Semiempirical scaling laws for diabatic energy levels of highly excited hydrogen atoms in high magnetic fields

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The "diabatic" levels responsible for the observation of quasi-Landau resonances in absorption spectra of strongly magnetized atoms obey some scaling laws, valid for the whole range of the magnetic field. This suggests again that it should be possible to find a fully separable approximate model to describe the considered system in a realistic way.

During the last few years, the structure of Rydberg atoms in the presence of an "intense" magnetic field has been the subject of many theoretical and experimental works.[1] In particular, much attention has been paid to the equally spaced structures,[2–6] so-called quasi-Landau resonances, which were initially found in the absorption spectrum of barium by Garton and Tomkins.[2] These resonances extend across the zero field series limit into the continuum with a spacing of about $1.5\hbar\omega_c$, ω_c being the cyclotron frequency. Such a spacing has been first explained by using a semiclassical model[7–9] in which the wave function is localized in a plane perpendicular to the magnetic field. Then, the connection between the quasi-Landau resonances and the low-magnetic-field energy-level structure has been investigated in three papers[10–12] which highly improved our knowledge of this old but still exciting problem.

First, by interpreting their data on diamagnetic structure of $m_l=1$ odd parity sodium Rydberg stages in the vicinity of $n=28$ (n is the principal quantum number, m_l is the magnetic orbital quantum number), Zimmerman *et al.*[10] showed that, in despite of the inter-n mixing induced by diamagnetic interaction, anticrossings between levels with same parity and same magnetic quantum numbers are very weak for highly excited hydrogenic states. This result is very important since, on the one hand, it suggests the existence of an approximate dynamical symmetry and, on the other hand, it shows that one can easily follow "diabatic" levels labeled by the same quantum numbers as in the low-magnetic-field limit, that is to say, parity, magnetic quantum numbers, n (the principle quantum number), and k, an additional label for distinguishing the various levels belonging to the same hydrogenic n manifold.

Then, two independent experimental studies, concerning, respectively, $m_l=-1,-2$ even-parity sodium spectra[11] and $m_l=\pm 3$ odd-parity cesium spectra,[12] showed that quasi-Landau resonances emerge by a concentration of oscillator strength into the diabatic level which, in the low-magnetic-field limit, rises fastest in energy with increasing the magnetic field. By convention, k is at minimum for that particular level. The object of this paper is to show that the diabatic levels leading to quasi-Landau resonances observed through optical excitation obey simple scaling laws which allow one to predict their energy for any values of n and the magnetic field B.

First, let us define by $\epsilon(n,k_<)$, the energy of the considered level corrected from the linear Zeeman shift. In the low-magnetic-field limit, $\epsilon(n,k_<)$ is given by[13]

$$\epsilon(n,k_<)=-\frac{1}{2n^2}+\tfrac{1}{8}a_n n^4 B^2 \; ; \tag{1}$$

a_n depends on n, but for values of n much larger than m_l, it can be approximated by $\frac{5}{2}$. Now, it is well known that the quantity $\beta=n^3B$ plays an important role in the considered problem since, in a classical picture, it represents the ratio between the Lorentz force and the Coulomb force.[8,9,14] In particular, semiclassical theory predicts that the level $(n,k_<)$ crosses the field-free ionization limit for $\beta=\beta_0\simeq 1.6$, a result in excellent agreement with the experimental data of Gay *et al.*[12] Equation (1) can be rewritten

$$\epsilon n^2=-\tfrac{1}{2}+\tfrac{5}{16}\beta^2 \; , \tag{2}$$

and it appears that in the low-magnetic-field limit, the quantity ϵn^2 is entirely determined by β.

In the high-field limit, Angelié and Deutsch[15] showed, by using virial considerations and WKB approximation, that ϵ can be approximated by

$$\epsilon = nB - (CB/n)^{1/2} , \tag{3}$$

with C being a constant, provided that n is much larger than m_l, a condition always fulfilled in Rydberg atoms produced in an optical way. Equation (3) can be rewritten

$$\epsilon n^2 = \beta - (C\beta)^{1/2} , \tag{4}$$

and again the quantity ϵn^2 depends on β only. In fact, Eq. (3) was first derived by O'Connell[14] from a simplified Bohr model. With such a model, C is equal to $\frac{1}{2}$. Moreover, Fonck *et al.*[6] used an expression equivalent to Eq. (4) to fit their data including observations in the $M_L = 0$ even-parity channels of Ba I and Sr I with $B = 2.5-4$ T and the $M_L = 1$ odd-parity channel of Ba I at $B = 4.7$ T. The agreement was found to be excellent; for values of β as small as 0.3, the corresponding value of C is obviously equal to β_0 in this approximation.

Now, considering Eqs. (2) and (4), it is strongly tempting to assume that, for the whole B range, the quantity ϵn^2 is a function of β only. Besides, this property is satisfied by the WKB solutions in a one-dimensional model[6] if one ignores the centrifugal energy contribution. To verify again this conjecture which was first used, in a different but equivalent form, by Fonck *et al.*,[14] we have plotted, in Fig. 1, the quantity ϵn^2 against β for some of the numerous data recently published by Castro *et al.*[11] and Gay *et al.*[12] The result is clear again: The assumption is verified by experiment.

Then, one may ask if it is possible to find an analytical expression for $\epsilon n^2 = f(\beta)$ that fits accurately the experimental data. After some unsuccessful attempts, we have searched $f(\beta)$ under the following form:

$$f(\beta) = (\beta^2 + t\beta + \mu^2)^{1/2} - (x\beta + y^2)^{1/2} . \tag{5}$$

By imposing that Eq. (2) be satisfied, only one free parameter, for example, $x = C$, remains to be adjusted to provide a best fit to the considered experimental data. The result of the fitting is quite surprising, since one obtains with an excellent approximation $x = 2$, an integer number, which leads of course to $y = 2$, $t = \mu = \frac{3}{2}$. Moreover, Fig. 1 shows that $f(\beta)$ reproduces very well the available experimental data, and in particular, one must notice that $f(\beta) = 0$ for $\beta = 1.6$, a value equal to β_0,

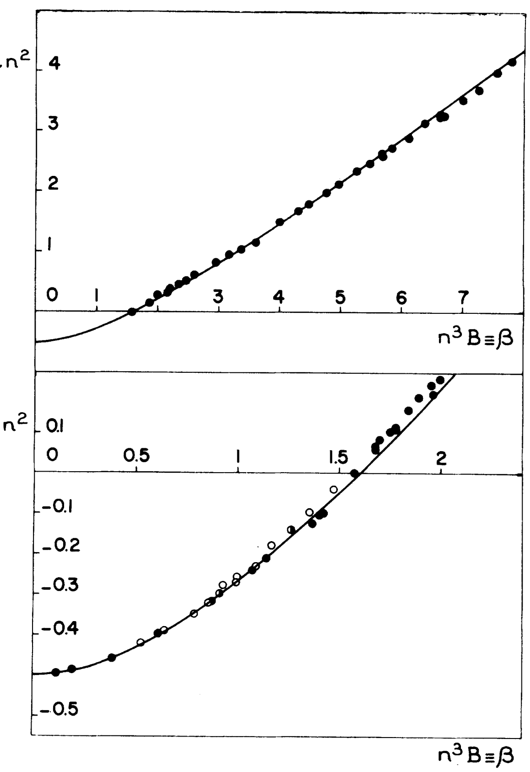

FIG. 1. ϵn^2 vs $n^3 B$. Values randomly chosen among the numerous data of Gay *et al.* (Ref. 12) (●) and of Castro *et al.* (Ref. 13) (○). Calculated values (—) from Eq. (5).

and that $\dot{f}(\beta_0) = \frac{1}{2}$, which leads to

$$(\partial\epsilon/\partial n)_{\epsilon=0} = |\, 3\dot{f}(\beta_0) - (2/\beta_0) f(\beta_0) \,|\, B$$
$$= (\tfrac{3}{2}) B .$$

Considering the simplicity of $f(\beta)$, it is hard to believe that the agreement observed between the values derived from $f(\beta)$ and the experimental data is fortuitous. Therefore, we are convinced that some physics is present in the particular form of $f(\beta)$ we have chosen.

One may remark that the knowledge of $f(\beta)$ allows us to determine the mean values of $1/r$, the Coulomb operator, and of ρ^2, the diamagnetic operator. More precisely, one gets from the Hellmann-Feynman theorem

$$\langle 1/r \rangle = (2/n^2)[\beta \dot{f}(\beta) - f(\beta)] , \tag{6}$$

$$\langle \rho^2 \rangle = (4n^4/\beta) \dot{f}(\beta) . \tag{7}$$

It is clear from Eq. (5) that in the strong magnetic field limit, the quantity $\langle \rho^2 \rangle \langle 1/r \rangle^2$, which depends on β only, goes to a limit in agreement with classical predictions. Moreover, from Eqs. (6) and (7), one directly obtains the mean values of the Coulomb energy V_C, of the diamagnetic energy V_B, and therefore, by difference, of the kinetic energy T:

$$V_C = -(2/n^2)[\beta\dot{f}(\beta) - f(\beta)] , \tag{8}$$

$$V_B = (1/2n^2)\beta\dot{f}(\beta) , \tag{9}$$

$$T = (1/n^2)[-f(\beta) + (\tfrac{3}{2})\beta\dot{f}(\beta)] . \tag{10}$$

The corresponding functions are illustrated on Fig. 2.

Let us finally notice that $f(\beta)$ appears as the sum of two contributions (one positive, one negative) which can be considered as eigenvalues of two separated Hamiltonians. This suggests again that it should be possible to find a fully separable model to describe the considered problem in a realistic way. From the present work, the spectrum of each of the separated Hamiltonians is entirely known and this should help to find them explicitly.

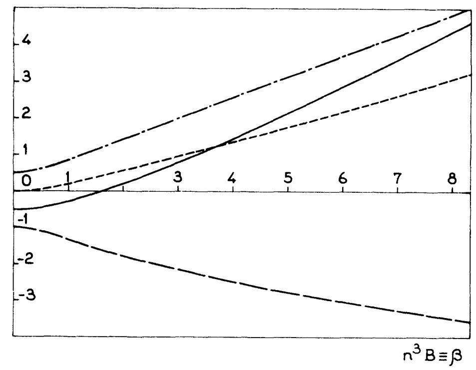

FIG. 2. Variations vs $\beta = n^3 B$ of the respective mean values, multiplied by n^2, of the Coulomb energy (— — —), the diamagnetic energy (- - - -), the kinetic energy (— - — - —), and the total energy (—).

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