

## CHAPTER X

### APPLICATION OF THE VFM TO THE ZEEMAN EFFECT IN HYDROGEN

#### §.33. Derivation of the variational functional

Let us consider a hydrogen atom of nuclear charge  $Z$ , placed in an external uniform magnetic field along the  $x_3 \equiv z$  direction. The Hamiltonian operator describing this system in the non-relativistic approximation, and with suitable units (Appendix H), is:

$$H_e = -\frac{1}{2} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{\partial^2}{\partial x_3^2} \right) + \frac{m^2}{2\rho^2} + \frac{\lambda^2}{8} \rho^2 + \frac{\lambda}{2} (L_{x_3} + g_s S_{x_3}) - \frac{Z}{r} \quad (33.1.)$$

where

$$r^2 = x_1^2 + x_2^2 + x_3^2 = \rho^2 + x_3^2 \quad (33.2)$$

Let  $E(Z, \lambda)$  denote the set of eigenvalues of that portion of  $H$  excluding the paramagnetic field terms (Eq. (31.1)), i.e.:

$$E(Z, \lambda) = \langle H(Z, \lambda) \rangle = \langle H_e \rangle - \frac{\lambda}{2} (m + g_s m_s); \quad m=0, \pm 1, \pm 2, \dots$$

$$m_s = \pm 1/2 \quad (33.3)$$

The importance of this problem was already widely discussed in §.30. As pointed out, the eigenvalue problem has no analytic solution due to the coupling of the two coulombic degrees of freedom ( $\rho$  and  $x_3$ ). Our purpose is to apply the VFM to derive valid approximate expressions for  $E(Z, \lambda)$ ,  $\forall \lambda \geq 0$  /1,2/.

From the Heisenberg inequalities (in cartesian coordinates), we found in §.22 an appropriate form of the VF, which here reduces to

$$F = \frac{A_1}{q_1^2} + \frac{A_2}{q_2^2} + \frac{A_3}{q_3^2} + \hat{V}(\bar{q}) \quad (33.4)$$

$$\bar{q} = (q_1, q_2, q_3) \quad (33.5)$$

with  $\{A_i\}$  constants not depending on  $\lambda$ . The parameters  $\{q_i\}$  are proportional to the uncertainties in each cartesian coordinate (see Chapter VI). In accordance with the BC defining the problem, such parameters satisfy the following proportionality relation:

$$q_i^2 \propto \langle x_i^2 \rangle \quad (33.6)$$

The functional  $\hat{V}(q)$  is the expectation value of the potential  $V = -\frac{Z}{r} + \lambda^2 \rho^2/8$  in terms of  $\{q_i\}$ .

In order to construct this functional we follow the procedure depicted in Chapter VI. Thus, the simplest choice is suggested at once by the expression of the potential function:

$$\hat{V}(q) = -C \frac{Z}{q} + \frac{\lambda^2}{8} (q_1^2 + q_2^2) B \quad ; \quad q = ||\bar{q}|| \quad (33.7)$$

Keeping ourselves within the simplified scheme employed up to now, we will assume that B and C are constants depending just on the quantum numbers. It must be noted that the two constants introduced in  $V(q)$  are not redundant, unlike the models studied in Chapter VII. This is due to the fact that these last models were reducible to 1D systems, while the present one demands a multidimensional functional. Up to certain point, the present state of affairs is quite similar to that found in Chapter VIII, where the finite BC made it necessary to modify the VF, with the introduction of an additional constant. It is well known that the exact eigenvalue  $E(Z, \lambda)$  fulfils two fundamental Theorems,

determining the dependence on the parameters contained within H: VT

$$\sum_{n=1}^3 \langle p_n^2 \rangle = \langle \frac{Z}{r} + \frac{\lambda^2}{4} \rho^2 \rangle, \quad (33.8)$$

and HFT

$$\frac{\partial E}{\partial Z} = - \langle \frac{1}{r} \rangle, \quad (33.9a)$$

$$\frac{\partial E}{\partial \lambda} = \frac{\lambda}{4} \langle \rho^2 \rangle. \quad (33.9b)$$

From Theorem 19.1, the F extreme condition

$$\left( \frac{\partial F}{\partial q_i} \right) (q_i = q_i^*) = 0 \quad ; \quad i = 1, 2, 3 \quad (33.10)$$

allows the fulfilment of VT and HFT-like equations, viz.

$$2 \sum_{i=1}^3 \frac{A_i}{q_i^*{}^2} = \frac{CZ}{q^*} + \frac{\lambda^2}{4} B (q_1^{*2} + q_2^{*2}), \quad (33.11a)$$

$$\left( \frac{\partial F}{\partial \lambda} \right) (q_i = q_i^*) = \frac{\lambda}{4} B (q_1^{*2} + q_2^{*2}), \quad (33.11b)$$

$$\left( \frac{\partial F}{\partial Z} \right) (q_i = q_i^*) = - \frac{C}{q^*}. \quad (33.11c)$$

The extreme values of variables  $q$  and  $\{q_i\}$  are determined from (33.10), which immediately allow one to obtain the couple of relationships

$$-2 \frac{A_i}{q_i^*{}^3} + \frac{\lambda^2}{4} B q_i^* + \frac{ZC}{q^*{}^3} q_i^* = 0 \quad ; \quad i = 1, 2, \quad (33.12a)$$

$$-2 \frac{A_3}{q_3^*} + \frac{ZC}{q_3^*} q_3^* = 0 \quad . \quad (33.12b)$$

The Hamiltonian's cylindrical symmetry for  $\lambda \neq 0$  does not permit the separate determination of  $q_1^*$  and  $q_2^*$ . Thus, it is natural to compute just  $q_1^{*2} + q_2^{*2}$  and  $q_3^*$ , since they are enough to describe completely the system. We start from Eqs. (33.12) to determine such coordinates, and we are led to

$$q_1^{*2} + q_2^{*2} = [A_1^{1/2} + A_2^{1/2}] \left\{ \frac{2q_3^{*3}}{\frac{\lambda}{4} Bq_3^{*3} + ZC} \right\}^{1/2}, \quad (33.13a)$$

$$q_3^* = \left[ \frac{2A_3 q_3^*}{ZC} \right]^{1/2}, \quad (33.13b)$$

The calculation is completed with Eq. (33.5)

$$q^{*2} = q_1^{*2} + q_2^{*2} + q_3^{*2} \quad (33.13c)$$

Once the constants  $A_3$ ,  $C$ ,  $B$  and  $(A_1^{1/2} + A_2^{1/2})$  are known, Eqs. (33.13) are solved iteratively.

As discussed in Chapter VI, the VFM allows one to approach the eigenvalue  $E(Z, \lambda)$  through the functional extreme. Using Eqs. (33.11a) (VT for F) and (33.13a) in F, such extreme can be expressed at once in terms of  $q^*$  and the aforesaid constants:

$$F(q^*) = \frac{-ZC}{2q^*} + \frac{\lambda^2}{4} |A_1^{1/2} + A_2^{1/2}| \left\{ \frac{2B^2 q_3^{*3}}{ZC + \frac{\lambda^2 B q_3^{*3}}{4}} \right\}^{1/2} \quad (33.14)$$

Finally, to complete the F construction it remains to determine the involved constants. Before discussing this problem, it is convenient to analyse some relations that will be useful later on.

From the HFT for F (Eqs.(33.11b, c)) and HFT for E (Eqs.(33.9)), we obtain the expectation values

$$\langle \rho^2 \rangle = B(q_1^{*2} + q_2^{*2}) \quad (33.15a)$$

$$\langle \frac{1}{r} \rangle = \frac{C}{q^*} \quad (33.15b)$$

for the state under consideration.

Applying the same procedure as in Chapters VII and VIII, we gather the constants involved within the functional from the knowledge of the system properties at zero field ( $\lambda=0$ ) and infinite field (which is equivalent to make  $Z=0$ ). From Eq.(33.14) we get:

$$\lim_{\lambda \rightarrow 0} F(\bar{q}^*) = -\frac{ZC}{2} \lim_{\lambda \rightarrow 0} q^{*-1} \quad (33.16)$$

and, on the other hand, Eqs. (33.13) allow one to deduce

$$\lim_{\lambda \rightarrow 0} q^{*-1} = \frac{ZC}{2A} ; \quad \sqrt{A} = \sum_{i=1}^3 A_i^{1/2} \quad (33.17)$$

so that Eq.(33.16) takes the form:

$$\lim_{\lambda \rightarrow 0} F(\bar{q}^*) = -\frac{Z^2 C^2}{4A} \quad (33.18)$$

Imposing the correlation between the VF and the correct eigenvalue at zero field:

$$E(Z, 0) = \lim_{\lambda \rightarrow 0} F(\bar{q}^*) \quad , \quad (33.19)$$

we derive a first relation to be satisfied by the constants

$$\frac{C^2}{A} = \frac{2}{n^2} \quad ; \quad n = n_r + \ell + 1 \quad ; \quad n_r \ell \geq 0 \quad (33.20)$$

where, as usual,  $n$  is the principal quantum number of the hydrogen-like atom. Since  $\{q_\pm\}$  satisfy the proportionality relationship (33.6) it could be concluded that

$$\langle r^2 \rangle \propto q^*{}^2 \quad . \quad (33.21)$$

But this relation, unlike (33.15) is not an equality for all  $\lambda$ , because now we have not any theorem relating derivatives of the VF with  $\langle r^2 \rangle$ . However, we can determine, without any loss of generality, the constant  $C$  so that (33.21) is obeyed at zero-field

$$\langle r^2 \rangle (\lambda=0) = \lim_{\lambda \rightarrow 0} q^*{}^2 \quad . \quad (33.22)$$

Substitution of (33.22) into (33.15b) permits the determination of the constant  $C$ :

$$C = \sqrt{\left\langle \left(\frac{1}{r}\right)^2 \right\rangle (\lambda=0)} = \frac{1}{n\sqrt{2}} \{5n^2 + 1 - 3\ell(\ell+1)\}^{1/2}, \quad (33.23)$$

since the involved expectation values are well-known in the hydrogen-like eigenfunctions basis set /3,4/. Notice that  $C$ -constant is  $Z$  independent.

Eqs. (33.20) and (33.23) allow us to fix the correct  $E$  and  $\langle r^2 \rangle$  values when  $\lambda \rightarrow 0$ . There is an additional relation for the correct behavior of  $\langle \rho^2 \rangle$  when  $\lambda \rightarrow 0$ .

The hydrogen atom fulfils /3/

$$\langle \rho^2 \rangle (\lambda=0) = \frac{2}{3} f \langle r^2 \rangle (\lambda=0) \quad (33.24a)$$

where

$$f = f(m, \ell) = 1 + \frac{3n^2 - \ell(\ell+1)}{(2\ell+3)(2\ell-1)} \quad (33.24b)$$

Inserting Eqs. (33.15a) and (33.22) in (33.24a), we obtain

$$\begin{aligned} B \lim_{\lambda \rightarrow 0} (q_1^{*2} + q_2^{*2}) &= \left[ \frac{2}{ZC} \right]^{1/2} B (A_1^{1/2} + A_2^{1/2}) \lim_{\lambda \rightarrow 0} q^{*3/2} = \\ & \frac{2f}{3} \lim_{\lambda \rightarrow 0} q^{*2} \quad , \end{aligned} \quad (33.25)$$

and together with Eqs. (33.17) and (33.20) yields other relationship among the constants:

$$B (A_1^{1/2} + A_2^{1/2}) = \frac{2^{1/2} n f C}{3} \quad . \quad (33.26)$$

In order to complete the functional's construction, we have to determine the constant  $A_1^{1/2} + A_2^{1/2}$ . Since such a constant appears in the purely cylindrical symmetry term of  $F$ , it seems appropriate to determine it from the knowledge of the energy at infinite field strength, where the term containing the constant is dominant. For  $\lambda \rightarrow \infty$  (equivalent to  $Z \rightarrow 0$ ), the functional extreme (Eq. (33.14)) follows

$$\lim_{Z \rightarrow 0} F(\bar{q}^*) = (2B)^{1/2} (A_1^{1/2} + A_2^{1/2}) \frac{\lambda}{2} \quad . \quad (33.27)$$

This behavior can be matched with the Landau spectrum by way of

$$E(0, \lambda) = \left( \frac{N+1}{2} \right) \lambda = \lim_{Z \rightarrow 0} F(\bar{q}^*) \quad (33.23)$$

and finally the desired result follows:

$$A_1^{1/2} + A_2^{1/2} = \frac{N+1}{(2B)^{1/2}}, \quad (33.29)$$

where  $N=0,1,\dots$  is the Landau quantum number (Appendix H), labelling the problem states with  $Z \rightarrow 0$ . In order to perform any computation, it is necessary to know the correlation among the quantum numbers  $(n, \ell, m)$  and  $N/4-6/$ . It must be pointed out that only  $m$  is a good quantum number, since the angular momentum  $L$  in the axis  $x_3$  is conserved. Notwithstanding, it is possible to correlate properly the Coulombic regime states with the Landau ones through the constants contained within  $F$ . The substitution of (33.29) in (33.26) and using (33.23), we get the  $B$  constant in closed form:

$$B = \frac{2}{9(N+1)^2} f^2 (5n^2 + 1 - 3\ell(\ell+1)) \quad . \quad (33.30)$$

Constant  $A_3$  is computed with the aid of Eqs. (33.17) and (33.20)

$$A_3^{1/2} = \frac{1}{2} \{5n^2 + 1 - 3\ell(\ell+1)\}^{1/2} - \frac{N+1}{(2B)^{1/2}} \quad , \quad (33.31)$$

and it concludes the calculation procedure.

Summing up, the constructed functional allows one to obtain a function satisfying HFT and VT and, furthermore, having the same behavior as the exact eigenvalue for  $\lambda \rightarrow 0$  and  $\lambda \rightarrow \infty$ . In addition, the insertion of an extra constant permits one to get the correct  $\langle \rho^2 \rangle$  ( $\lambda=0$ ) and  $\langle r^2 \rangle$  ( $\lambda=0$ ) values.

Since the functional obeys the first aforesaid expectation value, it is implied that the VFM yields the RSPT up to the first order. We will see that, on spite of its simplicity, the functional gives an excellent approximation to the exact eigenvalue  $E(Z, \lambda)$ .

It is appropriate to analyse some scaling properties fulfilled by  $F$ , through the extreme condition (33.10), before performing any actual



calculation.

To this end, let us denote with  $F(\bar{q}^* ; Z, \lambda)$  the minimum  $F$  value (Eq. (33.14)), representing the hydrogen-like atom energy with  $Z$  nuclear charge, in a field  $|\lambda|$ . Scaling the parameter  $q^*$  (see Appendix A) through Eq. (33.14), and re-writing the formula in an unitary equivalence form, we obtain

$$F(\bar{q}^*; Z, \lambda) = \lambda \left\{ -\frac{ZC^{-1}}{2q^*\lambda} + \frac{1}{4} (A_1^{1/2} + A_2^{1/2}) \left[ \frac{2B^2 q^{*3}}{\alpha \frac{3}{\lambda^2} + \frac{Bq^{*3}}{4}} \right]^{1/2} \right\} . \quad (33.32)$$

The choice

$$\alpha = \lambda^{-1/2} , \quad (33.33)$$

transforms Eq. (33.32) into

$$F(\bar{q}^*; Z, \lambda) = \lambda \left\{ -\frac{C}{2q^*} \left( \frac{Z}{\lambda^{1/2}} \right) + \frac{1}{4} (A_1^{1/2} + A_2^{1/2}) \left[ \frac{2B^2 q^{*3}}{\lambda^{1/2} + \frac{Bq^{*3}}{4}} \right]^{1/2} \right\} . \quad (33.34)$$

and it yields the following equivalence relationship

$$F(\bar{q}^*; Z, \lambda) = \lambda F(q^*; Z\lambda^{-1/2}, 1) . \quad (33.35)$$

Eq. (33.35) is the same as that satisfied by the exact eigenvalue  $E(Z, \lambda)$ . This property assures us that the VF will have an approximately correct dependence upon  $\lambda$  within the whole range of field intensities. Moreover, relationship (33.35) simplifies at a large extent the computation scheme, since they must only be done for  $Z=1$ .

### §.34. Results for several functions of physical interest.

Equations deduced in §.33 allow one to compute the eigenvalue  $E(1, \lambda)$  ( $Z=1$  in our calculations), within a reasonable accuracy, whenever the correlation among quantum numbers  $(n, m, \ell)$  and  $N$  is provided /4-6/. Besides, HFT makes up the way to obtain  $\langle \rho^2 \rangle$  and  $\langle r^{-1} \rangle$  plausible approximate values.

The computational scheme is as follows: After selecting the state under study (i.e. fix  $(n, m, \ell)$  and  $N$  values), the constants appearing in the functional are computed via Eqs. (33.23) and (33.29)-(33.31). Then  $q^*$  is determined through an iterative solution of the coupled equations (33.13), and energy as well as expectation values are obtained from Eqs. (33.14) and (33.15), respectively.

We can add another calculation based on the fact that (33.21) turns into a equality when  $\lambda \rightarrow 0$  (Eq. (33.22)). For  $\lambda \neq 0$  one could rigorously guess that it might still be a reasonable approximation to  $\langle r^2 \rangle$ . The goodness of this result is discussed in this paragraph. Let us remark that  $E, \langle r^2 \rangle$  and  $\langle \rho^2 \rangle$  are the most significant quantities from the physical viewpoint, because the first one stands for the atomic energy, and the two remaining ones describe the approximate atomic "shape".

Some results are shown in Figs. 10.1 and 10.2 for a large range of field intensities.

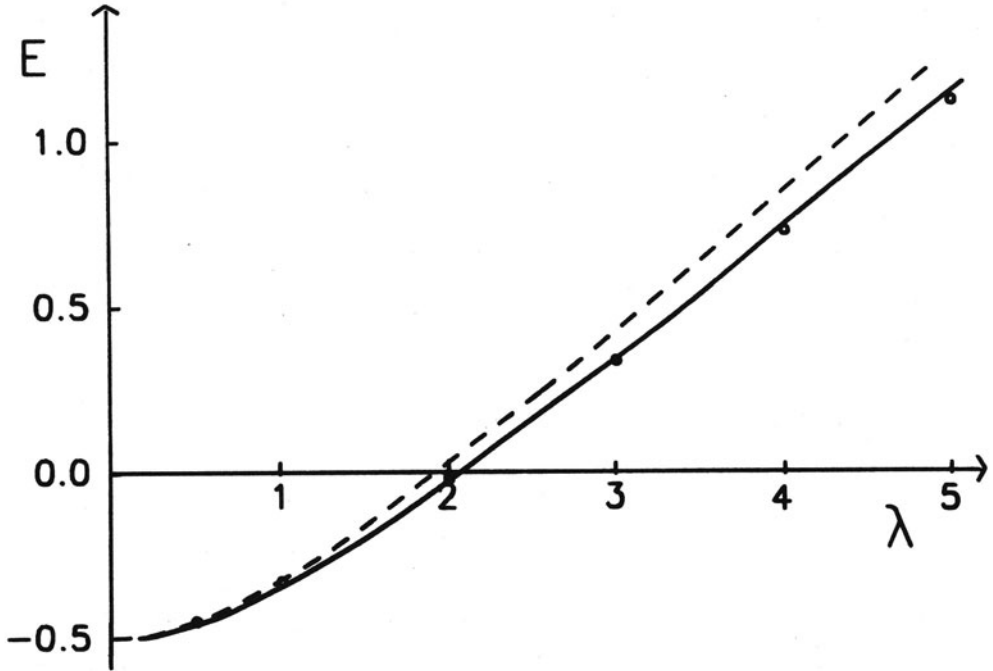


Fig. 10.1: Ground state energy of the Zeeman effect in the Hydrogen atom for low and middle field strengths.

- Results obtained from the VFM ( $n_r=l=m=0$ )
- Results obtained from the VFM ( $n_r \rightarrow \infty, l=m=0$ )
- o "Exact" results /7/.

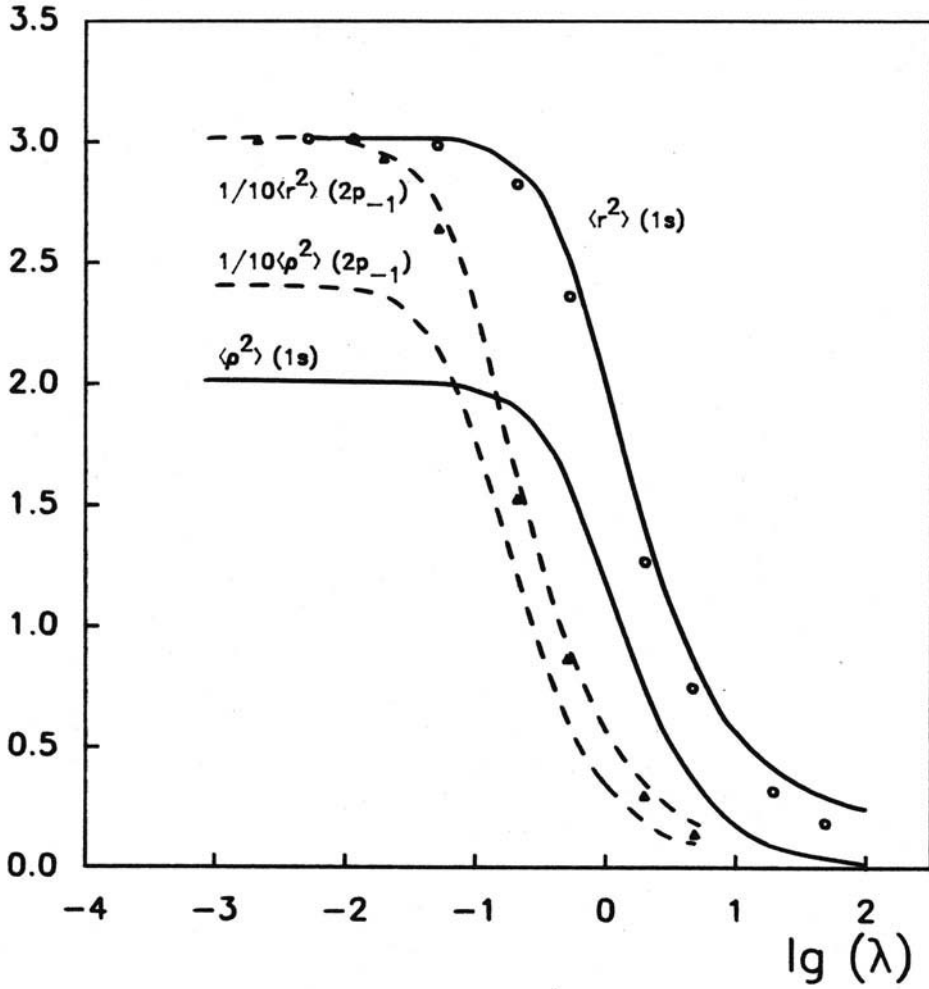


Fig. 10.2: Approximate average values of  $O^2$  and  $r^2$  for the Zeeman effect in Hydrogen atom states by way of the VFM.

— 1s state

-----  $2p_{-2}$  state

○ "Exact" results for the 1s state /7/

△ "Exact" results for the  $2p_{-1}$  state /7/

For the sake of simplicity, we have chosen the first two Landau states ( $N+m=0$ ), which are the two most studied tight-bound states (see Chapter IX). For  $\lambda \rightarrow 0$ , these states correlate with the hydrogen atom states  $1s$  and  $2p_{-1}$ . The quantum numbers assignments are

$$(n, m, \ell; N) = (1, 0, 0; 1) \rightarrow "1s" \text{ state} \quad (34.1a)$$

$$(n, m, \ell; N) = (2, -1, 1; 1) \rightarrow "2p_{-1}" \text{ state} \quad (34.1b)$$

The broken line in Fig. 10.1 shows the ground state energy change (34.1a) for low and intermediate field intensities. The results reveal some noteworthy features:

i) For  $\lambda \leq 1$  results agree satisfactorily with the exact ones obtained with the most accurate numerical, variational techniques available /7/. This is not surprising since the greatest information introduced within the functional corresponds to  $\lambda \rightarrow 0$ . Nevertheless, the agreement is remarkable, since we have only used the RSPT first-order information. It is well known that RSPT is asymptotically divergent, and this property hinders its practical application for  $\lambda \geq 0$  /8/. Consequently, the extension performed through the VFM is quite meaningful.

ii) For larger field intensities ( $\lambda \geq 1$ ) present results lack accuracy and yield an upper bound to the eigenvalue  $E(1, \lambda)$  (Eq. (34.1a)). However, it is worth noting that the curve shape obtained from the VFM is quite similar to the exact one. This result shows that the main dependence of  $E$  on  $\lambda$  may be guaranteed through the VT and HFT obeyed by the VF. The remaining differences could be removed by including higher orders of RSPT within the VF. This point will be discussed later on.

Fig. 10.2 displays the results for  $\langle \rho^2 \rangle$  and  $\langle r^2 \rangle$  within the field range  $10^{-3} \leq \lambda \leq 10^2$ , for those states described by Eqs. (34.1). Results show that  $q^*{}^2$  is an excellent approximation to  $\langle r^2 \rangle$  /7/, in the whole field intensity range. A similar conclusion can be reached for the present approximation to  $\langle \rho^2 \rangle$  (in principle more accurate than that obtained for  $\langle r^2 \rangle$ ), although there are not exact data available to make the necessary comparisons.

In closing this paragraph, we can remark that VFM makes up a quite simple formalism to describe up to a satisfactory degree the more important physical properties of the Zeeman effect in the hydrogen-like atoms. Present conclusions about the atomic "shape" for the two considered states are correct /9/: the atom distorts turning to be a "needle" oriented along the field direction. That is to say, the electronic density tends to concentrate on the nucleus, and in less proportion across the directions normal to the field. Additional results on the application of the VFM to this system can be seen in Refs. /1,2/.

### §. 35. Scaling laws and semiclassical behavior of the Variational functional.

Eq. (33.35) represents a scaling relationship in the magnetic field and it is fulfilled by the VF made an extreme in the configuration space.

As shown in Appendix H, this relationship can be expressed as a scaling law in the nuclear charge  $Z$ . There exists an additional relation satisfied by the exact eigenvalues at the semiclassical limit, i.e. for large  $n$  and  $N$  quantum numbers. This law is represented in an approximate fashion by Eq. (30.6) (it was discussed in Chapter IX regarding Rydberg atoms placed in magnetic fields). As analysed in §.31, and elementary semiclassical model allows one to account for such a law (cf. Eq. 31.25).

Let us discuss the VF behavior regarding the scaling in quantum numbers. Let us consider those states obeying the relation

$$n = N+1 \quad ; \quad (35.1)$$

redefining the functional constants and variables as follows

$$A_i' = A_i/n^2 \quad , \quad (35.2a)$$

$$\lambda' = n^3 \lambda \quad , \quad (35.2b)$$

$$q'^* = q^*/n^2 ; \bar{q}'^* = (q_1'^*, q_2'^*, q_3'^*) ; q'^* = ||\bar{q}'^*||, \quad (35.2c)$$

$$F'^* = n^2 F^* = n^2 F(\bar{q}'^*; Z, \lambda) . \quad (35.2d)$$

From Eqs. (35.1) and (35.2a) together with Eqs. (33.29), (33.31) and (33.23), we have

$$A_1'^{1/2} + A_2'^{1/2} = \frac{1}{(2B)^{1/2}} , \quad (35.3)$$

$$A_3'^{1/2} = 2^{-1/2} (C - B^{-1/2}) ; \quad (35.4)$$

$q_i'^*$  values are derived from Eqs. (33.13), (35.1) and (35.2):

$$q_1'^*{}^2 + q_2'^*{}^2 = (A_1'^{1/2} + A_2'^{1/2}) \left\{ \frac{2q'^*{}^3}{\lambda'^2 B q'^*{}^3} + ZC \right\}^{1/2} \quad (35.5a)$$

$$q_3'^*{}^2 = \left\{ \frac{2A_3 q'^*{}^3}{ZC} \right\}^{1/2} \quad (35.5b)$$

Finally, Eqs. (35.2a) and (33.14) yield the extreme functional expression  $F'^*$ :

$$F'^* = n^2 F^* = - \frac{ZC}{2q'^*} + \frac{\lambda'^2}{4} B^{1/2} \left\{ \frac{q'^*{}^3}{ZC + \frac{\lambda'^2 B q'^*{}^3}{4}} \right\}^{1/2} \quad (35.6)$$

Eq. (35.6) is the desired result:  $F'^*$  depends exclusively on  $n^3 \lambda$ , such as it is required by the scaling law (30.6). Then, the VFM obeys the relation (30.6) as well as other semiclassical approximations like (31.25) do.  $F'^*$  depends on  $\lambda'$  and its only explicit dependence on the quantum numbers is through  $C$  and  $B$ . This function  $F'^*$  behaves similarly to the ground state ( $n = N+1 = 1$ ), since it satisfies the same asymp-

otic relationships:

$$F'^* (\lambda' = 0) = -Z^2/2 \quad , \quad (35.7)$$

$$F'^* (Z = 0) = \lambda'/2 \quad . \quad (35.8)$$

Accordingly, there is an infinite family of curves  $F'^*$  with the same asymptotic behavior as the ground state. We can obtain a sole function not depending on  $n$  taking the limit  $n \rightarrow \infty$ . This is possible due to the fact that  $C$  and  $B$  have finite limits:

$$\lim_{n \rightarrow \infty} C = \left(\frac{5}{2}\right)^{1/2} \quad , \quad (35.9)$$

$$\lim_{n \rightarrow \infty} B = \frac{10}{9} f^2 \quad . \quad (35.10)$$

Substitution of (35.9) and (35.10) into (35.6), after taking the limit  $n \rightarrow \infty$ , allow one to express  $F'^*$  as a function depending on  $\lambda'$ ,  $m$  and  $\ell$ .

This last result is especially interesting, since it leads to a similar result to that obtained through semiclassical approximations in  $1/n$  power series expansions [10,11]. In such a approximation, the ground state is obtained with the limit  $n \rightarrow \infty$ ; accordingly, it seems plausible to use the limit  $n \rightarrow \infty$  in  $F'^*$  with  $m=\ell=0$  to approximate this particular state.

Fig.10.1 displays in broken line, the results for the lowest eigenvalue ( $N=m=\ell=0$ ) obtained via Eq. (35.6) at the limit  $n \rightarrow \infty$  ( $n_r \rightarrow \infty$ ) (Eqs. (35.9) and (35.10) with  $f=1$ ).

These results reveal the following characteristics:

- i) For  $\lambda \ll 1$  they are worse than those discussed in §.34. This behavior is quite understandable considering that  $(\partial F'^*/\partial \lambda)(\lambda'=0)$  differs from the correct value  $(\partial F^*/\partial \lambda)(\lambda=0) = (\partial E/\partial \lambda)(\lambda=0)$ . That if,  $F'$  scaled



with  $n_r \rightarrow \infty$  does not satisfy the perturbative expansion up to the first order.

ii) Within the interval  $1 < \lambda < 5$  results are extremely accurate. We can assume that in this range the dilatation effects on quantum numbers have the largest importance.

In §.30 we made a thorough discussion on recent physical applications of the Zeeman effect in hydrogen-like atoms for magnetic fields of arbitrary intensity, and it was commented that quasi-Landau resonances at the ionization threshold at zero field for Rydberg atoms possessed a deep interest /4,12-14, and Refs. Chapter IX/. Recently, Feneuille /15/ has developed an empirical law to join the Landau and Coulomb regimes from the quasi-Landau spectrum experimental data. This law fulfils the dependence on the quantum numbers (30.6), and on this basis the author conjectured that there should be a theoretical justification for his successful empirical law. We have proved in §.31 that an elemental semiclassical model predicts such a law, and recently it has been proved that the quantization method JWKB (for a plane normal to the magnetic field direction) explains quite well such dependence on the quantum numbers /16/. These authors have presented another different explanation of the Feneuille law through the employment of the variational method discussed in §.20 /16/. Then, the VFM, as presented in this section, is an alternative formulation to rationalize empirical laws like that of Ref. /15/. Precisely, Fig. 10.1 (broken line) shows that VFM describes very well the ionization limit zone ( $E=0$ ) to zero-field, which is that of greater interest for quasi-Landau resonances.

## REFERENCES OF CHAPTER X

- /1/ F.M. Fernández, G.A. Arteca and E.A. Castro, *Int. J. Quantum Chem.* 25 (1984) 1023.
- /2/ G.A. Arteca, F.M. Fernández and E.A. Castro, *Z. Physik A* 315 (1984) 255.
- /3/ H.A. Bethe and E.E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms*, Springer Verlag, Berlin, 1957.
- /4/ R.H. Garstang, *Rep. Prog. Phys.* 40 (1977) 105.
- /5/ J. Simola and J. Virtamo, *J. Phys. B* 11 (1978) 3309.
- /6/ M. Robnik, *J. Phys. A* 14 (1981) 3195.
- /7/ G. Wunner and H. Ruder, *J. Physique* 43 (1982) C2-137.
- /8/ H. Ruder, G. Wunner, H. Herold and M. Reinecke, *J. Phys. B* 14 (1981) L 45.
- /9/ W. Rosner, G. Wunner, H. Herold and H. Ruder, *J. Phys. B* 17 (1984) 29.
- /10/ L.D. Mlodinow and N. Papanicolaou, *Ann. Phys. (NY)* 128 (1980) 314.
- /11/ C.M. Bender, L.D. Mlodinow and N. Papanicolaou, *Phys. Rev. A* 25 (1982) 1305.
- /12/ W.R.S. Garton and F.S. Tomkins, *Astrophys. J.* 158 (1969) 839.
- /13/ J.C. Castro, M.L. Zimmerman, R.G. Hulet, D. Kleppner and R.R. Freeman, *Phys. Rev. Lett.* 45 (1980) 1780.
- /14/ J.C. Gay, D. Delande and F. Biraben, *J. Phys. B* 13 (1980) L 729.
- /15/ S. Feneuille, *Phys. Rev. A* 26 (1982) 673.
- /16/ J.A.C. Gallas, E. Gerck and R.F. O'Connell, *Phys. Rev. Lett.* 50 (1983) 324.