Quadratic Zeeman Effect for an s-electron Moving in a Screened Coulomb Potential

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Abstract

The s-level of a screened hydogenic atom in a uniform magnetic field of arbitrary strength B have been calculated accurately. First, the related spherical symmetric case $\frac{1}{2}\Omega^2 r^2 (\Omega \sim B)$ has been treated by using the linear variational method. The trial wave function is taken as linear mixture of hydogenic and 3D harmonic ascillator wave functions of s-symmetry. Second, the actual nonspherical case $\frac{1}{2}\Omega^2 (x^2+y^2)$ is studied by adopting the correction proposed by Mustafa and Chhajlany (Phys. Rev.A,50,(I994),2926). The latter accounts for the difference between the two cases in an appaximate way by utilizing the properties of the 2D and 3D harmonic oscillators.

We start our study with the unsceened hydrogen case to recover their shifted $\frac{1}{N}$ results and deal then with the more involved case of the screened hydrogen atom covering wide ranges of the applied field and of the screening length.

الخلاصة

لقد حسبت طاقة المستوى s لذرة الهايدروجين المحجوبة تحت تاثير مجال مغناطيسي خارجي B بدقة. لقد عولجت ابتداءا حالة التناظر الكروي $\left(\frac{1}{2}\Omega^2 r^2 (\Omega \sim B)\right)$ باستخدام طريقة التغاير الخطية ومزيج من دوال الهيدروجين والمتذبذب التوافقي ثلاثي الابعاد 3D ذات التناظر s ومن ثم درست الحالة اللاكروية$\left(\frac{1}{2}\Omega^2 (x^2+y^2)\right)$ باستخدام التصحيح الذي اقترحه كل من مصطفى وجاجلاني(Phys. Rev.A,50,(I994),2926). ان التصحيح الاخير يأخذ بنظر الاعتبار بصورة تقريبية الفرق بين الحالتين من خلال الاستفادة من خواص المتذبذبات الثنائية الثلاثية الابعاد .

اجريت دراسة تمهيدية لحالةالهايدروجين اللامحجوب لتأكيد نتائج سابقة بطريقة $\frac{1}{N}$ ثم عولجت الحالة الاكثر صعوبة للذرة المحجوبة وقد غطت الدراسة مديات واسعة للمجال المغناطيسي ولطول الحجب.

Introduction

A large number of physical problems require solving the schrodinger equation for spherically symmetric potential in order to determine the energy eigenvalues and eigenfunctions.

Since only a handful of potentials is exactly solvable, in general, one has to resort to numerical techniques or approximation schemes. A typical example of such a potential the one that arise in an atomic system under the effect of an external magnetic field B. The treatment of the quadratic Zeeman effect (~B^2) attracts most available perturbative techniques. These include the shifted $\frac{1}{N}$ expansion method based on logarithmic perturbation theory (Impo et. a1.(1984), Mustafa (1993), Mustafa et.al. (1994), Villalba et.al. (1998), (2001), (2002), Pino (1999), Elsaid (2002)), the shifted l-expansion technique (Mustafa et.al. (1999), Odeh et,al, (2004), Mustafa (2004)) and the so called PT-symmetric pseudo perturbation (Bender et.al. (1998,1999)), the semiclassical quantization method (Hasegawa et.al. (1998)) and the so called $\hbar$ expansion method (Dobrovolska et.al. (2002)). The eigenvalue problem for the Yukawa (or Debye-Huckel) potential falls into such a category (Rogers et.al. (1970), Iafrate (1969)). When a uniform static magnetic field act on the screened electron, the problem becomes much more complicated even for very weak screenings (Jiang (1987)). For example, the application of such a field to the hydrogen atom breaks the orbital symmetry, thus destroying the angular momentum as a good constant of motion (Mustafa and Chhajlany (1994)).

Conventional perturbation treatment of this problem can handle the weak and strong field limits where the problem becomes almost separable. However, the experimentally most important situation is the one in which the magnetic and the Coulombic fields are comparable. To bridge the two limits of the magnetic field, one has to rely on various approximations and interpolation techniques. One of such techniques is the linear variational method (Villalba et.a1.(2001)) which proves efficient in dealing with 2D doner problems. The 3D problem is much more complicated because the hamiltomian in this case is no longer spherically symmetric as in the 2D. As we all know, that most numerical and perturbative techniques such as the shifted 1/N method as an example, require spherical symmetric potentials as a prerequisite intial condition. To overcome this difficulty reasonably well, we utilize the proposal due to Mustafa and Chhajlani (1994). This proposal enables one to consider initially a related spherical symmetric problem close to the real non-spherical one and then account for the nonspherical character in an approximate manner. In the next section, we outline the basic idea behind such strategy. In sec.3, we present our calculational procedure. In sec.4, discuss our results and finally sec.5 concludes the paper.

The method

(i)- The Coulmb screening

Consider a positive point charge (+Z) that is immersed in a plasma. The Coulomb potential due to this charge, namely, Z/r is screened by the electrons surrounding it so that an electron experiences the presence of this positive charge as if Z is modified by this screening into an effective charge $Z_{eff} = Ze^{-sr}$, where s is a screening parameter. To see how this comes about, consider the expression (Ashcroft and Mermin (1976)):

$$V(r)=\frac{Z}{(2\pi)^3}\int d^3q\,\frac{4\pi}{q^2\varepsilon(\vec{q})}e^{i\vec{q}.\vec{r}} \qquad (1)$$

and that in the Thomas-Femi approximation, the dielectric constant is given by

$$\left.\begin{array}{l}\varepsilon(\vec{q})=1+\dfrac{s^2}{q^2}\\ and\\ s^2=\dfrac{3k_F}{\pi a_o}\end{array}\right\} \qquad (2)$$

Where

$a_o=\hbar^2\varepsilon/me^2$

is the Bohr radius. The screened potential by using (2) gives:

$$V(r)=\frac{Z}{(2\pi)^3}\int d^3q\,\frac{4\pi}{(q^2+s^2)}e^{i\vec{q}.\vec{r}}$$

Therefore

$$V(r)=\frac{Z}{r}e^{-sr} \qquad (3)$$

With

$$s=\left(\frac{16}{3\pi^2}\right)^{\frac{1}{3}}\left(\frac{r_s}{a_0}\right)^{\frac{1}{2}}K_F=\frac{2.95}{(r_s/a_0)^{\frac{1}{2}}}\overset{0}{A}{}^{-1} \qquad (4)$$

Corresponding to a screening length D=l/s. Taking into account that for most of cases, the ratio r_s/a_o is between 2 and 6, we have that $1.2 \leq s \leq 2.1$. The influence of the applied magnetic field B is a nontrivial problem and in the present article we assume that s is the same for all values of B.

(ii) The Hamiltonian

In the nonrelativistic scheme, the Hamiltonian for a screened hydrogen atom when a constant magnetic field B is applied perpendicular to the (x,y) plane can be written as

$$H=\frac{1}{2m}\left(\vec{p}+\frac{e}{2}\vec{B}\times\vec{r}\right)^2-\frac{Ze^2}{r}e^{-sr} \qquad (5)$$

Using atomic units (see the appendix) H becomes:

$$H=-\frac{1}{2}\nabla^2-\frac{Ze^{-sr}}{r}+\frac{1}{2}\Omega^2\rho^2 \qquad (6)$$

Where Ω is a dimensionless parameter which can be taken as a measure of the magnetic field, (in cgs) Ω =B/4.7x109 G. It is clear that H is not a spherical symmetric because of the presence of the last term in (6) and so the orbital quantum number 1 is no longer a good quantum number, The angular momentum is not conserved as a consequence of the noncommutivity between $\hat{H}$ and $\acute{L}^2$ namely $[\hat{H}, \acute{L}^2] \neq 0$. Furthermore, the solution of the eigenvalue problem with H defined by (6) cannot be obtained in a closed form or even numerically by conventional techniques, instead, we start with the related spherical symmetric counterpart, namely;

$$H_{sph}=-\frac{1}{2}\nabla^2-\frac{Ze^{-sr}}{r}+\frac{1}{2}\Omega^2 r^2 \qquad (7)$$

and try to solve the corresponding schrodingcr equation

$$H_{sph}\phi=E'\phi \qquad (8)$$

Even so the exact solution of (8) cannot be expressed in a closed from in terms of special functions. In the present paper we choose to use a mixed-basis variational method with trial function as linear combination of screened hydrogenic and 3D harmonic basis eigenfunction. Such a trial function will reduce to the screened hydrogen atom when Ω=0 and to that of the 3D harmonic oscillator for large values of Ω. In order to obtain an estimate to the actual energy E, we use the approximate formula (Mustafa and Chhajlany (7994))

$$E\approx\frac{2}{3}(E'-E_{coul})+E_{coul} \qquad (9)$$

Equation (9) is based on the fact that the ground state energies of an isotropic pure 2D harmonic oscillator, with the potential term $\Omega^2(x^2+y^2)/2$, are equal to two-thirds of the eigenvalues of an isotropic pure 3D harmonic oscillator with the potential term $\Omega^2(x^2+y^2+z^2)/2$ Thus for the ground state and for isotropic harmonic oscillator, the eigenvalues of $\Omega^2(x^2+y^2)/2$ contribute two- thirds of those of the spherically symmetric one, $\Omega^2 r^2/2$, to the coulomb energy eigenvalues, To derive a formula for E_{coul} , we start from $H\psi=E\psi$ with H given by (6) and impose the normalization condition $\langle\psi\,|\,\psi\rangle=1$, to obtain

$$E=\left\langle\psi\left|\frac{1}{2}\nabla^2-\frac{Ze^{-sr}}{r}+\frac{1}{2}\Omega^2(x^2+y^2)\right|\psi\right\rangle \qquad (10)$$

Using

$$\langle x^2\rangle=\langle y^2\rangle=\frac{1}{3}\langle r^2\rangle \qquad (11)$$

We obtain

$$\langle\rho^2\rangle\approx\frac{2}{3}\langle r^2\rangle \qquad (12)$$

Using(12) into (10) we get:

$$\begin{aligned}E&\approx\left\langle\psi\left|\frac{1}{2}\nabla^2-\frac{Ze^{-sr}}{r}+\frac{2}{3}\left(\frac{1}{2}\Omega^2r^2\right)\right|\psi\right\rangle\\&=\frac{2}{3}\left\langle\psi\left|-\frac{1}{2}\nabla^2-\frac{Ze^{-sr}}{r}+\frac{1}{2}\Omega^2r^2\right|\psi\right\rangle+\\&\frac{1}{3}\left\langle\psi\left|-\frac{1}{2}\nabla^2-\frac{Ze^{-sr}}{r}\right|\psi\right\rangle\end{aligned} \qquad (13)$$

Using equation (7) and (8), we obtain:

$$E \approx \frac{2}{3}E' + \frac{1}{3}\left\langle \psi \left| -\frac{1}{2}\nabla^2 - \frac{Ze^{-sr}}{r} \right| \psi \right\rangle$$

If we denote the second term by E_{coul}, we finally obtain (9) and

$$E_{coul} = \left\langle \psi \left| -\frac{1}{2}\nabla^2 - \frac{Ze^{-sr}}{r} \right| \psi \right\rangle \qquad (14)$$

It is clear that (13) cannot be evaluated exactly since Ψ is unknown. If Ψ is replaced by Φ from (8), we arrive at an approximate formula

$$E_{coul} \approx \langle -\frac{1}{2}\nabla^2 - \frac{Ze^{-sr}}{r} \rangle_{sph}$$

Where $\langle \quad \rangle_{sph}$ denotes the ground state expectation value by using Φ instead of Ψ. In the weak field limit $(\Omega \to 0)$, it can be shown (see the appendix) that

$$E_{coul}(\Omega \to 0) \approx -\frac{Z}{2}\langle \frac{e^{-sr}}{r} \rangle_{sph} \qquad (15)$$

The evaluation of E_{coul} in either formula require the knowledge of the screened hydrogenic eigenfunctions ϕ_{scH} satisfying

$$\left(-\frac{1}{2}\nabla^2 - \frac{Z}{r}e^{-sr} \right)\phi_{scH} = \varepsilon_{scH}\phi_{scH} \qquad (16)$$

Unfortunately (16) cannot be solved analytically to obtain exact ϕ_{scH} it can, however, be solved by numerical integration (Rogers et.a1.(1970)) This would yield ϕ_{scH} in a form of tables only.

Calculations:

If we attempt to apply the variational method using only ϕ_{scH} for the screened hydrogen atom. we will obtain a good agreement with accurate results for small values of Ω, but this approach fails for large Ω even if we consider a basis with many terms. Analogous situation occurs if we use pure oscillator basis for large Ω, which converges very slowly for small values of Ω. In order to overcome such difficulties, we use mixed basis approach to represent Φ of equation (8)

$$\phi = \sum_i C_i \phi_i \qquad (17)$$

Φ_i either belongs to the screened hydrogen atom $(\phi_i = \phi_{scH})$ or belongs to the 30 harmonic oscillator $(\phi_i = \phi_{osc})$ where C_i are varied so as to get minimum energy. It is worth noticing that our mixed basis are not orthogonal under inner product i,e $\langle \phi_i \mid \phi_j \rangle \neq 0$ We proceed to minimize the expectation value $\langle \phi | H_{sph} | \phi \rangle$ with the normalization condition

$\sum_i |C_i|^2 = 1$ fulfilled,

After performing a variation on the basis coefficients C_i we reduce our problem to that of solving the matrix equation

$$\lfloor H_{ij} - \lambda s_{ij} \rfloor\lfloor C_j \rfloor = 0 \qquad (18)$$

Where $H_{ij} = \langle \phi_i | H_{sph} | \phi_j \rangle$ and $S_{ij} = \langle \phi_i | \phi_j \rangle$ Using the definition (7) in (18) and solving the secular equation $|H_{ij} - \lambda S_{ij}| = 0$ to obtain the lowest value of λ. $E' \leq \lambda$ can be obtained in terms of H_{ij} and S_{ij}.

The advantage of this approach is two fold. First we have a lower bound for our energy E'. Second we obtain a relatively simple expression for the normalized eigenfunction.

In this paper we choose to work with a two term mixed variational basis. In order to compute the binding energy for the ground state, we use a two term (1S) like states, namely ϕ_{scH}^{1s} and ϕ_{osc}^{1s} i.e

$$\phi_{1s} = c_1\phi_{scH}^{1s} + c_2\phi_{osc}^{1s} \qquad (19)$$

substituting (19) into (18): we get

$$\begin{pmatrix} H_{11} - \lambda & H_{12} - \lambda s_2 \\ H_{21} - \lambda s_{21} & H_{22} - \lambda \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad (20)$$

Where

$$H_{11} = \langle \phi_{scH}^{1s} \left| H_{sph} \right| \phi_{scH}^{1s} \rangle \qquad (21)$$

$$H_{22} = \langle \phi_{osc}^{1s} \left| H_{sph} \right| \phi_{osc}^{1s} \rangle \qquad (22)$$

$$s = s_{12} = s_{21} = \langle \phi_{osc}^{1s} \left| \phi_{scH}^{1s} \right\rangle \qquad (23)$$

$$H_{21} = H_{12} = \langle \phi_{scH}^{1s} \left| H_{sph} \right| \phi_{osc}^{1s} \rangle \qquad (24)$$

The solution of the secular equation (18) is given by

$$2(1-S^2)\lambda = H_{11} + H_{22} - 2SH_{12} - \sqrt{(H_{11}+H_{22}-2SH_{12})^2 - 4(1-S^2)(H_{11}H_{22}-H_{12}^2)2(1-S^2)} \qquad (25)$$

By solving (20) for C_i with the normalization $\sum |C_i|^2 = 1$, w get:

$$C_1 = \left[1 + \left(\frac{H_{11}-\lambda}{H_{12}-\lambda S} \right)^2 - 2S \left(\frac{H_{11}-\lambda}{H_{12}-\lambda S} \right) \right]^{-1/2} \qquad (26)$$

$$C_2 = -\left(\frac{H_{11}-\lambda}{H_{12}-\lambda S} \right) \left[1 + \left(\frac{H_{11}-\lambda}{H_{12}-\lambda S} \right)^2 - 2S \left(\frac{H_{11}-\lambda}{H_{12}-\lambda S} \right) \right]^{-1/2} \qquad (27)$$

H_{11}, H_{12} and S for the screened hydrogen may by evaluated numerically since ϕ_{scH}^{1s} is in the form of tables.

Results and discussion

(i) Th s=0 case (the unscreened Coulomb potential)

As a primenary stage let us start with the bare Coulomb potential $\left(-\frac{Z}{r} \right)$ i.e with s=0. The computation of the energy by equation (25) is greatly simplified for this special case. Using ϕ_H^{1s} and ϕ_{osc}^{1s} given by

$$\phi_H^{1s} = \frac{1}{\sqrt{\pi}} e^{-r}, \phi_{osc}^{1s} = \left(\frac{\Omega}{\pi} \right)^{3/4} e^{-\frac{1}{2}\Omega r^2} \qquad (28)$$

We get:

$$H_{11} = \langle \phi_H^{1s} \left| -\frac{1}{2}\nabla^2 - \frac{1}{r} + \frac{1}{2}\Omega^2 r^2 \right| \phi_H^{1s} \rangle = -\frac{1}{2} - \frac{3}{2}\Omega^2 \qquad (29)$$

$$H_{22} = \langle \phi_{osc}^{1s} \left| -\frac{1}{2}\nabla^2 - \frac{1}{r} + \frac{1}{2}\Omega^2 r^2 \right| \phi_{osc}^{1s} \rangle = -\frac{3}{2}\Omega - 2\sqrt{\frac{\Omega}{\pi}} \qquad (30)$$

$$H_{12} = \frac{3}{2}\Omega S + 4\left(\frac{1}{\Omega\pi} \right)^{\frac{1}{4}} \left\{ 1 - \sqrt{\frac{2}{\Omega}} e^{\frac{1}{2\Omega}} \int_{1/\sqrt{2\Omega}}^{\infty} e^{-x^2} dx . \right\} \qquad (31)$$

Where S is given by:

$$S = 4\sqrt{2} \left(\frac{1}{\pi\Omega^3} \right)^{\frac{1}{4}} \left\{ \left(1 + \frac{1}{\Omega} \right) e^{\frac{1}{2\Omega}} \int_{1/\sqrt{2\Omega}}^{\infty} e^{-x^2} dx - \frac{1}{\sqrt{2\Omega}} \right\}$$

(32)

The details for getting (31) and (32) appear in the appendix. The integral in (31) and (32), as a function of the applied field, can either be evaluated numerically or taken from tables. Using equation (25), we can evaluate an upper bound for $E'_{1s} \left(E'_{1s} \le \lambda \right)$ and the eigenfunction ϕ_{1s} by using C_1 and C_2 from (26) and (27) respectively. E_{coul} Reduces to:

$$E_{coul} \approx \langle \phi_{1s} \left| -\frac{1}{2}\nabla^2 - \frac{Z}{r} \right| \phi_{1s} \rangle = -\frac{1}{2}C_1^2 - C_1 C_2 S - C_2^2 \left(\frac{3}{2}\Omega - 2\sqrt{\frac{\Omega}{\pi}} \right) \qquad (33)$$

(see the appendix).

The result (33) is suitable for intermediate Ω. For very small Ω, $E_{coul} \approx 0.167$, according to equation (15). For very large Ω the Coulomb effect is negligible and we approximately have $E \approx \frac{3}{2} E'$.

In table (1), we list the results of our calculations for the special case s=0 according to equations (29-33) for various values of Ω. E_{1s} is evaluated by using equation (9) and listed in the last two columns where it has been obtained by using two sets of values for E_{coul} as stated above. As seen, these sets are very close in the range (Ω=0.1-1.0) because the Coulomb interaction overwhelms the magnetic, As Ω grows up, the values calculated according to equation (33) becomes more valid. In table (2) these calculations are extended to higher values of Ω. For such high values, E_{coul} becomes negligible compared with the effect of the magnetic field and so E is approximately equals to 2E'/3. It is also shown in table (2) the results of other workers namely those due to Rosen (1986) and Mustafa and Chhajlani (1994), It is seen that our results indicate very close to those of Rosen in the low field region but Slightly differ from Mustafa and Chhajlani being lower than ours in the low field region. The latter authors used the shifted 1/N method due to Imbo et.a1(1984) and as pointed out by Villalba and Pino (1998) this method overestimate the energy of the ground state for low field and also in the high field. The variational solution obtained using the hydrogen basis is in good agreement with the results obtained by Martin et.al. . The impressive feature of our results as a whole is that the energies have the coulomb limit of E_{1s}=-0.5 at very low field and approach the outcome of the Londau level E_{1s}= Ω in the high field, thus describing the spectrum of the electron in a uniform large magnetic field strength.

(ii) The screened electron

In order to obtain ϕ^{1s}_{scH} in (9), we have to solve equation (16) numerically.

ϕ^{1s}_{scH} is given by

$$\phi^{1s}_{scH} = \frac{1}{\sqrt{4\pi}}\frac{1}{r}R_{1s}(r) \qquad (34)$$

Where R_{1s} satisfies the radial schrodinger equation

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} - \frac{Ze^{-sr}}{r}\right)R_{1s} = \varepsilon^{1s}_{scH}R_{1s} \qquad (35)$$

Equation (35) has no analytic solution in a closed form in terms of special functions; It assumes an approximate analytic solution as a series in powers of the screening parameter, s but such solution is only valid in the asymptotic region (Kasssim (1994)) In order to compute R_{1s} and ε^{1s}_{scH}, (35) has to be solved numerically using for example Numerov method (Kassim(l976)). All integrals involving ϕ^{1s}_{scH} will be evaluated numerically accordingly. To calculate E_{1s} variationally, we follow similar steps using the relations (21-27) to obtain the matrix elements H_{ij} and S_{ij}, and then λ by numerical integration. To calculate E_{coul} we use equation (33) with suitable replacements, in the form:

$$E_{coul} = \varepsilon^{1s}_{scH}C_1^2 - C_1C_2S +$$

$$C_2^2\left\{\frac{3}{2}\Omega - \langle\phi^{1s}_{osc}\left|\frac{Ze^{-sr}}{r} + \frac{1}{2}\Omega^2r^2\right|\phi_{osc}\rangle\right\}$$

Where ε^{1s}_{scH} and, S are obtained numerically and C_i are calculated accordingly,

Evidently, the E_{1s}, depends on two parameters, the screening length D=1/s and the magnetic field strength through Ω. The range of the former is taken as $1 \leq D \leq 10$.

In table (3). We have listed the results of our calculations for the values s=0.1,0.2,....,1.0 for a wide range of Ω ($0.05-10^3$) .It can be seen that the Yukawa potential shifts up the energy level as long as the screening parameters increases. For s-1 the presence of the magnetic field shifts the E_{1s} level away twords the continuum. As s increases, the contribution of the magnetic field becomes more important and the energy eigenvalues are closer to those given by the oscillator energy expression i.e to Landau levels. Therefore a critical value for s (or D≈1) for which it stops binding the electron in the s-state.

As a whole, the above results show that the presence of bounded states in a Yukawa hydrogenic atom strongly depends on the strength of the screening. The inclusion of the magnetic field permits one to recover the Landau energy levels. In summary, the mixed variational approach gives the most accurate numerical results even for large Ω values.

Table (1): Hydrogenic ground state energy (in Hartees) E_{1s} calculated by the method of the linear variation using a trial wave function as a mixture of pure hydrogenic and pure 3D harmonic oscillator of s-symmetry as a function of the external magnetic field strength represented by the unitless parameter Ω

Ω	H_{11}	H_{22}	S_{12}	H_{12}	E'	C_1	C_2	E_{coul}	$E_{1s} \approx \frac{2}{3}E' - \frac{0.5}{3}$	$E_{1s} \approx \frac{2}{3}E' + \frac{1}{3}E_{coul}$
0.10	**-0.48500**	**-0.20675**	**0.68722**	**-0.32011**	**-0.48567**	**1.03411**	**-0.05062**	**-0.49944**	**-0.49045**	**-0.49026**
0.15	**-0.46630**	**-0.21119**	**0.79641**	**-0.34658**	**-0.46909**	**1.08870**	**-0.11435**	**-0.49770**	**-0.47939**	**-0.47863**
0.2	**-0.44000**	**-0.20452**	**0.86412**	**-0.34546**	**-0.44682**	**1.16380**	**-0.19523**	**-0.49446**	**-0.46455**	**-0.46269**
0.25	**-0.40630**	**-0.18908**	**0.90789**	**-0.32768**	**-0.41797**	**1.24960**	**-0.2874**	**-0.49013**	**-0.44531**	**-0.44202**
0.3	**-0.36500**	**-0.16791**	**0.93662**	**-0.29914**	**-0.38035**	**1.32600**	**-0.36564**	**-0.48640**	**-0.42023**	**-0.41570**
0.35	**-0.31630**	**-0.14242**	**0.95535**	**-0.26337**	**-0.33110**	**0.35770**	**-0.38103**	**-0.48620**	**-0.38741**	**-0.38281**
0.4	**-0.26000**	**-0.11350**	**0.9672**	**-0.22265**	**-0.26910**	**1.30110**	**-0.31460**	**-0.49144**	**-0.346066**	**-0.343212**
0.45	**-.196310**	**-0.08178**	**0.97414**	**-0.17847**	**-0.19805**	**1.13730**	**-0.14140**	**-0.49840**	**-0.29870**	**-0.29820**
0.5	**-0.12500**	**-0.04772**	**0.97753**	**-0.13188**	**-0.12597**	**0.90140**	**0.10070**	**-0.49922**	**-0.2506**	**-0.25039**
0.6	**0.03990**	**0.02614**	**0.97706**	**-0.03427**	**-0.00098**	**0.45110**	**0.55460**	**-0.47524**	**-0.16732**	**-0.15951**
0.7	**0.23500**	**0.10612**	**0.97050**	**-0.06631**	**0.09941**	**0.18300**	**0.82160**	**-0.44524**	**-0.10039**	**-0.08214**
0.8	**0.03980**	**0.02614**	**0.97707**	**0.16774**	**0.19012**	**0.05234**	**0.94960**	**-0.41799**	**-0.03991**	**-0.01258**
0.9	**0.50210**	**0.29870**	**0.9534**	**0.21076**	**0.2325**	**0.04632**	**0.97670**	**-0.38761**	**0.03602**	**-0.06762**
1.0	**1.00000**	**0.37184**	**0.93538**	**0.36867**	**0.37110**	**0.03540**	**1.03300**	**-0.36997**	**0.08074**	**-0.12408**

Table (2): E_{1s} (in atomic units with Z =1), the energy of the ground state of an electron in (1s) state in the hydrogen atom that is subjected to an external magnetic field Ω compared the results of the references (14, 21)

Ω	Mustafa and Chhajlany Ref (14)	Rosen Ref (21)	Present Work
0.05	-0.49754	-0.498800	-0.49751
0.25	-0.44872	-0.470300	-0.44202
0.50	-0.33685	-0.331200	-0.25039
1.00	-0.04429	-0.165200	-0.12408
1.25	0.12078	0.152450	0.24045
2.50	1.03356	1.119600	1.14126
5.00	3.05150	2.623000	3.15018
25.0	21.00130	19.87000	20.62900
50.0	44.46250	42.80000	43.95300
500	483.08610	477.50000	482.23900
1000	976.19370		975.27000
2000	1966.45250		1965.29000
3000	2958.96550		2957.90700
5000	4947.10917		4945.52300
10000	9925.3057		9925.48000

Table (3) E_{1s} of an electron that is moving in a screened Coulomb potential under the action of an external magnetic field of strength Ω for various screening lengths D=1/s (All energies are measured in Hartrees)

Ω	D = 10	D= 5	D =3	D=2	D=1
0.05	-0.40447	-0.32414	-0.23383	-0.14445	0.01514
0.10	-0.39732	-0.31663	-0.22558	-0.13450	0.05858
0.15	-0.38609	-0.30491	-0.21263	-0.118120	0.09291
0.20	-0.37096	-0.28896	-0.19442	-0.09322	0.12441
0.25	-0.35122	-0.26774	-0.16910	-0.05720	0.15531
0.30	-0.32529	-0.23935	-0.13455	-0.01228	0.18627
0.35	-0.29127	-0.23937	-0.09112	0.03406	0.21750
0.40	-0.24879	-0.15715	-0.04364	0.07600	0.24911
0.45	-0.20102	-0.10910	0.00173	0.11267	0.28110
0.50	-0.18392	-0.11974	0.04204	0.14364	0.31346
0.55	-0.13793	-0.07332	0.07766	0.17658	0.34619
0.60	-0.09423	-0.03328	0.11013	0.20664	0.37928
0.65	-0.05491	0.00396	0.14087	0.23650	0.41270
0.70	-0.01829	0.03367	0.17084	0.26644	0.44644
0.75	0.01661	0.07240	0.20064	0.29673	0.48049
0.80	0.05065	0.10778	0.23058	0.32740	0.51482
0.85	0.08442	0.14459	0.26084	0.35850	0.54943
0.90	0.11829	0.17881	0.29149	0.39009	0.58430
0.95	0.15249	0.20880	0.32257	0.42206	0.61941
1.00	0.18713	0.24530	0.35409	0.45440	0.65476
1.25	0.36804	0.42513	0.49289	0.62175	0.83472
2.5	1.23670	1.46963	1.54269	1.62470	1.82363
5.00	3.24622	3.33500	3.9349	4.02440	4.25427
25.0	21.16220	21.26080	21.3746	21.50500	21.83344
50.0	44.61220	44.70410	44.82000	44.95300	45.29440
500	483.110	483.202	483.313	483.455	483.543
1000	976.130	976.217	976.310	976.410	976.876

Appendix

(i) Derivation of Equation (6)

By using $\hat{P} = -i\hbar\hat{\nabla}$ in Equation (5), we obtain

$$H = \frac{1}{2m}\left[-i\hbar\hat{\nabla} + \frac{1}{2}e\left(\vec{B}\times\vec{r}\right)\right] - \frac{Ze^2e^{-sr}}{r} \quad \text{(A1)}$$

If the applied magnetic field is in the z- direction, then

$$\vec{B} = B\vec{k} \quad \text{(A2)}$$

And

$$\vec{B}\times\vec{r} = B(-y,x,0) = B\rho\vec{e_\phi} \quad \text{(A3)}$$

Nothing $\hat{\nabla}.(\rho\vec{e_\phi}) = 0$ and employing $\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi}$, we get:

$$\hat{H} = -\frac{\hbar^2}{2m}\hat{\nabla}^2 + \frac{eB}{2m}\hat{L}_z + \frac{e^2}{8m}B^2\rho^2 - \frac{Ze^2e^{-sr}}{r} \quad \text{(A4)}$$

For states with s-symmetry, $(l = 0, m_l = 0)\hat{L}_z\,\phi_s = 0$, we get

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{e^2B^2}{8m}\rho^2 - \frac{Ze^2e^{-sr}}{r} \quad \text{(A5)}$$

Expressing Ĥ in atomic units (energy in $\frac{me^4}{\hbar^2}$ and distances in Bohr units $\frac{\hbar^2}{me^2}$), we get:

$$\hat{H} = -\frac{1}{2}\nabla^2 + \frac{1}{2}\Omega^2\rho^2 - \frac{Ze^{-sr}}{r} \quad \text{(A6)}$$

Where Ω is measure of the strength of B and is given (in CGS) by

$$\Omega = \frac{B}{4.7\times10^9G} \quad \text{(A7)}$$

(ii) Derivation of Equations (12, 15)

The virial theorem $2 < -\nabla^2/2 > = < \vec{r}.\vec{\nabla}V >$ with respect to Equation (14, 17) yield respectively:

$$< \nabla^2 + \frac{Ze^{-sr}}{r} + \Omega^2(x^2+y^2) > = 0 \quad \text{(A8)}$$

$$< \nabla^2 + \frac{Ze^{-sr}}{r} + \Omega^2r^2 >_{sph} = 0 \quad \text{(A9)}$$

Using the Hellmann - Feynman theorem on Equations (14, 17) we respectively obtain

$$\left.\begin{aligned}\frac{\partial E(\Omega,z)}{\partial z} &= -<\frac{e^{-sr}}{r}> \\ \frac{\partial E(\Omega,z)}{\partial\Omega} &= \Omega < x^2+y^2 >\end{aligned}\right\} \quad \text{(10)}$$

and

$$\left.\begin{aligned}\frac{\partial E'(\Omega,z)}{\partial z} &= -\langle\frac{e^{-sr}}{r}\rangle_{sph} \\ \frac{\partial E'}{\partial z} &= \Omega\langle r^2\rangle_{sph}\end{aligned}\right\} \quad \text{(A11)}$$

Provided all wave functions are normalized.

The Euler homogeneity condition associated with Equations (A8, A9) yields:

$$< \nabla^2 > = z\left(\frac{\partial E'}{\partial z}\right) - \Omega\left(\frac{\partial E'}{\partial z}\right) \quad \text{(A12)}$$

$$< \nabla^2 >_{sph} = z\left(\frac{\partial E'}{\partial z}\right) - \Omega\left(\frac{\partial E'}{\partial z}\right) \quad \text{(A13)}$$

respectively.

Using Equations (14, 17) we obtain

$$E = \frac{1}{2}z\frac{\partial E}{\partial z} + \Omega\frac{\partial E}{\partial\Omega} \quad \text{(A14)}$$

$$E = \frac{1}{2}z\frac{\partial E'}{\partial z} + \Omega\frac{\partial E'}{\partial\Omega} \quad \text{(A15)}$$

By substituting Equations (A14, A15) into Equation (15), we obtain

$$\frac{1}{2}z\frac{\partial E}{\partial z} + \Omega\frac{\partial E}{\partial\Omega} \approx \frac{2}{3}\left(\frac{1}{2}z\frac{\partial E'}{\partial z} + \Omega\frac{\partial E'}{\partial\Omega}\right) + \frac{1}{3}E_{coul} \quad \text{(A16)}$$

Substituting Equations A12 and A13 into A16, we get:

$$\frac{1}{2}z < -\frac{e^{-sr}}{r} > + \Omega^2 < x^2+y^2 > \approx$$

$$\frac{2}{3}\left(\frac{-z}{2} < \frac{e^{-sr}}{r} >_{sph} + \Omega^2 < r^2 >_{sph}\right) + \frac{1}{3}E_{coul} \quad \text{(A17)}$$

Consider now two limiting cases for Equation (A17).

(a) The limit $\Omega \to 0$: Equation (A17) reads

$$E_{coul} \approx 3z\left\{\frac{1}{3} < \frac{e^{-sr}}{r} >_{sph} - \frac{1}{2} < \frac{e^{-sr}}{r} >\right\}$$

Assuming

$$< \frac{e^{-sr}}{r} >_{sph} \approx < \frac{e^{-sr}}{r} >$$

Provided that

$$H \approx -\frac{1}{2}\nabla^2 - \frac{ze^{-sr}}{r}$$

We obtain

$$E_{coul} \approx -\frac{z}{2} < \frac{e^{-sr}}{r} >_{sph} \qquad \text{(A18)}$$

(a) The limit $\Omega \to \infty$: Equation (A17) reads

$$\Omega^2 < x^2 + y^2 > \approx \frac{2}{3}\Omega^2 < r^2 >_{sph} \qquad \text{(A19)}$$

Provided that

$$H \approx \frac{1}{2}\nabla^2 + \frac{1}{2}\Omega^2 r^2$$

Equation (A19) furnish a sound justification for the validity of approximate formula (15) and equation (A18) provides an approximation for E_{coul} at low field

(iii) Evaluation of S$_{12}$ and H$_{12}$

$$S_{12} = < \phi_H^{1S} \Big| \phi_{osc}^{1S} > = 4(\frac{\Omega^3}{\pi})^{\frac{1}{4}} \int_0^\infty r^2 e^{-(\frac{1}{2}\Omega r^2 + r)} dr$$

(A20)

$$H_{12} = \frac{3}{2} S_{12}\Omega - 4(\frac{\Omega^3}{\pi})^{\frac{1}{4}} \int_0^\infty r\ e^{-(\frac{1}{2}\Omega r^2 + r)} dr$$

(A21)

Integrating the second integral by parts once and the first integral twice, we finally obtain single integral of the form

$$\int_0^\infty e^{-(ax^2+bx+c)} dx = \frac{1}{2}\sqrt{\frac{\pi}{a}} e^{(b^2-4ac)/2a} erfc(\frac{b}{2\sqrt{a}})$$

(A22)

Where

$$erfc(p) = \frac{2}{\sqrt{\pi}} \int_p^\infty e^{-x^2} dx \qquad \text{(A23)}$$

Using (A22), (A23) in (A20), (A21) obtain:

$$S_{12} = \sqrt{32}(\frac{1}{\pi\Omega^3})^{\frac{1}{4}} \left\{ (1 + 1/\Omega) e^{\frac{1}{2\Omega}} \int_{\frac{1}{\sqrt{2\Omega}}}^\infty e^{-x^2} dx - \frac{1}{\sqrt{2\Omega}} \right\}$$

(A24)

$$H_{12} = \frac{3}{2}\Omega S_{12} - 4(\frac{1}{\pi\Omega^3})^{\frac{1}{4}} \left\{ 1 - \sqrt{\frac{2}{\Omega}} e^{\frac{1}{2\Omega}} \int_{\frac{1}{\sqrt{2\Omega}}}^\infty e^{-x^2} dx \right\}$$

(A25)

(iv) Derivation of Equation (46):

$$E_{coul} = < \psi | h | \psi > \qquad \text{(A26)}$$

where

$$h = \frac{1}{2}\nabla^2 - \frac{z}{r} \qquad \text{(A27)}$$

$$\psi = c_1\phi_H^{1s} + c_2\phi_{osc}^{1s} \qquad \text{(A28)}$$

$$E_{coul} \approx c_1^2 < \phi_H^{1S} | h | \phi_H^{1S} > +$$

$$2c_1c_2 < \phi_H^{1S} | h_0 | \phi_{osc}^{1S} > + c_2^2 < \phi_{osc}^{1S} | h | \phi_{osc}^{1S} >$$

$$= -\frac{1}{2}c_1^2 - c_1c_2S_{12} +$$

$$\frac{3}{2}c_2^2\Omega - c_2^2 < \phi_{osc}^{1S} \left| \frac{Z}{r} + \frac{1}{2}\Omega^2 r^2 \right| \phi_{osc}^{1S} >$$

(A29)

The integral in the last step maybe evaluated as follows:

$$< \phi_{osc}^{1S} \left| \frac{z}{r} + \frac{1}{2}\Omega^2 r^2 \right| \phi_{osc}^{1S} >$$

$$= 4(\frac{\Omega^3}{\pi})^{1/2} \left\{ z\int_0^\infty re^{-\Omega r^2} dr + \frac{1}{2}\Omega^2 \int_0^\infty r^4 e^{-\Omega r^2} dr \right\}$$

(A30)

Using the result:

$$\int_0^\infty x^m e^{-ax^2} dx = \frac{\Gamma(\frac{m+1}{2})}{2a^{(\frac{m+1}{2})}} \qquad \text{(A31)}$$

we finally obtain

$$E_{coul} \approx \frac{1}{2}c_1^2 - c_1c_2S_{12} + c_2^2(\frac{3}{2}\Omega - 2\sqrt{\frac{\Omega}{\pi}}$$

(A32)

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