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SEMICLASSICAL MODEL FOR THE ZEEMAN RESONANCES IN HYDROGEN AT THE ZEROFIELD IONIZATION THRESHOLD

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ABSTRACT

An analytical implicit expression for the Zeeman resonances in hydrogen at the zerofield ionization threshold is obtained by means of the semiclassical Bohr model. Upon solving the semiclassical equations of motion no approximation is made that is not contained in the foundations of the model. As a result, it is shown that the agreement between previous theoretical calculations using the Bohr atom and experiment is fortuituous and a consequence of invalid assumptions.

RESUMEN

Se obtiene una expresión analítica implícita para las resonancias Zeeman en hidrógeno en el umbral de campo cero de ionización usando el mo-

delo semiclásico de Bohr. No se hace ninguna aproximación que no esté contenida en las bases del modelo al resolver las ecuaciones de movimiento semiclásicos. Como resultado, se demuestra, que el acuerdo entre cálculos teóricos previos usando el átomo de Bohr y el experimento es fortuito y consecuencia de suposiciones ilegítimas.

1. INTRODUCTION

The Zeeman effect in hydrogen is an old quantum mechanical problem which has received a renewed attention because it is a useful model in studying a number of physical phenomena that are of great interest nowadays. Among them we can mention the magneto-optical properties of some dopped semiconductors, Rydberg atoms (*i.e.* atoms with a highly excited electron) in magnetic fields and properties of the matter on the surface of white dwarfs and neutron stars[1,2]. A simple approximate model to deal with these phenomena is a hydrogenlike atom in a very strong magnetic field. A common feature to all these problems is that the interaction between the electron and the field is larger than the Coulomb interaction.

Since the stationary Schrödinger equation for the Zeeman effect in hydrogen is found to be non-separable, only approximate solutions can be obtained. To this end several methods have been tried, such as perturbation theory, the Rayleigh-Ritz variational procedure, the adiabatic approximation and semiclassical methods. Comprehensive reviews on the subject are available[1,2].

In 1969 Garton and Tomkins[3] investigated the quadratic Zeeman effect in the BaI absorption spectrum. Their measurement extended to quantum numbers as high as $n = 75$ and they used a magnetic field of 2.4 T. One of the most striking features of the fascinating spectrum they obtained is the existence of a series of σ lines, extending across the zerofield series limit into the continuum, with a regular spacing of about $1.5\ \hbar\omega$, where ω is the cyclotron frequency defined below. Obviously, the Landau spacing $\hbar\omega$ does not offer a theoretical explanation of such experimental observation. Since the spectrum is due to an electron in a highly excited energy level, it seems to be reasonable to suppose that a semiclassical study

of the Zeeman effect in a hydrogenlike atom must be useful in understanding it.

In fact, the Bohr atom and the Bohr-Sommerfeld quantization rule led to the first theoretical explanation of the quasi-Landau resonances[1,4,5]. Though this model is a very rough approach to the actual problem, the predicted spacing between the energy levels appears to agree closely with experiment. The purpose of the present paper is to show that such an agreement is fortuituous as it is a consequence of invalid assumptions. To this end the Bohr atom in a magnetic field is discussed in Sec. 2 and the suppositions that lead to the experimental quasi-Landau spacing are criticized. The semiclassical equations of motion are rigorously solved in Sec. 3 and the predicted spacing is shown to be quite different from that obtained previously[1,4,5].

We deem that the present treatment of the problem might be of great pedagogical value for undergraduate students since it does not require a large mathematical background and the model offers a nice physical insight into the phenomenon. Besides, it is very instructive to realize that some careless simplifying assumptions on a rough model may lead to a strikingly accurate prediction. In addition to this, the Bohr atom is in many ways a more realistic model of an atom than the isotropic oscillator that has been recently used to illustrate some physical properties of atoms in uniform magnetic fields[6].

2. THE BOHR ATOM AND THE ZEEMAN EFFECT IN HYDROGEN

The classical Hamiltonian for a hydrogenlike atom with nuclear charge Z is

$$H = p^2/2m - Ze^2/Dr \quad , \tag{1}$$

where $\vec{p} = m\vec{v}$, m, $\vec{v}$, e and r are, respectively, the electron classical linear momentum, mass, velocity, charge and distance from the coordinate origin, and D is the dielectric constant of the medium.

In the first approximation the electron motion along the field

direction is neglected and the electron is supposed to move along a circular orbit in a plane perpendicular to the magnetic induction $\vec{B}$. This situation occurs when the Lorentz force $F_L = eBv/c$, the centripetal force mv^2/r and the Coulomb force Ze^2/Dr^2 obey the relationship

$$mv^2/r = Ze^2/Dr^2 + eBv/c \quad . \tag{2}$$

The allowed energies are given by Bohr-Sommerfeld quantization condition

$$\oint \vec{P} \cdot d\vec{s} = nh \quad , \qquad n = 1,2, \ldots , \tag{3}$$

where the integral is over the whole circular path, h is the Planck constant and $\vec{P} = \vec{p} - e\vec{A}/c$. Since the vector potential $\vec{A}$ and the magnetic induction $\vec{B}$ are related through $\vec{B} = \text{rot } \vec{A}$, then the left-hand side in Eq. (3) is easily integrated by invoking the Stokes theorem. The result is

$$mvr - eBr^2/2c = n\hbar \quad , \tag{4}$$

where $\hbar = h/2\pi$.

If Eq. (4) is solved for v and the result is introduced into Eq. (2) the following relationship is obtained

$$r/a_0 + r^4/4R^4 = n^2 \quad , \tag{5}$$

where $a_0 = \hbar^2 D/Zme^2$ and $R = (c\hbar/eB)^{\frac{1}{2}}$ are the Bohr and Landau radii, respectively. The only possitive real root of Eq. (5) gives us the radius of the only allowed electron orbit for each n and B values. It is very easy to show that

$$\lim_{B \to 0} r = n^2 a_0 \quad , \tag{6}$$

$$\lim_{Z \to 0} r = (2n)^{\frac{1}{2}} R \quad . \tag{7}$$

The semiclassical eigenvalues are obtained by introducing Eqs. (4) and (5) into the classical Hamiltonian function (1). A straighforward algebraic manipulation leads to

$$E_n(Z,B) = n\hbar eB/2mc + e^2B^2r^2/4mc^2 - Ze^2/2Dr \quad , \tag{8}$$

where r is the possitive real root of Eq. (5). The semiclassical eigenvalues, Eq. (8), fulfil

$$E_n(Z,B) = BE_n(ZB^{-\frac{1}{2}}, 1) \quad , \tag{9}$$

and

$$E_n(Z,B) = n^{-2}E_1(Z,b) \quad , \quad b = Bn^3 \quad . \tag{10}$$

Eq. (9) is exact in the sense that it is also obeyed by the eigenvalues of the quantum-mechanical Hamiltonian operator. On the other hand, Eq. (10) is approximate and it has been verified experimentally[7]. This equation is very instructive because it clearly shows that high-field effects occur at smaller fields when large n values are considered. Both Eqs. (9) and (10) follow immediately from the change of variables $r = ax$ where $a = B^{-\frac{1}{2}}$ and $a = n^2$, respectively.

At zero magnetic field Eqs. (5) and (8) yield exactly the eigenvalues of the isolated hydrogenlike atom:

$$E_n(Z,0) = - Ze^2/2Da_0n^2 \quad , \tag{11}$$

On the other hand, in the very large magnetic field limit we obtain

$$E_n(Z,B) = n\hbar\omega - (\hbar Be^3Z/2mncD)^{\frac{1}{2}} + O(1) \quad , \tag{12}$$

where $\omega = Be/mc$ is the cyclotron frequency. The leading term in Eq. (12) gives us the celebrated Landau formula for the large-field energy level spacing[1,2].

In what follows we will obtain the energy level spacing in the neighbourhood of the ordinary series limit ($E \cong 0$) predicted by the Bohr model according to the treatment given in Refs. 1 and 5.

For large n values, the influence of the magnetic field dominates and the effect of the Coulomb field on the orbit radius is supposed to be negligible. Therefore, if r in Eq. (8) is replaced by $(2n)^{\frac{1}{2}}R$ we have[5]

$$E_n \cong n\hbar\omega - (Z^2e^5B/8D^2n\hbar c)^{\frac{1}{2}} \quad , \tag{13}$$

which leads to the following energy level spacing

$$dE_n/dn = 3\hbar\omega/2 - E_n/2n \quad . \tag{14}$$

The close agreement between Eq. (14) and the experimental value $\Delta E/\Delta n \cong 3\hbar\omega/2$[3] is striking. However, there is a mistake in the reasoning given above. It immediately follows from the condition $E_n = 0$ that $B \propto n^{-3}$ (cf. Eq. (10)). Therefore, if a rigorous power series in $n^{-3/2}$ for the energy is tried (as suggested by the change of variables $r = n^{\frac{1}{2}}q$ in Eq. (5)) it is realized that every term in the expansion is of the same order ($O(n^{-2})$). This fact can be easily verified without any calculation by noticing that $E_n(Z,B) = BnE_1(Z/B^{\frac{1}{2}}n^{3/2}, 1)$ (cf. Eqs. (9) and (10)). Due to this, the truncation of the power series expansion leading to Eq. (13) omits an infinite number of terms which are not negligible at all. This conclusion is supported by Garstang's earlier remark[1] that a numerical calculation for B = 2.4 T and $E_n \cong 0$ (n = 44) yields $dE\omega/dn = 1.97\ \hbar\omega$ instead of $1.5\ \hbar\omega$.

It is surprising that a rigorous algebraic manipulation of the semiclassical equations of motion has not been tried. We will do this in Sec. 3.

3. RIGOROUS CALCULATION OF THE LEVEL SPACING AT $E_n = 0$

Let us suppose that a hydrogenlike atom is placed in a uniform magnetic field and that the energy level spacing $E_{n+1} - E_n$ is measured in

the neighbourhood of $E_n \cong 0$. An analytical expression for the energy level spacing in terms of n and B is obtained by differenciating Eq. (10) with respect to n:

$$dE_n/dn = -2n^{-1}E_n + n^{-2}(dE_1(Z,b)/dn) \quad , \tag{15}$$

where

$$E_1(Z,b) = \hbar eb/2mc + e^2b^2x^2/4mc^2 - Ze^2/2Dx \quad , \tag{16}$$

and $x = r/n^2$ is the positive real root of

$$x/a_0 + b^2e^2x^4/4c^2\hbar^2 = 1 \quad . \tag{17}$$

Clearly, E_1 depends on n implicitly through b and x. Therefore,

$$dE_n/dn = -2n^{-1}E_n + 3bn^{-3}\{(\partial E_1/\partial b)_x + (\partial E_1/\partial x)_b\,(\partial x/\partial b)\} \quad , \tag{18}$$

which leads to

$$dE_n/dn = E_n/n + 3Ze^2/2Dn^3x \quad . \tag{19}$$

On eliminating b between Eqs. (16) and (17) we obtain

$$m^2E_1^2x^3/\hbar^4 + 3m^2Ze^2E_1x^2/D\hbar^4 + \{9m^2Z^2e^4/4D^2\hbar^4 - 2mE_1/\hbar^2\}x$$
$$- 2mZe^2/D\hbar^2 = 0 \quad , \tag{20}$$

which tells us that x depends on n and b implicitly through E_1. Therefore, it is very easy to obtain the radius of the electron orbit when $E_n = 0$ (cf. Eq. (10)):

$$x_0 = x(E_1 = 0) = 8D\hbar^2/9Ze^2m \quad . \tag{21}$$

It follows from Eqs. (17) and (21) that the quantum number for

which $E_{n} \cong 0$ is the integer that lies most closely to n_0, where

$$n_0 = (27/32\gamma)^{1/3} \tag{22}$$

In this last equation $\gamma = B/B_0$ is the dimensionless field in units of $B_0 = Z^2e^3m^2c/D^2\hbar^3 = 2.35 \times 10^5$ T.

When B = 2.35 T Eq. (22) yields $n_0 \cong 44$ which agrees with Garstang's numerical calculation[1].

Upon using Eqs. (16) and (17), Eq. (19) can be rewritten as

$$dE_n/dn = (\hbar\omega/2)\ \{1 + (1 - x/a_0)^{-\frac{1}{2}}\} \quad , 0 \leq x < a_0 \quad , \tag{23}$$

which gives us the energy level spacing for each n and B. In the series limit $E_n = 0$ we obtain

$$(dE_n/dn)\ (E_1 = 0) = 2\hbar\omega \tag{24}$$

which differs markedly from O'Connell's prediction[5] and from the Landau spacing. Eqs. (23) and (24) are completely rigorous and show that O'Connell's assumptions, which lead to the actual experimental energy level spacing, are not valid. Besides, when B = 2.35 T Eq. (24) agrees with Garstang's numerical result $(dE_n/dn)\ (E_n \cong 0\ ) = 1.97\ \hbar\omega$.

In order to verify that our analytical results are correct, we have calculated $E_n - E_{n-1}$ numerically for B = 2.35 T and the results are compared with those obtained using Eq. (23) in Table I.

TABLE I

n	$(E_n - E_{n-1})^a$	$(dE_n/dn)^b$
40	2.3798	2.3261
41	2.2762	2.2282
42	2.1835	2.1404
43	2.1003	2.0615
44	2.0254	1.9905
45	1.9579	1.9264
46	1.8969	1.8684
47	1.8416	1.8158

Table I. Energy level spacing in units of $\hbar\omega$ for B = 2.35 T and Z = 1. (a) numerical calculation, (b) Eqs. (17) and (24).

4. CONCLUSIONS

It was shown that the Bohr model does not predict the experimental Zeeman resonances at the zerofield ionization threshold as suggested by O'Connell[5] and the failure of his simplifying assumptions were made clear.

The model just discussed is an oversimplified picture of the actual problem since the electron motion along the field direction is completely neglected. Inclusion of such a motion is a quite difficult task because the semiclassical equations are found to be non-separable. However this is possible[8,9] using the Einstein-Brillouin-Keller quantization theory[10].

In closing, we want to remark that the present prediction that $n_0\gamma^{1/3} \cong 0.95$ is quite similar to that obtained using the two-dimensional JWKB method: $n_0\gamma^{1/3} \cong 1.16$[11,12].

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