curve is very similar to the calculated magnetic field dependence which shown in Fig. 2.

Throught the process for solving the equations of motion,it is also found that the numbers of the splitting lines changes rather drastically, depending on the magnetic field strength. This effect is reflected upon the results through the discriminant in the formula for the roots of the equation of motion.

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