ACCURATE EIGENENERGIES FOR THE MAGNETIZED HYDROGEN ATOM

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The year of 1986 was extremely fruitful in results for the quadratic Zeeman effect. We mention three examples: first, quasi-Landau resonances having a closer spacing than $1.5\ \hbar\omega$ near the zero-energy threshold have been reported experimentally by the Bielefeld group[1,2] and explained theoretically.[3-6] The second example is the investigations connected with the manifestation of quantum chaos, i.e. how does classical deterministic chaos manifest itself in the quantum spectrum of energies.[4,7,8] Connected with this is the very interesting work of Wintgen[9] showing the existence of long-range correlations in the quantum spectrum. These contributions are particularly interesting because in contrast to previous studies of model Hamiltonians, they are based on a real physical system which can be investigated in the laboratory. As observed by Professor Friedrich in his lecture at this Conference, the magnetized hydrogen atom is becoming the system par excellence to investigate quantum chaos. The third example is the beautiful results of O'Mahony and Taylor on the quadratic Zeeman effect for nonhydrogenic systems.[10,11] The central point in almost all the aforementioned theoretical works was the calculation of the energy spectrum of a magnetized atom.

The purpose of this paper is to present a single variational function capable of producing very accurate approximations to the eigenenergies of a hydrogen atom in a uniform magnetic field. In fact, to the best of our knowledge, the trial function presented here is the only single function capable of consistently generating eigenenergies with at least 5 significant digits in the whole parameter range $0 \leq \gamma < \infty$, where γ is the magnetic field strength in units of 2.35×10^5T. Our

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function is based on an expansion in parabolic coordinates proposed by one of us,[12] using a basis combining characteristics of both the Coulomb and Landau regimes. Calling

$$f(x,y) = 1 + x_1c(x+y) + x_2c^2xy + x_3c^2(x^2 + y^2) + x_4c^3xy(x+y) + x_5c^3(x^3+y^3) + x_6c^4x^2y^2 + x_7c^4xy(x^2+y^2) + x_8c^4(x^4+y^4) + x_9c^5(x^5+y^5) + x_{10}c^5xy(x^3+y^3) + x_{11}c^5x^2y^2(x+y) + x_{12}c^6x^2y^2(x^2+y^2) + x_{13}c^6xy(x^4+y^4) + x_{14}c^6x^3y^3,$$

the trial function is given by $\psi(x,y) = f(x,y)\exp[-\frac{1}{2}a(x+y+acxy)]$, where $x\equiv\xi$ and $y\equiv\eta$ are the usual parabolic coordinates and a trivial normalization constant has been omitted. The great advantage of this trial function is having the exponential dependence appropriate to the symmetry of the problem.

Table 1. Comparison of binding energies (in a.u.) for a magnetized hydrogen atom. E_{RWHR} are the energies of Rösner, Wunner, Herold and Ruder.[14] The number in parenthesis indicates the number of configurations needed to guarantee their quoted digits. E_N are energies obtained by us using N configurations of the basis proposed by Gallas.[12]

γ	E_{RWHR}	E_6	E_{12}	E_{15}
1	0.831169(7)	0.83117	0.83117	0.831169
2	1.022214(11)	1.02220	1.02221	1.022214
3	1.164533(11)	1.16451	1.16453	1.164533
4	1.280798(12)	1.28077	1.28080	1.280798
10	1.747797(19)	1.74774	1.74780	1.747797
20	2.215398(20)	2.21533	2.21539	2.215398
40	2.801029(24)	2.80094	2.80102	2.801028
100	3.78905 (12)	3.78952	3.78977	3.789799
200	4.72655 (12)	4.72626	4.72709	4.727134
300	5.36030 (12)	5.35920	5.36074	5.360799
1000	7.66205 (12)	7.65562	7.66231	7.662388
2000	9.30448 (12)	9.29149	9.30462	9.304706
10000		14.09563	14.14038	14.140629
20000		16.63834	16.70516	16.705632

Peculiarities of the basis being used were already discussed by us in the literature.[12,13]

Using the above function a generalized 15×15 matrix eigenvalue problem was solved for the eigenenergies. The last column in Table 1 presented the results of such a calculation. In this table our results are compared with the results of the very detailed 1984 eigenfunction expansion of Rösner, Wunner, Herold and Ruder.[14] Their results are the most accurate available in the literature covering the whole range $0 \leq \gamma < \infty$, and were obtained by expanding the eigenfunction either in a Coulomb basis (for $\gamma \leq 40$) or in a Landau basis (for $\gamma > 40$). The number in parenthesis after their energies indicates the number of expansion terms that they needed to guarantee the quoted digits in the energy. In their calculations it was important to obtain first starting functions for the computation (thereby needing to solve numerically an eigenvalue equation), then to solve the actual problem, and, finally, to study the convergence of the procedure as a function of the terms in the spherical and the cylindrical basis. In contrast, our method involves a search for the minimum of $E = E(a,c)$ as a function of the two non-linear variational parameters a and c. The procedure involves a trivial and stable diagonalization of a 15×15 matrix. Altogether, our calculation involves 16 variational parameters (14 linear + 2 non-linear) but, obviously, 14 of them are automatically determined by the diagonalization procedure. To give an idea of convergence properties within the basis being used, Table 1 presents two further columns obtained by considering (i) a 6×6 matrix formed only with terms involving x_1, x_2, x_4, x_6 and x_7 in the above equation, and (ii) the 12×12 matrix obtained by neglecting x_{12}, x_{13} and x_{14} in the trial function.

From the energies presented in Table 1 one can assess the accuracy of the calculation of Rösner et al.[14] One sees that the region roughly between $10 \leq \gamma \leq 200$ is a "difficult" region for their calculations: up to about $\gamma = 40$ they had to greatly increase the size of the basis in order to maintain the same number of significant digits in the eigenvalues. For $\gamma = 100$ their value obtained using 12 configurations is not as good as ours obtained with just 6 configurations (involving 7 variational parameters). At this point it would be useful to know how to compare the effort needed to obtain eigenvalues of the same accuracy by both methods. This question is difficult to answer but it seems safe to say that for equal number of terms in the expansions our method is much easier to implement than that of Herold et al. Therefore we

believe our results involving 12 configurations to be much simpler to obtain than the corresponding ones obtained by Herold et al., also from 12 configurations. It is also worth mentioning that the non-relativistic model on which all calculations are based imposes a limit on the strength of the magnetic field for the energies to remain meaningful. As mentioned in Ref. 12, a limit on the magnetic field strength for the model to remain reliable is obtained by estimating the field required to produce an energy difference of mc^2 between neighbouring Landau levels. This defines the threshold $\gamma_{th} \cong 18700$, which is therefore the upper limit for the variation of γ. That is why our table includes results up to $\gamma \cong \gamma_{th}$. A further noteworthy point is the existence of calculations based on high-field expansions as, for example, that of Baye and Vincke.[15] Using at least 18 variational parameters they reported $E_B = 7.662405$ and 9.30475 for $\gamma = 1000$ and 2000, respectively. Being results of a specific high-field calculation, these 2 energies are better than the corresponding ones of Rösner et al. They are also better than the more accurate results being reported here. However it is important to realize that they use a larger basis and that their calculations are totally unable to deal with the Coulomb limit.

In summary, we presented binding enegies E_6, E_{12} and E_{15} for a magnetized hydrogen atom, based on variational calculations involving 7, 13, and 16 variational parameters, respectively. These energies cover the whole range of magnetic field strengths, from the Coulomb to the Landau limit. Our energies were compared with the most accurate results presently available in the literature, namely with the results of Rösner et al.[14] Our results obtained from the 13-parameter calculation are as good as the ones obtained by Rösner et al. The energies obtained from the 16-parameter calculation agree to at least 7 significant digits for γ less than about 40, and are superior for all other γ. We have also investigated the excited states obtaining similar results. A detailed report of our findings will be presented elsewhere.

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