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PERTURBATIVE APPROACH TO THE HYDROGEN ATOM IN A STRONG MAGNETIC FIELD

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We consider states of the hydrogen atom with the principal quantum number $n \leq 3$ and zero magnetic quantum number in a constant homogeneous magnetic field $\mathcal{H}$. The perturbation theory series is summed using the Borel transformation and conformal mapping of the Borel variable. Convergence of the approximate energy eigenvalues and their agreement with the corresponding existing results are observed for external fields up to $n^3\mathcal{H}/\mathcal{H}_0 \sim 5$, where $\mathcal{H}_0$ is the atomic magnetic field. The possibility of restoring the asymptotic behavior of energy levels using perturbation theory coefficients is also discussed.

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The own magnetic fields of some astrophysical objects reach very high values [1, 2]. If we are interested in the atomic spectra in these external fields, it is convenient to introduce the natural measure of field strength, the atomic magnetic field

$$\mathcal{H}_0 \equiv \frac{e^3m^2c}{\hbar^3} = 2.55 \cdot 10^9 \text{ G}.$$

The fields $\mathcal{H}$ up to one half of $\mathcal{H}_0$ are detected in the vicinity of some white dwarves. Neutron stars possess fields up to the order of $10^4\mathcal{H}_0$. For the correct interpretation of the observation results, it is desirable to know the atomic hydrogen spectrum in this range of external fields. For this aim, computations based on the adiabatic approach with a Landau level as the initial approximation were performed [3]. In what follows, we show which part of the desired external field range can be covered using the standard expansion in powers of $\mathcal{H}$, starting from the Coulomb levels of the hydrogen atom. The computation involves many orders of the perturbation theory (up to the 75th order). Summation of the series is performed using the Borel transformation supplemented by a conformal mapping of the Borel variable.

The Borel summation method was introduced into quantum field theory relatively long ago (see, e.g., [4]). It has been tested on some quantum-mechanical problems (one of the numerous examples is described in [5]) and is still applied in modern works [6]. Great hopes of the possibility to advance into the strong-coupling region were related with the Borel summation of the perturbation series. Some rather simple problems where the details can be traced and compared with the corresponding exact results supported this optimism. For example, for the funnel potential

$$V(r) = -\frac{1}{r} + gr,$$

applying a conformal mapping of the Borel variable and Padé summation of the Borel transformant gives the ground state energy as $g \to \infty$ in the form

$$E(g) = Cg^\nu$$

with the precision about 0.2 % for the index ν and about 5 % for the coefficient C [5]. It became clear later that such a successful summation presents a special but not the general case. We can guess that this success is a consequence of simplicity of this problem. In contrast, the asymptotic behavior of energy levels in the Stark and Zeeman effects establishes at very large values of the external fields. For the Stark effect, it is now practically impossible to reach the region of the truly asymptotic behavior by perturbation series summation. An intermediate linear asymptotic behavior is observed instead [7, 8].

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To introduce the notation and the scale, we write the Hamiltonian

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r} + \frac{1}{8}g(r^2 - z^2) \equiv \hat{H}_0 + g\hat{H}_1, \qquad (1)$$

where $g \equiv \mathcal{H}^2/c^2$ and we use the atomic units $\hbar = m = e = 1$ hereafter. In (1), we drop the elementary contribution of the electron spin and consider only states with the magnetic quantum number $m \equiv 0$. We can expand $E(g)$ as a formal power series in g,

$$E(g) = \sum_{k=0}^{\infty} E_k g^k. \qquad (2)$$

We must then obtain hypersusceptibilities E_k. We can use the moment method for this aim. This method is especially useful in the cases where variables cannot be separated in the Schrödinger equation. Obviously, the Zeeman effect is precisely such a problem. In the previous work [9], the moment method was applied to the recurrent evaluation of hypersusceptibilities. A somewhat different version of the moment method was introduced in [10].

For the lower four «isolated» hydrogen levels, we immediately use the results of Ref. [9]. Unfortunately, the computer code employed in [9] for the relatively more complicated case of degenerate $3s$ and $3d$ states contained a mistake[1)]. We therefore performed a new computation of the $3s$ and $3d$ hypersusceptibilities. Results of the computation for some orders are presented in Table 1. These results are in agreement with results in [11], where high-order hypersusceptibilities were obtained for the first time (but the method used in [11] is much more complicated than the moment method).

As the order k increases, hypersusceptibilities grow as a factorial [12],

$$E_k \to \tilde{E}_k = (-1)^{k+1} C_{nl} a_n^k \Gamma(2k + \beta_{nl}), \qquad (3)$$

where

$$a_n = \left(\frac{n^2}{\pi}\right)^2, \quad \beta_{nl} = 2n - 1 + \frac{(-1)^l}{2},$$

and C_{nl} are not essential for us; their values can be found in [9] and references therein. Equation (3) implies that series (2) is asymptotical, and the formal sum of such a series is therefore ambiguous. But the choice of the summation method is in fact restricted: from physical considerations, the function $E(g)$ must have analytical properties that are to be reproduced by the true sum of series (2). In the unphysical region $g < 0$, the diamagnetic perturbation $g\hat{H}_1$ changes its sign, the total Hamiltonian becomes «open», and the possibility of a spontaneous ionization of the atom emerges. The energy eigenvalue must therefore have an imaginary part at $g < 0$ and the function $E(g)$ must have a cut along the negative real semiaxis in the g plane. Summation using the Borel transformation results in a function that has the left cut and is a smooth function of g except for the discontinuity at this cut.

The Borel transformant $B(w)$ of $E(g)$ is a series

$$B(w) = \sum_{k=0}^{\infty} B_k w^k \qquad (4)$$

with the coefficients

$$B_k = E_k/\Gamma(2k + b_0),$$

where b_0 is an arbitrary constant. The choice of b_0 can in principle affect the numerical results, but because changing its value within the interval about $0.5 \le b_0 \le 5$ has a weak effect, we fixed b_0 by convenience. The numerical calculations in this work were performed at $b_0 = 3$. Series (4) converges, as usual, inside the circle $|w| < 1/a_n$. Substituting asymptotic

Table 1. Hypersusceptibilities of degenerate states

k	E_k *for 3s state*
1	19.578514767111954772299244883 94
2	−7992.558488642566993349104381687
3	9951240.466276842310264046307800
4	−20931559882.53444368634980579917
5	58826900682409.79349115290157121
25	$1.37932338518206094144637879132 15 \cdot 10^{94}$
50	$-9.32271326968896166177886769035 16 \cdot 10^{211}$
75	$2.80535339708117043265749308311 76 \cdot 10^{340}$
k	E_k *for 3d state*
1	5.171485232888045227700755116050
2	−1017.425886357433006650895618312
3	738127.824738782689735953692 1995
4	−923576528.554411294118944200 8231
5	1677908319019.727217770438272530
25	$1.04312177717586140118123118583 95 \cdot 10^{92}$
50	$-6.07219785614468843000727265530 11 \cdot 10^{209}$
75	$1.73025529950554326807310876350 37 \cdot 10^{338}$

[1)] We are thankful to Prof. V. D. Ovsyannikov for drawing our attention to this mistake.

coefficients $\tilde{E}_k$ for E_k, it is easy to verify that the singularity of $B(w)$ is located at $w = -1/a_n$. The energy of the level is related to the function $B(w)$ by the integral transformation

$$E(g) = \int_0^\infty e^{-x} B(gx^2) x^{b_0 - 1} dx. \tag{5}$$

For the numerical integration in the right-hand side to be successful, $B(w)$ must be analytically continued from its convergence disk to the domain containing the image of the entire positive real w semiaxis. For this, we performed a conformal mapping of the Borel variable w. Many sufficiently effective versions of this mapping are appropriate. The main point is that the nearest singularity of the Borel transformant must be removed to infinity. We used the mapping

$$y = \frac{a_n w}{1 + a_n w} \tag{6}$$

that was employed in [6]. As explained in [6], this transformation is optimal in the sense that it diminishes the influence of all possible singularities of $B(w)$ from the unphysical region. Transformation (6) is equivalent to the following series rearrangement:

$$\begin{aligned} B(w) &= \sum_{m=0}^{\infty} D_m y^m, \quad D_0 = B_0, \\ D_m &= \sum_{k=1}^{m} \frac{(m-1)!}{(k-1)!(m-k)!} \frac{B_k}{a^k}, \quad m \geq 1. \end{aligned} \tag{7}$$

To improve convergence, we applied the Padé summation to rearranged series (7),

$$B(w) \approx [M/N]\,(y) \equiv \frac{P_M(y)}{Q_N(y)}, \tag{8}$$

where P_M and Q_N are polynomials of the respective degrees M and N.

We performed computations using various Padé approximants and a straightforward summation of rearranged series (7). To illustrate the effect of computational accuracy on summation results, we compared those done with double precision (16 decimal digits) and quadruple precision (32 decimal digits).

Some graphs of the obtained binding energy

$$\mathcal{E}(\gamma) = \frac{1}{2}\gamma - E(\gamma^2)$$

as a function of the parameter $\gamma \equiv n^3\mathcal{H}/c$ are given in Figs. 1–3. Compared with the previous work [9], the region of external field values for which these eigenvalues are successfully recovered is extended by a factor of about 5. As usual, the precision of the sum considerably increases at lower $\mathcal{H}$ values. The accuracy of the summation method described above is illustrated in Table 2.

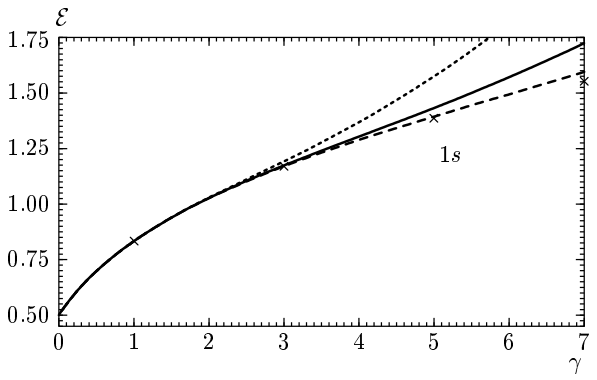

Fig. 1. Binding energy for the $1s$ state in atomic units. The data is evaluated with the double precision (using the Padé approximant [30/30], solid curve, and by straightforward summation, dotted curve) and with the quadruple precision (using the Padé approximant [30/30], dashed curve). Crosses denote the data in Ref. [13]

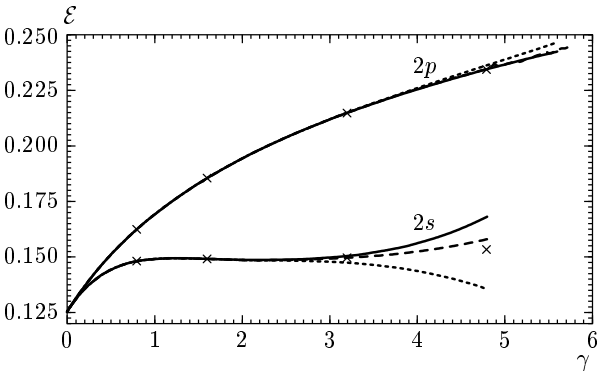

Fig. 2. Binding energy for the $2s$ and $2p$ states in atomic units. Notation is the same as in Fig. 1

We note that in [9], Padé approximants were immediately applied to summation of divergent series (2). These approximants imitate the discontinuity on the cut $g < 0$ by a set of delta functions, which is a very rough approximation. On the other hand, the same discontinuity is represented by a smooth function of g as a result of the Borel summation. Our calculations confirmed that mapping (6) is indeed very efficient: after this mapping, Padé summation of the Borel transformant improves the convergence only slightly, and its straightforward summation appears to be sufficient in some cases, see Figs. 1–3.

Table 2. Values of the binding energy for $2p$ state

$[M/N]$	$\mathcal{E}$ at $\gamma = 1.12$	[M/N]	$\mathcal{E}$ at $\gamma = 3.20$	$\mathcal{E}$ at $\gamma = 4.80$	$\mathcal{E}$ at $\gamma = 8.00$
[28/28]	0.172618226340	[30/30]	0.214270	0.23396	0.2655
[29/29]	0.172618226340	[37/36]	0.214257	0.23371	0.2612
[30/30]	0.172618226339	[37/37]	0.214265	0.23370	0.2610
[31/31]	0.172618226343				
[32/32]	0.172618226340				
Ref. [13]	0.17261822	Ref.[13]	0.2142655	0.233675	0.260006

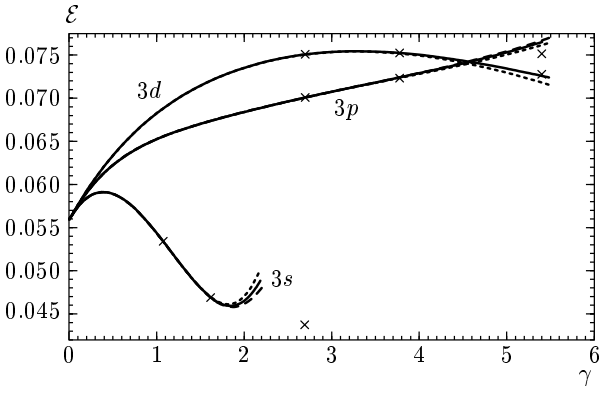

Fig. 3. Binding energy for the $3s$, $3p$, and $3d$ states in atomic units. Notation is the same as in Fig. 1

One technical detail is of principal importance for the perturbation series summation by any method. The precision of the entire chain of computations must increase as the number of the involved successive terms increases. This is simply a consequence of the fact that the sum, being of the order of unity, is the result of a compensation of very large terms with alternating signs.

At a first glance, it seems that the high-precision requirement is not necessary for the Borel transformant because all the essential alternating sign coefficients B_k have approximately the same order. But any numerical procedure of analytic continuation usually requires a high precision. Turning to series rearrangement (7), we see that binomial coefficients entering the sum for D_k change by 20 orders of magnitude (in the present case). Obviously, an enormous loss of precision occurs in performing the sum for D_k in (7). Therefore, if we want to use all B_k up to the 75th order, the precision of the B_k coefficients must be better than about 10^{-20}. In our calculations, the precision of E_k, and consequently, the precision of B_k was about 10^{-30}, and the precision of D_k therefore decreased from 10^{-30} at $k = 0$ to approximately 10^{-10} at $k = 75$.

We now turn to the problem of restoring the $E(g)$ dependence at large values of g and focus on the ground state. We first note that an interpolation expression for the ground (tightly bound) state energy was obtained in [3]. In spite of multiple anticrossings at $\gamma \leq 300$ and of the related computational complications, the fit in [3] provides precision within 10^{-3}–10^{-2} in the range $0.1 \leq \gamma \leq 10^4$.

The asymptotic form of the ground level energy at large g (equivalently, at large γ) is given by

$$E(\gamma) \to \frac{1}{2}\gamma - \frac{1}{2}\ln^2(\lambda\gamma) + \dots, \qquad (9)$$

where λ is a dimensionless constant (see, e.g., [14]). We first consider the possibility of restoring the leading term parameters in (9) — the power index and the constant multiplier — using the perturbation theory. Methods applicable to this problem are considered in [5, 6]. We note that for the asymptotic regime to establish, the leading term in (9) must be large compared with the correction term. We refer to the results in [13] (where the values of $\mathcal{E}(\gamma)$ were obtained by a variational procedure), which show that the binding energy is less than 20 % of $(1/2)\gamma$ only if $\gamma > 10^2$. We can therefore speculate about restoring the asymptotic parameters only if we succeed in summing $E(g)$ in this region of external fields. But we failed to do this using only 75 coefficients E_k, and the linear asymptotic behavior could not therefore be restored. This was confirmed in our attempts to apply the methods proposed in [5, 6]: no plausible result was obtained. In the method in [6], parameters of the asymptotic form of $E(g)$ are related to the large-k behavior of the coefficients D_k. Namely, if $E(g) \to Cg^\nu$ as $g \to \infty$, we obtain similarly to [6] that

$$D_k \to \frac{Ck^{\nu-1}}{a_n^k \Gamma(\nu)\Gamma(2\nu + b_0)}.$$

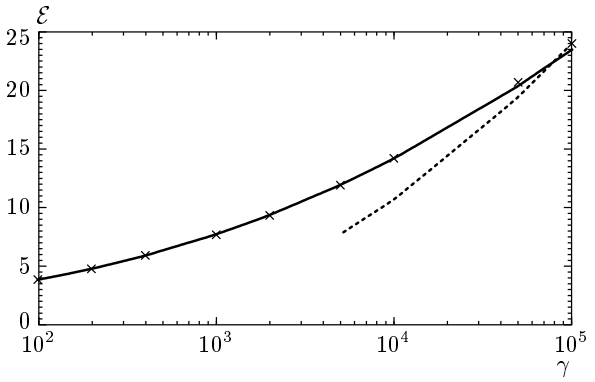

Fig. 4. Binding energy and its asymptotic form. The solid curve is plotted using Eq. (6) in Ref. [3]. Crosses denote the data in Ref. [13]. The dotted curve is the logarithmic asymptotic behavior with $\lambda = 0.010$

It was then suggested to perform the fit of C and ν using the known D_k coefficient and their errors by means of the χ^2 method. But in our case, the value of χ^2 at its minimum is extremely large (about 10^8 even if we try to fit only 5 coefficients D_k at the statistical error $\sigma = 10^{-10}$, and we have no reason to increase this value of σ). This result indicates that the asymptotic regime of D_k establishes at values of k much larger than 75.

The power index in the asymptotic form of $E(g)$ could also be traced using the method in [5]. This method consists in taking the limit of the expression $wB'(w)/B(w)$ as $w \to \infty$ (or equivalently, the limit of $y(1-y)B'(y)/B(y)$ as $y \to 1$), which gives the exact value of ν. But numerical calculation showed that we did not obtain a reasonable precision for the limit value in the region where $B(y)$ was recovered (for y close to 1, the error must obviously increase because of a finite number of D_k used).

It thus appears to be impossible to obtain asymptotic parameters corresponding to a Landau level on the base of all the known perturbation theory coefficients. Nevertheless, taking all possible information into account (including that contained in the interpolation formula [3] and the variational calculation results [13]), it is natural to raise the question whether it is possible to subtract the Landau level energy from the «exact» function $E(g)$ and trace the second term of the asymptotic expression. In other words, at which external field values does the logarithmic term in Eq. (9) become noticeable? An illustration to the answer is given in Fig. 4, where we plotted the binding energy and its logarithmic asymptotic form. The constant λ is chosen such that the value of the logarithmic term $(1/2)\ln^2(\lambda\gamma)$ in the asymptotic expression coincides with the data in [13] at $\gamma = 10^5$. This occurs at $\lambda = 0.01$ and the smallness of this constant indicates that the value of γ is too small for speaking about the asymptotic regime. We can see that the asymptotic curve and the curve of exact data have considerably different slopes.

Thus, for the Zeeman effect, perturbation theory does not allow recovering even the linear part of the ground state energy asymptotic behavior in a strong field and the logarithmic term becomes essential at huge fields beyond the neutron star range.

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