TRANSMITTED PROBABILITY AND SOME EXPECTATION VALUES FOR THE HYDROGEN ATOM IN INTENSE MAGNETIC FIELDS

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ABSTRACT

We present here a calculation of the binding energies of a hydrogen atom in magnetic fields of the order of $10^{10}-10^{12}$ gauss that are presumed to exist on the surfaces of neutron stars. The trial wave functions that we use are extensions of the products of Landau functions and hydrogenic functions. We also employ these improved wave functions to calculate transition probabilities and oscillator strengths and the ground-state expectation values of $r^n$ for $n = -1, 1, 2$ for various values of the magnetic fields. All the matrix elements involved are estimated variationally using an extremum principle.

Subject headings: atomic processes — magnetic fields — stars: neutron — transition probabilities

I. INTRODUCTION

The discovery of magnetic fields of the order of $10^{12}$ gauss at the surfaces of neutron stars (Trimper et al. 1977) has made the study of the hydrogen atom (and its isoelectronic sequence) in intense magnetic fields a topic of current interest (Garstang 1977). Slightly less intense magnetic fields of the order of $10^{10}$ gauss are also seen in white dwarfs. Even laboratory fields of the order of $10^{6}$ gauss can simulate the conditions of intense magnetic fields on exotrons in solids, where a small effective mass $m^*$ and a large dielectric constant $K$ can cut down the electric forces relative to the magnetic forces. A study of various properties of the hydrogen isoelectronic sequence serves as a useful guide in the understanding of atomic behavior in such extreme conditions. In particular, quite elaborate calculations have been performed for various low-lying energy levels of hydrogenic atoms in intense magnetic fields (Surmelian and O'Connell 1974). However, only limited results are available for other atomic properties such as transition rates.

A good review of the various trial wave functions used in the Rayleigh-Ritz evaluation of energy levels of hydrogenic atoms in intense magnetic fields is given by Rau and Spruch (1976). A particularly convenient trial wave function, the product of a Landau function and a hydrogenic function, was proposed by Rau, Mueller, and Spruch (1975). In the present paper, we have used an extension of this trial wave function to obtain variational estimates of the expectation values of $r^n$ for $n = -1, 1, 2$ and 2 for hydrogen atoms in intense magnetic fields. These matrix elements are related to various atomic properties such as diamagnetic susceptibility, polarizability, etc. We have also used these improved wave functions to obtain transition probabilities and oscillator strengths for transitions between low-lying levels of hydrogen. The transition probability and the oscillator strength can be written in terms of $S$, the strength of transition, as

$$A_{01} = \frac{e^2}{\hbar} \frac{(E_1 - E_0)}{e^2/\alpha_0} S \tau$$ \hspace{1cm} (la)

and

$$f_{01} = 2 \left( \frac{E_1 - E_0}{e^2/\alpha_0} \right) S \tau$$ \hspace{1cm} (lb)

where

$$S = \langle \mathbf{r} \rangle_{\alpha_1} \cdot \mathbf{\hat{r}}_{0} / \alpha_0$$ \hspace{1cm} (lc)

and

$$\tau = \alpha_0 / \alpha c , \quad \alpha = e^2 / \hbar c .$$

The strength of the magnetic field is conveniently measured in terms of the dimensionless parameter $\gamma$, which is twice the square of the ratio of $\alpha_0$, the Bohr radius for hydrogen, to $\beta$, the cyclotron radius of a free electron in a uniform magnetic field; $\beta = (2\mu_0 e B)^{1/2}$. In an intense magnetic field, $\beta$ is smaller than $\alpha_0$. Our calculations are nonrelativistic and therefore restricted to fields up to about $10^{13}$ gauss, since $\beta$ becomes comparable to $\lambda_0$, the Compton wavelength of the electron, only when the magnetic field is of the order of $9 \times 10^{13}$ gauss.

It is well known that matrix elements of various Hermitian operators, calculated by using Rayleigh-Ritz wave functions, are not as accurate as the energy estimate. However, using simple trial wave functions and auxiliary functions in an extremum principle, it is possible to obtain variational estimates of matrix elements comparable in accuracy to the energy estimate. In § II, we give a summary of the extremum principle for the variational estimate of the matrix elements. Our choice of the wave functions and the auxiliary functions that appear in the extremum principle is given in § III; a discussion of the results follows, in § IV.

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II. THE EXTREMUM PRINCIPLE

We present here only a brief summary of the extremum principle for a diagonal matrix element, since a detailed derivation, as well as the generalization to the off-diagonal case, has been given by Gerjuoy, Rau, and Spruch (1973) and Gerjuoy et al. (1974). Let \( \phi_1 \) denote a normalized approximation to \( \phi_1 \), the true ground-state wave function of the Hamiltonian \( H \), and let \( E_{11} = \phi_1 \dagger H \phi_1 \) be the corresponding variational estimate of the ground-state energy. We seek a variational estimate of the expectation value, \( \langle W \rangle = \phi_1 \dagger W \phi_1 \), of a Hermitian operator \( W \). Note that \( \langle W \rangle_{11} = \phi_1 \dagger W \phi_1 \) differs from \( \langle W \rangle \) by first order in \( \delta \phi_1 = \phi_1 - \phi_1 \). A variational estimate \( \langle W \rangle \) is given by

\[
\langle W \rangle = \langle W \rangle_{11} + 2 \text{ Re } L_{11}(H - E_{11})\phi_{11}.
\]

(2)

A singularity-free equation defining the auxiliary function \( L_{11} \) is (Gerjuoy et al. 1974)

\[
(H_{\text{mod}}, - E_{11})L_{11} = (\langle W \rangle_{11} - E_{11}c_{11} - W)\phi_{11},
\]

(3)

where \( H_{\text{mod}}, - E_{11} = H - H\phi_1 \phi_{11} \dagger H \phi_1 \) and \( c_{11} = L_{11} \phi_{11} \) is arbitrary. A particular choice \( c_{11} = \langle W \rangle_{11} / E_{11} \) provides a useful check on numerical calculations and simplifies equation (3) to

\[
(H_{\text{mod}}, - E_{11})L_{11} = -W\phi_{11}.
\]

(4)

If \( \phi_{11} \) is sufficiently accurate (for an exact meaning, see Gerjuoy et al. 1974), then the operator \( (H_{\text{mod}}, - E_{11}) \) is positive definite; therefore, the functional

\[
M(L_{11}) = L_{11}(H_{\text{mod}}, - E_{11})L_{11}
+ 2 \text{ Re } L_{11} \dagger W \phi_{11},
\]

achieves its minimum value for \( L_{11} = L_{11} \). For numerical applications of this extremum principle, see Shakeshaft, Rosenzweig, and Spruch (1976) for diagonal matrix elements and Wadehra, Spruch, and Shakeshaft (1978) for off-diagonal elements.

III. TRIAL WAVE FUNCTION AND AUXILIARY FUNCTIONS

Rau, Muller, and Spruch (1975) suggested a one-parameter wave function of the form \( \psi = \psi_{1m} \), where

\[
\psi_{m} = N_{mn} f_{m}^{\text{La}(n)}(r, \phi) P_{n}(r) Z_{n};
\]

(6)

\( f_{m}^{\text{La}(n)}(r, \phi) \) is the normalized ground-state Landau function of a free electron in a magnetic field,

\[
f_{m}^{\text{La}(n)}(r, \phi) = (n|m|l)^{-1/2}(\rho^{m})|l^{n+1}(l+1)
\times \exp(-\rho^{2}/2\rho^{2}) \exp(im\phi);
\]

(7)

\( P_{n}\) is the radial hydrogenic function with a (nonlinear) variational parameter \( Z_{n} \), and \( N_{mn} \) is the overall normalization constant. This wave function has the merit of accommodating the limit of both weak and intense magnetic fields and gives results for the energy that are comparable to more elaborate calculations (Rau and Spruch 1976).

One can improve this trial wave function by including radial parts of successively higher hydrogenic functions. Our choice of trial wave function is

\[
\psi_{1} = c_{1}\psi_{m}(r, \rho, \phi; Z_{1}) + c_{2}\psi_{n}(r, \rho, \phi; Z_{2}),
\]

(8)

where \( \psi_{mn} \) and \( \psi_{nn} \) are normalized orbitals, given by equation (6), with \( n = 1 \) and \( n = 2 \), respectively. \( Z_{1} \) and \( Z_{2} \) are nonlinear variational parameters; \( c_{1} \) and \( c_{2} \) are linear variational parameters, but they are not independent, since the normalization of the trial wave function implies

\[
c_{1}^{2} + 2c_{1}c_{2}S_{12} + c_{2}^{2} = 1,
\]

(9)

where \( S_{12} \), the overlap integral, is

\[
S_{12} = \langle \psi_{m}(Z_{1}) | \psi_{n}(Z_{2}) \rangle.
\]

(10)

The variational upper bound on the energy is given by

\[
E \leq c_{1}^{2}H_{11} + 2c_{1}c_{2}H_{12} + c_{2}^{2}H_{22},
\]

(11)

where

\[
H_{mn} = \langle \psi_{mn}(Z_{1}) | H | \psi_{mn}(Z_{2}) \rangle.
\]

(12)

Minimization of equation (10) with respect to the linear parameters \( c_{1} \) and \( c_{2} \), subject to the normalization condition (9), gives two values of energy

\[
E_{\pm} = \frac{\alpha_{+}^{2}H_{11} + 2\alpha_{+}H_{12} + H_{22}}{\alpha_{+}^{2} + 2\alpha_{+}S_{12} + 1},
\]

(11)

corresponding to the two values of \( \alpha \)

\[
\alpha_{\pm} = [-B \pm (B^{2} - AC)^{1/2}] / A,
\]

(11)

where

\[
A = H_{11}S_{12} - H_{12}, \quad 2B = H_{11} - H_{22},
\]

\[
C = H_{12} - H_{22}S_{12}.
\]

The linear parameters are given by

\[
c_{1} = \alpha(\alpha^{2} + 2\alphaS_{12} + 1)^{-1/2},
\]

(11)

\[
c_{2} = (\alpha^{2} + 2\alphaS_{12} + 1)^{-1/2}.
\]

(11)

Each of the two values of energy is a function of \( Z_{1} \) and \( Z_{2} \). The minimization of the lower of these two values with respect to \( Z_{1} \) and \( Z_{2} \) gives the required energy estimate. It is worth noting that \( H_{11}, H_{12}, H_{22} \), and \( S_{12} \) can be easily expressed in terms of confluent hypergeometric functions. For the particular cases \( m = 0 \) and \( m = -1 \), these functions can be reexpressed in terms of exponential integrals which are tabulated in the standard references (Abramowitz and Stegun 1964).

The auxiliary function that appears in the variational estimation of the expectation values of \( r^{n} \) for \( n = -1, 1, \) and 2 is taken to be

\[
L_{11} = f_{c}^{\text{La}(n)}(r, \phi) g(r),
\]

(12)
TABLE 1

<table>
<thead>
<tr>
<th>( \gamma )</th>
<th>( B ) (gauss)</th>
<th>( Z_1 )</th>
<th>( Z_2 )</th>
<th>( c_1 )</th>
<th>( c_2 )</th>
<th>( S_{12} )</th>
<th>( E ) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m = 0 )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20 . . .</td>
<td>4.7 (10)</td>
<td>3.87</td>
<td>5.17</td>
<td>-1.067</td>
<td>0.578</td>
<td>0.383</td>
<td>-56.81</td>
</tr>
<tr>
<td>100 . . .</td>
<td>2.35 (11)</td>
<td>5.00</td>
<td>7.19</td>
<td>-1.217</td>
<td>0.584</td>
<td>0.578</td>
<td>-97.41</td>
</tr>
<tr>
<td>200 . . .</td>
<td>4.7 (11)</td>
<td>2.93</td>
<td>7.77</td>
<td>-1.062</td>
<td>0.183</td>
<td>0.413</td>
<td>-122.03</td>
</tr>
<tr>
<td>500 . . .</td>
<td>7.05 (11)</td>
<td>2.94</td>
<td>9.21</td>
<td>-1.041</td>
<td>0.139</td>
<td>0.353</td>
<td>-138.83</td>
</tr>
<tr>
<td>1000 . .</td>
<td>2.35 (12)</td>
<td>3.31</td>
<td>14.74</td>
<td>-1.018</td>
<td>0.083</td>
<td>0.253</td>
<td>-200.54</td>
</tr>
<tr>
<td>( m = -1 )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100 . . .</td>
<td>2.35 (11)</td>
<td>4.11</td>
<td>5.85</td>
<td>-1.115</td>
<td>0.546</td>
<td>0.445</td>
<td>-67.34</td>
</tr>
<tr>
<td>200 . . .</td>
<td>4.7 (11)</td>
<td>2.34</td>
<td>6.61</td>
<td>-1.035</td>
<td>0.175</td>
<td>0.279</td>
<td>-85.99</td>
</tr>
<tr>
<td>1000 . .</td>
<td>2.35 (12)</td>
<td>2.78</td>
<td>12.24</td>
<td>-1.013</td>
<td>0.092</td>
<td>0.187</td>
<td>-147.00</td>
</tr>
</tbody>
</table>

where

\[
g(r) = b_1 \exp(-\alpha r/a_0) + b_2(2 - \beta r/a_0) \exp(-\beta r/2a_0);
\]

(13)

\( b_1, \ b_2, \ \alpha, \ \beta \) are the parameters to be varied to obtain the lowest value of the functional \( M \) (see eq. [5]).

The variational estimation of an off-diagonal matrix element requires the determination of two auxiliary functions, which can be determined independently. These two functions in the variational estimation of the transition probability and the oscillator strength are taken to be

\[
L_{1\mu} = f_{1a}^{\mu\alpha}(\rho, \phi)g(r),
\]

(14a)

\[
L_{2\mu} = f_{2a}^{\mu\alpha}(\rho, \phi)g(r),
\]

(14b)

where \( g(r) \) is given in equation (13).

IV. RESULTS AND DISCUSSION

Table 1 shows the variational upper bounds on the ground-state \( (m = 0) \) and the first excited state \( (m = -1) \) energies of the hydrogen atom, using the improved trial wave function, in magnetic fields ranging from about \( 10^{10} \) to \( 10^{12} \) gauss. (All energy values are given relative to the ground-state energy of a free electron in a magnetic field.) The table also gives the optimum values of the variational parameters in the trial wave function. The total energy is necessarily lower than that obtained by using the one-parameter trial wave function of Rau et al. A few features of Table 1 are worth noting. As the magnetic field \( B \) increases, the overlap between the two orbitals in the trial wave function becomes smaller, as indicated by the values of \( S_{12} \). In the limit of infinite magnetic field, \( S_{12} \) behaves as

\[
S_{12} = (2x)^{3/2}(x + 1)^2 + O(1/B),
\]

(15)

where \( x = 2Z_1/Z_2 \). In this limit, \( S_{12} \) is effectively the matrix element of \( r^{-2} \) between the radial hydrogenic functions, as can be seen by expanding the integrand in \( S_{12} \) as a power series in \( \beta \). Furthermore, as expected, \( c_1 \) becomes much larger than \( c_2 \).

Table 2 gives the zeroth order and the variational estimates of the ground-state expectation values of \( r^4 \) for \( n = -1, 1, \) and \( 2 \) for the hydrogen atom for different values of the magnetic field (in atomic units).

TABLE 2

<table>
<thead>
<tr>
<th>( \gamma )</th>
<th>( \langle r^4 \rangle )</th>
<th>( \langle r \rangle )</th>
<th>( \langle r^{-2} \rangle )</th>
<th>( \langle r^8 \rangle )</th>
<th>( \langle r \rangle )</th>
<th>( \langle r^{-2} \rangle )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20 . . .</td>
<td>0.3820</td>
<td>0.5309</td>
<td>2.7609</td>
<td>0.3857</td>
<td>0.5317</td>
<td>2.7613</td>
</tr>
<tr>
<td>100 . . .</td>
<td>0.1586</td>
<td>0.3304</td>
<td>4.8091</td>
<td>0.1620</td>
<td>0.3321</td>
<td>4.8176</td>
</tr>
<tr>
<td>200 . . .</td>
<td>0.1155</td>
<td>0.2755</td>
<td>6.0909</td>
<td>0.1159</td>
<td>0.2754</td>
<td>6.1052</td>
</tr>
<tr>
<td>500 . . .</td>
<td>0.0956</td>
<td>0.2477</td>
<td>6.9923</td>
<td>0.0959</td>
<td>0.24779</td>
<td>7.0039</td>
</tr>
<tr>
<td>1000 . .</td>
<td>0.0580</td>
<td>0.1865</td>
<td>10.3812</td>
<td>0.0573</td>
<td>0.1857</td>
<td>10.3881</td>
</tr>
</tbody>
</table>

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functions are effectively functions of \( z \). The infinite field limits for \( \langle r^2 \rangle \) and \( \langle r \rangle \) are

\[
\langle r^2 \rangle = 2 \frac{Z^2}{x^2} \left[ \frac{c_1^2}{z} + 2c_2^2 + \frac{16c_1c_2(2x)^{1/2}}{(x+1)^3} \left( \frac{x-2}{x+1} \right) \right] + O(1/B),
\]

\( \langle r \rangle = \frac{1}{2} \left[ \frac{c_1^2}{x} + c_2^2 + \frac{8c_1c_2(2x)^{1/2}}{(x+1)^3} \left( \frac{x-1}{x+1} \right) \right] + O(1/B),
\]

where, as before, \( x = 2Z^2/2 \). The limiting expressions like equations (15) and (16) assist in the semi-quantitative understanding of the results of Tables 1 and 2. For example, for \( \gamma = 1000 \), equations (15) and (16) give for \( S_{22} \), \( \langle r^2 \rangle \), and \( \langle r \rangle \) the values 0.405, 0.0496, and 0.165 plus terms of order \( 1/B \) and higher, respectively. These expressions become quantitatively more meaningful only when \( \gamma > 10^5 \), a regime which is only of academic interest in the present calculations, since, for such high values of the magnetic field, relativistic effects must be taken into account.

Table 3 provides the zeroth order and the variational estimates of the transition probabilities and the oscillator strengths for the transition between the ground state and the first excited state. The present calculations are the first attempt to obtain these transition rates in such high magnetic fields; previous calculations were restricted to smaller fields (Smith et al. 1973). Our results indicate that the transition probability decreases with increasing fields, which is contrary to the results for smaller magnetic fields (Smith et al. 1973). This difference, however, can be explained by the fact that, in intense magnetic fields, the sums of the oscillator strengths are different for left and for right circular polarizations. It has been shown (Hasegawa and Howard 1961) that, in the infinite field limit, all transitions from the ground state are prohibited for right circular polarization, like the one under consideration. However, for weak magnetic fields (\( B < B_0 \)) considered by Smith et al., this difference is not significant and the strength of the transition is governed by the Coulomb potential. Furthermore, the results of Hasegawa and Howard (1961) indicate that the oscillator strength should fall as \( (E_2 - E_1)/\gamma \). The results in Table 3 for \( f_{01} \) indeed show this behavior.

A few comments should be made regarding the choice of the auxiliary functions that appear in the variational principle. The "form" of the auxiliary functions is suggested by the differential equation they satisfy. In particular, the angular dependence of the auxiliary functions is determined by the operator under consideration and by the angular dependence of the wave functions. The fact that the variational correction to the matrix elements is small simply reflects the inadequacies of the auxiliary functions; more parameters in the auxiliary functions are needed to show any appreciable departure from the zeroth order results. The variational results in the present calculations, therefore, may not be a significant improvement over the zeroth order results. However, we have also done the zeroth order and the variational calculations of transition probabilities and oscillator strengths using one-parameter \( (c_4 = 1, c_4 = 0) \) wave functions and one-parameter \( (b = 1, b_2 = 0) \) auxiliary functions. The present results shown in Tables 2 and 3 are reasonably more accurate than those employing one-parameter functions.

One can use properly antisymmetrized products of the present wave functions for other elements, notably helium and its isoelectronic sequence. Calculations employing such wave functions for the energy spectrum and the transition probabilities for two-electron systems are under way.

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