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Rydberg states in strong electric and magnetic fields

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We have previously presented a semiclassical treatment of highly excited atoms in a magnetic field (for application to an analysis of the observed Zeeman effect in the Ba I absorption spectrum) and a similar treatment of a one-dimensional Coulomb field with an electric field in the same direction (of interest for the study of far-infrared emission from Si inversion layers, and also for the discussion of electrons outside a free surface of liquid helium). Since the latter experiment has also been carried out in the presence of a magnetic field, an analysis is now presented, based on the simultaneous presence of both electric and magnetic fields, which is applicable to low-lying as well as highly excited states.

For atomic electrons in high Rydberg states, the influence of a typical laboratory-size field of $\approx 10^4$ G can be as strong as the Coulomb field. In fact, the Ba spectrum was observed under such circumstances and it was found[1] that the magnetic field B produced a pattern of equally spaced lines with a separation $\frac{3}{2}\hbar\omega$ (where $\omega = eB/mc$). We have already given a semiclassical explanation of this result.[2,3] Recently, our semiclassical method was applied to electric field effects[4,5] in one-dimensional hydrogenic atoms, which are of interest for the analysis of various recent experiments—in particular, the study of far-infrared emission from Si inversion levels[6-8] and the spectra of electron states outside liquid helium in the presence of an electric field.[9-11] Since the latter experiments have also been carried out in the presence of a magnetic field,[10] we are thus motivated to extend our previous work to the case where both electric and magnetic fields are simultaneously present. Brief discussions of this problem already exist[5,12] but here we wish to present a more detailed analysis. Our results will be applicable to both low-lying and highly excited states.

For definiteness, we will, first of all, consider that the Coulomb potential is three-dimensional. However, as we will later point out, the results we obtain hold also, with minor modifications, for the case of the one-dimensional Coulomb potential.

The appropriate Hamiltonian for a hydrogenic atom in magnetic ($B = B_z$) and electric ($\mathcal{E} = \mathcal{E}_x$) fields may be written as

$$H = \frac{1}{2m}\left(\vec{\mathrm{P}} + \frac{e}{c}\vec{\mathrm{A}}\right)^2 - \frac{ze^2}{r} + e\mathcal{E}x\,, \tag{1}$$

where $\vec{\mathrm{P}}$, m, and $-e$ denote the momentum, mass, and charge of the electron.

Even in the case of just two of these fields, the Schrödinger equation cannot be solved analytically. Of course, if one of the fields dominates then perturbation theory may be used. However, we are interested in treating situations where all of these fields may be, more or less, equally important. For this purpose, we will use the semiclassical approach outlined in Ref. 2, because of its success in treating the highly excited states in Ba (Refs. 2 and 3) (where we had $\mathcal{E} = 0$) and the spectra outside helium in the presence of an electric field[4,5] (where we had $B = 0$).

In the case of a pure magnetic field,[13] the energy, E_m say, is given by

$$E_m = n\hbar\omega \quad (n = 0, 1, 2, \ldots)\,, \tag{2}$$

and the corresponding radius of the "true circular orbit" is

$$R_m = (2nB_0/B)^{1/2}a_0\,, \tag{3}$$

where

$$\omega = eB/mc\,, \tag{4}$$

is the cyclotron frequency, a_0 is the Bohr radius, and

$$B_0 \equiv (m^2ce^3/\hbar^3) = 2.350 \times 10^9\ \mathrm{G}\,. \tag{5}$$

Since we are interested in treating a range of total energies E, we will assume that the magnetic field either dominates or is always at least about as strong as the other fields (while emphasizing that, in situations where the other fields are dominant, one may modify the procedure in an obvious way, as we shall see later). Thus, we are led to write the total energy as

$$E = E_m + E_c + E_F\,, \tag{6}$$

where E_m is given in Eq. (2),

$$E_c = -ze^2\langle 1/r\rangle \approx -ze^2/R_m\,, \tag{7}$$

and

$$E_F = e\mathcal{E}\langle x\rangle \approx \pm\frac{1}{\sqrt{3}}\,e\mathcal{E}R_m\,, \tag{8}$$

and where the ± refers to the sign of x. Noting that

$$e^2/a_0 = \hbar\omega(B/B_0)^{-1} \quad (9)$$

and

$$e\mathcal{E}a_0 = (e^2/a_0)(\mathcal{E}/\mathcal{E}_0)\,, \quad (10)$$

where

$$\mathcal{E}_0 \equiv e/a_0^2 = 5.142\times10^9 \text{ V/cm}\,, \quad (11)$$

we use Eqs. (3) and (6)–(8), to obtain [in a.u. (Ref. 14), where $e = m = \hbar = 1$ so that $a_0 = 1$ and $\mathcal{E}_0 = 1$]

$$E = \omega[n - n^{-1/2}z(2B/B_0)^{-1/2} \pm n^{1/2}(\tfrac{2}{3})^{1/2}\mathcal{E}(B/B_0)^{-3/2}]\,. \quad (12)$$

It is now convenient to define "critical" fields

$$B_c \equiv \tfrac{1}{2}z^2B_0\,, \quad (13)$$

and

$$\mathcal{E}_c \equiv \tfrac{1}{4}3^{1/2}z^3\mathcal{E}_0 \approx 0.43z^3\mathcal{E}_0\,. \quad (14)$$

As we shall see later, in the case where $n = 1$, B_c, and $\mathcal{E}_c$ are approximately the same as B^* and $\mathcal{E}^*$, respectively, [see Eqs. (37) and (39)], where B^* ($\mathcal{E}^*$) denotes the value for which the magnetic (electric) field becomes as dominant as the Coulomb field.

It follows that the energy can be written in the simple form

$$E = \hbar\omega[n - n^{-1/2}(B/B_c)^{-1/2} \pm n^{1/2}(\mathcal{E}/\mathcal{E}_c)(B/B_c)^{-3/2}]\,. \quad (15)$$

This is one of our key results. Of course, the last two terms on the right-hand side of Eq. (15) are off by unknown numerical factors but this is not of primary interest to us. What is of interest is the *spacing* between energy levels (particularly at $E \approx 0$) and this is determined essentially by the power dependence of n in the various terms. In fact, in the case of $E_F = 0$, this was verified by Garstang[15] who obtained a different numerical factor than us[2,3] for the $n^{-1/2}$ term but still obtained the same energy spacing of $\frac{3}{2}\hbar\omega$ for the Ba spectrum in the region of $E \approx 0$. In fact, we suggest that the simplest way to interpret our results is to take Eq. (15) for E as being exact in form, but where the critical fields, as defined in Eqs. (13) and (14) are uncertain by numerical factors (which we expect are not too much different from unity).

From Eq. (15) it immediately follows that the energy spacing is given by

$$\frac{\delta E}{\delta n} = \hbar\omega[1 + \tfrac{1}{2}n^{-3/2}(B/B_c)^{-1/2} \pm \tfrac{1}{2}n^{-1/2}(\mathcal{E}/\mathcal{E}_c)(B/B_c)^{-3/2}]\,. \quad (16)$$

Hence

$$\frac{\delta E}{\delta n} = \frac{1}{n}(E_m - \tfrac{1}{2}E_c + \tfrac{1}{2}E_F)\,. \quad (17a)$$

Next, using Eq. (6) to eliminate E_c, we finally obtain

$$\frac{\delta E}{\delta n} = n^{-1}(\tfrac{3}{2}E_m + E_F - \tfrac{1}{2}E)\,. \quad (17b)$$

It follows that, for $E \approx 0$,

$$\frac{\delta E}{\delta n} = \frac{3}{2}\hbar\omega\left(1 + \frac{2}{3}\frac{E_F}{E_m}\right)\,. \quad (17c)$$

This formula gives a generalization of our previous result[2,3] for the energy spacing in the region $E \approx 0$. It will be noticed that, for positive (negative) values of $x\mathcal{E}$, the effect of the electric field is to increase (decrease) the energy spacing in the region of $E \approx 0$. An experimental verification of this prediction would be of interest.

Turning now to the case of the one-dimensional Coulomb potential, the results will be exactly the same, except that Eq. (7) will be modified to reflect the fact that $\langle x^{-1}\rangle \approx \pm 3^{-1/2}R_m^{-1}$. However, in the case of the spectra of electron states outside liquid helium, for example, $x > 0$ is the only situation of interest. So, from now on, we will assume that $x > 0$ and thus we can use all the above results without essential modification.

It is also of interest to consider the one-dimensional problem in the case where the electric field generally dominates. In the case of a pure electric field, the energy levels are given by[16] (for $x > 0$)

$$E_F \approx \tfrac{1}{2}(3\pi n\mathcal{E})^{2/3} \quad (n = 1, 2, 3, \ldots)\,. \quad (18)$$

Thus, in the case where all three fields are present but with the electric field either dominant or at least about as strong as the other fields, we may use Eq. (6) again, with E_F given by Eq. (18) and with

$$E_c = -z\left\langle\frac{1}{x}\right\rangle \approx -\frac{2\mathcal{E}^{1/3}z}{(3\pi n)^{2/3}}\,, \quad (19)$$

and

$$E_m \equiv E_m^{(2)} + E_m^{(1)} = \tfrac{1}{8}\omega^2\langle x^2 + y^2\rangle + \tfrac{1}{2}\omega\langle L_z\rangle \approx \frac{1}{16}\left(\frac{B}{B_0}\right)^2(3\pi n)^{4/3}\mathcal{E}^{-2/3} + \frac{1}{2}\omega\langle L_z\rangle\,, \quad (20)$$

where the superscripts 1 and 2 on E_m indicate the terms linear and quadratic in B and, where L_z is the z component of the angular momentum operator (for the particular case of highly excited states—large n values—$E_m^{(1)}$ is often negligible compared to $E_m^{(2)}$). It follows that

$$E=\tfrac{1}{2}(3\pi\mathcal{E})^{2/3}\left[n^{2/3}-\frac{4z}{(3\pi)^{4/3}}\mathcal{E}^{-1/3}n^{-2/3}+\frac{1}{8}(3\pi)^{2/3}\left(\frac{B}{B_0}\right)^2\mathcal{E}^{-4/3}n^{4/3}\right]+E_m^{(1)}. \quad (21)$$

We will now introduce critical fields B_c' and E_c' in such a way that they are of the same order as B_c and E_c (and also of the same order as B_c'' and E_c'', to be introduced below for the case where the Coulomb field generally dominates). We are thus led to choose

$$B_c'\equiv B_c \quad (22)$$

and

$$\mathcal{E}_c'\equiv(3\pi)^{1/2}2^{-15/4}z^3\mathcal{E}_0\approx 0.53\mathcal{E}_c\approx 0.23z^3\mathcal{E}_0. \quad (23)$$

Hence, using the fact that $2^{13/4}(3\pi)^{-3/2}\approx 0.33$, we may write Eq. (21) in the form

$$E=\tfrac{1}{2}(3\pi\mathcal{E})^{2/3}[n^{2/3}-0.33(\mathcal{E}/\mathcal{E}_c')^{-1/3}+(B/B_c')^2(\mathcal{E}/\mathcal{E}_c')^{-4/3}]+E_m^{(1)}. \quad (24)$$

We now return to Eq. (21) to evaluate energy spacings between levels of the same $\langle L_z\rangle$. Hence, we obtain

$$\frac{\delta E}{\delta n}=\frac{1}{n}\left(\tfrac{2}{3}E_F-\tfrac{2}{3}E_c+\tfrac{4}{3}E_m^{(2)}\right). \quad (25)$$

Next, using Eq. (6) to eliminate E_c, we obtain

$$\frac{\delta E}{\delta n}=\frac{4}{3n}\left[(E_F+\tfrac{3}{2}E_m-\tfrac{1}{2}E)-E_m^{(1)}\right]. \quad (26)$$

Hence, for $E\approx 0$,

$$\frac{\delta E}{\delta n}=\tfrac{2}{3}(3\pi\mathcal{E})^{2/3}n^{-1/3}\left[\left(1+\frac{3}{2}\frac{E_m}{E_F}\right)-\frac{E_m^{(1)}}{E_F}\right]. \quad (27)$$

Finally, we consider the one-dimensional problem in the case where the Coulomb field generally dominates. In the case of a pure Coulomb field, the energy levels are given by[17] (for $x>0$)

$$E_c=-z^2/2n^2 \quad (n=1,2,3,\ldots). \quad (28)$$

Thus, in the case where all three fields are present but with the Coulomb field either dominant or at least about as strong as the other fields, we may use Eq. (6) again, with E_c given by Eq. (28) and with

$$E_F=\mathcal{E}\langle x\rangle\approx(2\mathcal{E}/z)n^2, \quad (29)$$

and

$$E_m=\tfrac{1}{8}\omega^2\langle x^2+y^2\rangle+E_m^{(1)}\approx\frac{1}{z^2}\left(\frac{B}{B_0}\right)^2n^4+E_m^{(1)}. \quad (30)$$

Hence

$$E=-\frac{z^2}{2}\left[n^{-2}-\frac{4\mathcal{E}}{z^3}n^2-\frac{2}{z^4}\left(\frac{B}{B_0}\right)^2n^4\right]+E_m^{(1)}\equiv-\tfrac{1}{2}z^2[n^{-2}-(\mathcal{E}/\mathcal{E}_c'')n^2-(B/B_c'')^2n^4]+E_m^{(1)}, \quad (31)$$

where

$$B_c''\equiv 2^{1/2}B_c\approx 1.4B_c, \quad (32)$$

$$\mathcal{E}_c''\equiv 3^{-1/2}\mathcal{E}_c\approx 0.58\mathcal{E}_c. \quad (33)$$

In addition

$$\frac{\delta E}{\delta n}=\frac{1}{n}(-2E_c+2E_F+4E_m^{(2)}), \quad (34)$$

so that, using Eq. (6) to eliminate, say $E_m^{(2)}$, we obtain

$$\frac{\delta E}{\delta n}=-\frac{6}{n}\left[E_c+\tfrac{1}{3}E_F-\tfrac{2}{3}E)+\tfrac{2}{3}E_m^{(1)}\right]. \quad (35)$$

Hence, for $E\approx 0$,

$$\frac{\delta E}{\delta n}=+\frac{3z^2}{n^3}\left[\left(1+\frac{1}{3}\frac{E_F}{E_c}\right)+\frac{2}{3}\frac{E_m^{(1)}}{E_c}\right]. \quad (36)$$

The question of which of the variety of results we have obtained should be used in a particular instance is answered simply from a knowledge of the parameters appropriate to the particular problem being considered. As already noted, in the case of $\mathcal{E}=0$, Eq. (17c) gives the $\frac{3}{2}\hbar\omega$ spacing, at $E\approx 0$, observed by Garton and Tomkins[1] for the Ba spectrum in B fields $\approx 10^4$ G. It would be of interest to extend this work to include the presence of an electric field.

In the case where $B=0$, the appropriate formulas to be used are either Eqs. (21)–(27) or (31)–(36) depending on whether the electric or Coulomb fields dominate. From an examination of Eq. (31), we see that the electric field dominates over the Coulomb field for $\mathcal{E}$ values greater than about

$$\mathcal{E}^*\equiv\tfrac{1}{4}n^{-4}z^3=\mathcal{E}_c''n^{-4}, \quad (37)$$

as we had previously noted.[4] In the case of liquid helium, for which the appropriate value of z is[9,10] 7×10^{-3}, this corresponds to a value of

$$\mathcal{E}^*=441n^{-4}\ \text{V/cm}, \quad (38)$$

so that for $n=1,2,3$ we have that $\mathcal{E}^*=441$, 27.5, and 5.5 V/cm, respectively, which in turn implies that the present experiments[9] which use fields as high as 300 V/cm are already in the strong-electric-field region. In fact semiclassical analysis in the latter region was shown[4] to give agreement with the experimental results, in the case of $B=0$.

We turn now to the liquid-helium problem in the presence of a magnetic field. From Eq. (31), we see that the magnetic field dominates over the Coulomb field for B values greater than about

$$B^* \equiv 2^{-1/2} n^{-3} z^2 B_0 = n^{-3} B_c'' . \quad (39)$$

In the case of liquid helium, this corresponds to a value of

$$B^* = 8.5 \times 10^4 n^{-3} \text{ G} , \quad (40)$$

so that for $n = 1, 2, 3$ we have that $B^* = 8.5 \times 10^4$, 1.1×10^4, and 3.1×10^3 G, respectively. Thus, we see that the existing experiments,[10] which use fields as high as 2 kG, are close to the strong-magnetic-field region. Since much higher fields than 2 kG are now available for laboratory experiments, we urge their use for the liquid-helium experiment, in anticipation that phenomena as fascinating as those occurring in the Ba spectrum will manifest themselves.

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