THE HYDROGEN ATOM IN A SUPERSTRONG MAGNETIC FIELD

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A new method for energy-level calculations of the H-atom in a superstrong magnetic field is proposed. The method is based on perturbation theory. The finite-difference technique is used to solve the resulting equations.

Recently the existence of a superstrong magnetic field (SMF) ($\sim 10^{12}$ G) near surfaces of neutron stars was supposed. This caused an increasing interest in the problem of the properties of matter in such fields [1–4]. The nonrelativistic motion of an electron in the field of a fixed nucleus and in the presence of a SMF is the most simple problem to study the effects of a SMF. The well-known relation $E(Z, B) = Z^2 \times E(1, B/Z^2)$ reduces this problem to calculation of the H-atom energy levels for a wide range of magnetic fields. Here $E(Z, B)$ is the energy of a one-electron atom with nuclear charge Z in the presence of an external magnetic field B. Nowadays the energy levels of the H-atom in a SMG are known with rather high accuracy [3,4], but the methods applied to solve this problem become inefficient under a more realistic formulation of the latter or under application to many-electron systems.

In this note we propose a new method for calculation of the energy levels of the H-atom in a SMF, which uses perturbation theory (PT). A considerable simplification of the calculations is achieved by making use of the finite difference (FD) technique. We suppose the method proposed to be more suited for various generalizations, particularly for taking into account the motion of the nucleus and relativistic corrections.

The equation describing the nonrelativistic motion of an electron in the field of an infinitely heavy nucleus and an external uniform magnetic field directed along the Oz axis have the form

$$\left\{-\frac{1}{2}\frac{\partial^2}{\partial z^2} - \frac{1}{2}\frac{\partial^2}{\partial \rho^2} + \frac{1}{8}\left[(4m^2-1)\rho^{-2} + B^2\rho^2\right] - Z/(\rho^2+z^2)^{1/2}\right\} F(z,\rho) = (E - \tfrac{1}{2}Bm)\,F(z,\rho). \quad (1)$$

The function $F(z, \rho)$ satisfies the boundary conditions

$$F(z,\rho) = 0, \quad \text{if } z = \pm\infty \text{ or } \rho = 0, \infty. \quad (2)$$

Here z and ρ are the polar coordinates of the electron, m is the quantum number of the projection of the angular momentum on the Oz axis, B is the strength of the magnetic field in units of $B_0 = c|e|^3M^2/h^3 = 2.35 \times 10^9$ G, M and e are the mass and the charge of the electron. We separate the total hamiltonian into a zero-order part and the perturbation:

$$H = H_0 + V, \quad (3)$$

$$H_0 = H_1 + H_2, \quad (4)$$

$$H_1 = -0.5\,\partial^2/\partial\rho^2 + 0.125\left[(4m^2-1)\rho^{-2} + B^2\rho^2\right] + 0.5\,Bm, \quad (5)$$

$$H_2 = -0.5\,\partial^2/\partial z^2 - Z/(\rho_m^2 + z^2)^{1/2}, \quad (6)$$

$$V = Z/(\rho_m^2+z^2)^{1/2} - Z/(\rho^2+z^2)^{1/2}, \quad (7)$$

to take into account that the electron motion for large B is well localised near the cylindrical surface of radius $\rho_m = [(2m+1)/B]^{1/2}$ [1]. Here H_1 is the hamiltonian for the free motion of the electron in the x–y plane in the presence of a uniform magnetic field. The hamiltonian H_2 describes the motion of the electron in a one-dimensional Coulomb potential which is cut at ρ_m. The z and ρ variables may be sep-

arated in the zero-order operator. This simplifies considerably the solution of the problem via PT. The given choice of H_0 leads to better convergence of the perturbation series for higher B values. For example, the third-order correction for the ground-state energy for $B = 20B_0$ is about 1% of E_0, whereas for $B = 2000 \times B_0$ it is of order 10^{-5}% of E_0. The corresponding ratio of the first-, second- and third-order corrections is, respectively, 2 : 3 : 0.1 for $B = 20B_0$ and 1 : 0.1 : 0.001 for $B = 2000B_0$. Thus for $B \geqslant 10^{10}$ G it is sufficient to calculate the energy through the third-order of PT.

The third-order energy correction may be easily calculated if the first-order wave function $F^{(1)}(z, \rho)$ is known. $F^{(1)}(z, \rho)$ satisfies the inhomogeneous differential equation

$$[H_1(\rho) + H_2(z) - E_0]\, F^{(1)}(z,\rho) = (E_1 - V)\, F^{(0)}(z,\rho)\,, \tag{8}$$

where $F^{(1)}(z, \rho)$ and $F^{(0)}(z, \rho)$ satisfy the boundary conditions (2). We represent $F^{(1)}(z, \rho)$ in terms of a series expansion using the basis $\{f_{mn}(\rho) g_k(z)\}$. Here $f_{mn}(\rho)$ are the exact functions for Landau's states [7] which are orthonormalized without weight function ρ, and $g_k(z)$ are the eigenfunctions of H_2 in the FD approximation. The same approach was used earlier for the solution of the atomic pair radial equations [6] and yielded very accurate results. The eigenvalue problem for the H_2 operator takes the form

$$[-0.5\, \partial^2/\partial z^2 - Z/(\rho_m^2 + z^2)^{1/2}]\, f_k(z) = \epsilon_k f_k(z)\,, \tag{9}$$

$$f_k(\infty) = f_k(-\infty) = 0\,. \tag{10}$$

To apply the FD approximation to eq. (9) we replace the infinite domain of $f_k(z)$ by a finite one by introducing the new variable x ($-\frac{1}{2}\pi < x < \frac{1}{2}\pi$),

$$x = \operatorname{arctg}(\alpha z)\,. \tag{11}$$

We divide the interval $(-\frac{1}{2}\pi, \frac{1}{2}\pi)$ by $N + 2$ internal points into $N + 3$ equal parts. The functions $f_k(z)$ are equal to zero in the points $x = \pm\frac{1}{2}\pi$ due to the boundary conditions. By appropriate choice of the parameter α in eq. (11) we make the unknown functions negligible at the first and the last internal points. Such a condition enables us to use without any difficulties the fourth-order FD approximation for the second derivative operator

$$f''(i) = \tfrac{1}{12} h^{-2}[-f(i-2) + 16f(i-1) - 30f(i) + 16f(i+1) - f(i+2)]\,. \tag{12}$$

Here $f(i)$ is the value of the function f at the ith grid point, h is the step of the FD scheme. Using eq. (12) we reduce the problem (9), (10) to the eigenvalue problem for an $N \times N$ five-diagonal matrix. Given the eigenvectors of this matrix, the coefficients of the series expansion of $F^{(1)}(z, \rho)$ may be easily calculated. Thus the first-order correction for the wave function with quantum numbers m, n, k includes the function $f_{mn}(\rho)\, g_k(z)$ with the coefficient

$$C^{mnk}_{n'k'} = V^m_{nk,n'k'}/(E^0_{nk} - E^0_{n'k'})\,, \tag{13}$$

where

$$V^m_{nk,n'k'} = \langle f_{mn'}(\rho)\, g_{k'}(z) | V | f_{mn}(\rho)\, g_k(z) \rangle\,. \tag{14}$$

A simple trapezoidal rule must be used to perform the integration over the z variable in (14). The integration over ρ is performed using Gauss–Laguerre formulae. To increase the accuracy we use Richardson's extrapolation [5]. This procedure includes the solution of the problem for several h values and the extrapolation to $h = 0$. We take the h-dependence of the energy in the form

$$E(h) = E + E'h^4 + E''h^6 + \ldots\,. \tag{15}$$

The energy depends also on the knot number n in the Gauss–Laguerre quadrature formula:

$$E(1/n) = E + (1/n)\, E' + (1/n)^2 E'' + \ldots\,. \tag{16}$$

This enables us to put $n \to \infty$.

The method described was used to calculate the ionisation potentials for the ground and several excited states of the H-atom in a wide range of magnetic fields. The results are listed in table 1. To obtain these results a series of grids with $N = 50, 60, 70, 80$ and the quadrature formula with $n = 38, 40, 42$ were used. The obtained results are in good agreement with the best values known up to date. The most significant error in our results is due to a nonoptimal distribution of the grid points in the z-variable. It may be reduced by a suitable choice of the transformation (11). We did not use this possibility because the accuracy of the obtained results is quite sufficient in the frame of the employed approximation. In other words, the corrections to the energy from the motion of the nucleus

Table 1
Ionisation energies (in au) for several states of the H-atom in a magnetic field B (in units of B_0). m, n, k are the quantum numbers characterising the states of the H-atom in a magnetic field and showing from which states of the zero-order hamiltonian they are generated.

n	m	k	B				
			2 [a]	2	20	200	2000
0 [a]	0	1		1.022	2.215 3 4	4.727 0 3	9.304 67 10
0	0	1	1.022 21	1.014 32	2.214 46	4.729 04	9.274 05
0	0	2	0.297 70	0.297 50	0.413 35	0.476 54	0.495 63
0	0	3	0.174 03	0.174 08	0.223 79	0.267 84	0.300 72
0	0	4	0.096 94	0.096 82	0.114 05	0.122 13	0.121 76
0	−1	1	0.599 59	0.599 28	1.465 46	3.347 15	6.951 80
0	−1	2	0.245 27	0.245 21	0.376 12	0.461 82	0.492 20
0	−1	3	0.142 54	0.142 47	0.198 86	0.248 97	0.289 81
0	−1	4		0.087 28	0.108 85	0.120 28	0.121 22
0	−2	1	0.471 22	0.471 12	1.193 62	2.802 02	5.968 63
0	−2	2		0.217 44	0.352 19	0.450 58	0.489 29
0	−2	3		0.128 68	0.186 37	0.238 47	0.282 18
0	−2	4		0.081 66	0.105 33	0.118 86	0.120 77

[a] The results in the first column and in the first row were obtained in refs. [3] and [4], respectively.

and relativistic effects are expected to be larger than the errors in our results.

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