

## IONIZATION ENERGIES OF HYDROGEN IN MAGNETIC WHITE DWARFS

A. K. RAJAGOPAL, G. CHANMUGAM,  
 R. F. O'CONNELL, AND G. L. SURMELIAN

Department of Physics and Astronomy, Louisiana State University, Baton Rouge  
 Received 1972 February 28; revised 1972 May 22

### ABSTRACT

The variational principle is used to determine the ionization energy of a hydrogen atom in its ground state, in the presence of magnetic fields of the order of those found in magnetic white dwarfs and some neutron stars. The results are shown to be better than those obtained by using perturbation theory for all fields and significantly better than those of Cohen *et al.*, for fields less than  $\sim 3 \times 10^{10}$  gauss. A general procedure for obtaining the energies of higher levels is outlined.

### I. INTRODUCTION

The discovery of strong magnetic fields ( $\sim 10^7$  gauss) in some white dwarfs (Kemp 1970a; Kemp *et al.* 1970) and the possible existence of superstrong magnetic fields ( $\sim 10^{12}$  gauss) in neutron stars has stimulated interest in the behavior of matter in intense magnetic fields. Of particular importance is the study of the behavior of atoms in strong magnetic fields because many stellar characteristics are affected by the presence of magnetic fields. The behavior of atoms in low fields can be adequately described using hydrogenic wave functions in perturbation theory. On the other hand, for superstrong magnetic fields ( $B \gtrsim 3 \times 10^{10}$  gauss) the Coulomb interaction becomes negligible in comparison with the magnetic energy so that the wave functions are essentially oscillator-like (Cohen, Lodenquai, and Ruderman 1970). It is clearly of importance to understand at what field strengths perturbation theory using hydrogenic wave functions breaks down and to devise a scheme for analyzing the system in fields of intermediate strength. Kemp (1970b) has emphasized the importance of this difficult intermediate case ( $B \approx 10^8$ - $10^9$  gauss) for magnetic white dwarfs. To our knowledge, this problem has not been investigated before.

It is our purpose here to determine the ionization energy of hydrogen in magnetic fields  $B$  of intermediate strength, i.e., up to those values of  $B$  where the theory of Cohen *et al.* becomes applicable. The precise region of demarcation between intermediate and strong fields will be determined in the analysis. In addition, we shall show that our method gives better results than the perturbation results for all fields.

### II. VARIATIONAL CALCULATION

The Hamiltonian for the hydrogen atom (we neglect spin) in a magnetic field  $B$  oriented along the  $z$ -axis is given by

$$H = p^2/2m - e^2/r + \omega_L L_z + \frac{1}{2}m\omega_L^2 r^2 \sin^2 \theta, \quad (1)$$

where  $\omega_L = eB/2mc$ . We calculate the energy of the system using a variational calculation which should give better results than perturbation theory for a sensible choice of trial wave functions. In their calculation Cohen *et al.* used a trial wave function which was essentially oscillator-like, since their concern was high fields where the Coulomb interaction is small compared with the magnetic-field effects. On the other

hand, for fields  $B \lesssim 10^{10}$  gauss which is our main concern, the Coulomb interaction dominates. For this reason, in contrast to Cohen *et al.*, we use a *hydrogen-like* wave function.

Initially, we choose a normalized trial wave function for the ground state in the form

$$\psi_1 = \beta_1^{3/2} R_{10}(\beta_1 r) Y_{00}(\theta, \phi). \quad (2)$$

Our variational parameter is  $\beta_1$ , which depends on  $B$ . We note that  $\beta_1 = 1$  corresponds to the well-known normalized hydrogen-atom wave function for the ground state, in the absence of a magnetic field. We expect that the effect of the magnetic field is to increase the binding and decrease the mean radius of the atom. It is this idea that physically motivated the present choice of the trial solution.

The expectation value of  $H$  with respect to  $\psi_1$  is given by

$$\langle H \rangle = \frac{\hbar^2}{2ma_0^2} (\beta_1^2 - 2\beta_1) + \frac{1}{\beta_1^2} m\omega_L^2 a_0^2, \quad (3)$$

where  $a_0$  is the Bohr radius. Minimizing  $\langle H \rangle$  with respect to  $\beta_1$ , we obtain

$$\beta_1^3(\beta_1 - 1) = \frac{1}{2} \frac{e^2}{c^2 \hbar^2} a_0^4 B^2. \quad (4)$$

For given  $B$ , there exist two complex roots, one negative root, and only one positive root  $\beta_0$ , of equation (4). We note that  $\beta_0 > 1$  and that  $\partial^2 \langle H \rangle / \partial \beta_1^2$ , evaluated at  $\beta_1 = \beta_0 > 1$ , is positive and hence our extremum corresponds to a minimum.

Using equations (3) and (4), we can express the minimum energy corresponding to the variational trial wave function (2) in the convenient form

$$E_V = -\frac{\hbar^2}{2ma_0^2} + Am\omega_L^2 a_0^2, \quad (5)$$

where

$$A \equiv (2\beta_0 - 1)/\beta_0^3.$$

On the other hand, if we calculate the energy in first-order perturbation theory, we find that the energy is given by

$$E_P = -\frac{\hbar^2}{2ma_0^2} + m\omega_L^2 a_0^2. \quad (6)$$

Since  $\beta_0 > 1$ , it follows that  $0 < A < 1$  and hence  $E_V < E_P$ . Thus, the variational result is better than the perturbation result, as it should be.

The ionization energy  $E_I$  of atoms plays an important role in the study of white-dwarf atmosphere models. Since the lowest energy of an electron at infinity in the same field is  $\hbar\omega_L$ , the ionization energy for the hydrogen atom in the ground state is given by

$$E_I \equiv \hbar\omega_L - E_V = \frac{\hbar^2}{2ma_0^2} - m\omega_L^2 a_0^2 A + \hbar\omega_L. \quad (7)$$

In figure 1 we compare our results (curve *c*) for  $E_I$  for the ground state with the results of Cohen *et al.* (1970) (curve *e*) and with those obtained by using perturbation theory (curve *a*). We note that for  $B \lesssim 1.5 \times 10^{10}$  gauss, our value for  $E_I$  is greater than that of Cohen *et al.* (1970). This implies that our value for the ground-state energy is lower than theirs for such values of  $B$ . The physical reason for this is that for such lower values of  $B$  the wave function is more hydrogen-like whereas for higher values of  $B$  it is oscillator-like.

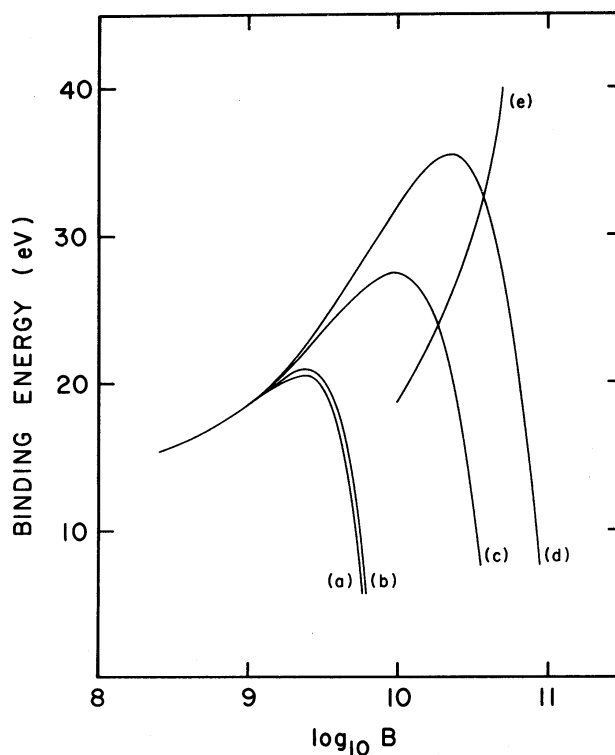


FIG. 1.—The ionization energy of the ground state of hydrogen as a function of the magnetic field  $B$  calculated using (a) perturbation theory, (b) two linear parameter ( $c_1$  and  $c_2$ ) variational calculation, (c) one nonlinear ( $\beta_1$ ) parameter variational calculation, (d) two linear ( $c_1$  and  $c_2$ ) and two nonlinear ( $\beta_1$  and  $\beta_2$ ) parameter variational calculation (see eq. [8]), and (e) the work of Cohen *et al.*

### III. IMPROVED TRIAL WAVE FUNCTIONS

Clearly, one can improve our results by using trial wave functions which include successively the higher hydrogenic states. Let us therefore choose a trial wave function of the form

$$\psi = c_1\psi_1 + c_2\psi_2, \quad (8)$$

where  $\psi_1$  is given by equation (2) and

$$\psi_2 = \beta_2^{3/2} R_{20}(\beta_2 r) Y_{00}(\theta, \phi).$$

Here, for  $\beta_2 = 1$ ,  $\psi_2$  is the  $2s$  hydrogen wave-function. We shall refer to  $c_1$  and  $c_2$  as the linear parameters and to  $\beta_1$  and  $\beta_2$  as the nonlinear parameters. The normalization condition is then given by

$$c_1^2 + c_2^2 + 2c_1c_2\langle\psi_1|\psi_2\rangle = 1, \quad (9)$$

where

$$\langle\psi_1|\psi_2\rangle = \frac{64}{2^{1/2}} \frac{(\beta_1\beta_2)^{3/2}}{(2\beta_1 + \beta_2)^4} (\beta_1 - \beta_2). \quad (10)$$

Also,

$$\langle\psi|H|\psi\rangle = c_1^2\langle\psi_1|H|\psi_1\rangle + c_2^2\langle\psi_2|H|\psi_2\rangle + 2c_1c_2\langle\psi_2|H|\psi_1\rangle. \quad (11)$$

Setting  $B_0 \equiv \alpha^2 m^2 c^3 / e \hbar = 2.350 \times 10^9$  gauss, we obtain (in Rydbergs)

$$\langle \psi_2 | H | \psi_2 \rangle = -\frac{1}{4}(2\beta_2 - \beta_2^2) + \frac{7}{\beta_2^2} \left( \frac{B}{B_0} \right)^2 \quad (12)$$

and

$$\begin{aligned} \langle \psi_2 | H | \psi_1 \rangle &= \frac{16}{2^{1/2}} \frac{(\beta_1 \beta_2)^{3/2}}{(2\beta_1 + \beta_2)^4} [\beta_2^2(1 - \beta_1) + 4\beta_1^2(\beta_2 - 1)] \\ &+ 512 \left( \frac{B}{B_0} \right)^2 \frac{(\beta_1 \beta_2)^{3/2}}{2^{1/2}(2\beta_1 + \beta_2)^6} (\beta_1 - 2\beta_2). \end{aligned} \quad (13)$$

The variation of  $\langle \psi | H | \psi \rangle$  with respect to  $c_1, c_2$  subject to the condition (9) gives two values of the energy, which are functions of  $\beta_1, \beta_2$ . The minimum of the lower of these values in the  $(\beta_1, \beta_2)$ -space gives the ground-state energy of the system. This is done numerically. The corresponding ionization energy is also given in figure 1 (curve *d*).

#### IV. DISCUSSION

These results are clearly better than those obtained by using  $\psi_1$  alone. Furthermore, in figure 1 we note that the turnover point for  $E_I$  has been moved to the right. This demonstrates that by including successively higher states,  $E_I$  can be made to approach the values of Cohen *et al.* for very high fields.

We have considered only spherically symmetric trial functions. Inclusion of the  $p$ - and  $d$ -states would introduce cylindrical symmetry and would be expected to give even better results for  $E_I$  for  $B > 10^{10}$  gauss. Furthermore, it would also result in  $\langle z \rangle \neq \langle (x^2 + y^2)^{1/2} \rangle$ , thereby showing the approach to the cigar-shaped wave function that the system is supposed to have for very high fields. The attractive feature of the method is the feasibility of improving the answers to any degree of accuracy.

We have also calculated  $E_I$  using equation (8) when  $\beta_1 = \beta_2 = 1$  (curve *b*). However, this leads only to slight improvement over the one-state-perturbation result. The reason for this is that when one varies the  $\beta$ 's the change in the mean radius is taken into account in a simple and direct manner. A plot of the mean radius as a function of  $B$ , corresponding to the wave function given in equation (8), is given in figure 2.

Recently, Preston (1970) and Trimble (1971) have estimated the magnetic fields in some white dwarfs using perturbation-theory results for the quadratic Zeeman effect. For the ground state, the perturbation-theory results are in good agreement with our variational-calculation results for  $B \lesssim 10^9$  gauss. This is because the quadratic Zeeman contribution is negligible for the ground state for  $B < 10^9$  gauss. For the higher excited states, as is well known, the quadratic Zeeman terms become important at lower fields. It is therefore important to determine the energy levels of the higher excited states more accurately than by using perturbation theory. One aspect of our calculation, which is very useful as a practical procedure, is that we identify the spectrum of the hydrogen atom in strong magnetic fields ( $B \lesssim 10^{10}$  gauss) in terms of that of the atom in zero fields.

The wave functions and energies of higher levels may be obtained by simply extending the number of terms in equation (8) to include more basis functions.

The Hamiltonian (1) is invariant under rotations about the  $z$ -axis and under inversion. So all the eigenstates of it can be labeled by the eigenvalues of  $L_z$  and the parity. This suggests that the most general form of the trial solution would be to employ the following function:

$$\psi_m^\pm(\mathbf{r}) = \sum_{nl} C_{nl}^\pm R_{nl}(\beta_{nlm}^\pm r) Y_{lm}(\theta, \phi). \quad (14)$$

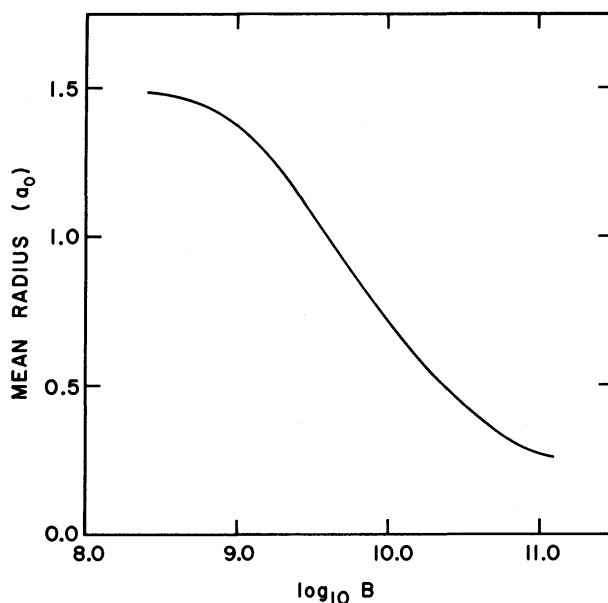


FIG. 2.—The mean radius  $\langle r \rangle$  in units of the Bohr radius, for our best variational calculation ( $\psi$  given by eq. [8]) as a function of the magnetic field  $B$ .

The sum on  $l$  in (14) over all even integers leads to the state with even parity (+), and the sum over odd  $l$  to the odd parity (−) state. Here  $m$  is the eigenvalue of  $L_z$ .  $R_{nl}$  is, in general, any suitable function. In this paper, we chose the radial hydrogenic solutions, with the associated scaling  $\beta_{nlm}^{(\pm)}$ , in view of the expected change in the effective radius of the electron in the magnetic field. It is perhaps convenient to choose instead of  $R_{nl}(\beta_{nlm}^{(\pm)}r)$  the function

$$r^l e^{-(\beta_{nlm}^{(\pm)}r)}. \quad (15)$$

This choice is dictated by the condition that the solution associated with  $Y_{lm}$  in the hydrogen atom must have the behavior  $r^l$  near  $r = 0$ . The choice (15) makes possible explicit evaluation of matrix elements entirely in terms of the well-known gamma functions. However, because of the use of the additional parameters  $\beta_{nlm}^{(\pm)}$ , the higher states must be made orthogonal by means of the Schmidt method; see, for instance, Kemble (1958). This involves extensive numerical work, and such a program is now in progress. The method presented here can also be generalized to examine the ground states of other atoms and ions (e.g., He,  $H^-$ ).

A. K. R. and G. C. thank J. Callaway for discussions.

#### REFERENCES

- Cohen, R., Lodenquai, J., and Ruderman, M. 1970, *Phys. Rev. Letters*, **25**, 467.  
 Kemble, E. C. 1958, *The Fundamental Principles of Quantum Mechanics* (New York: Dover Publications).  
 Kemp, J. C. 1970a, *Ap. J.*, **162**, 169.  
 ———. 1970b, *Ap. J. (Letters)*, **162**, L69.  
 Kemp, J. C., Swedlund, J. B., Landstreet, J. D., and Angel, J. R. P. 1970, *Ap. J. (Letters)*, **161**, L77.  
 Preston, G. W. 1970, *Ap. J. (Letters)*, **160**, L143.  
 Trimble, V. 1971, *Nature Phys. Sci.*, **231**, 124.

*Note added in proof.*—The numerical program discussed above has now been carried out for hydrogen (Smith, Henry, Surmelian, O'Connell, and Rajagopal, 1972, *Phys. Rev. D*, in press). In particular, the energy spectrum for the ground and the next thirteen excited states has been obtained.