Perturbative approach to the hydrogen atom in strong magnetic field

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Abstract

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

The own magnetic fields of some astrophysical objects reach very high values [1, 2]. If we are interested of the atomic spectra in these external fields, it is convenient to introduce natural measure of field strength – the atomic magnetic field $\mathcal{H}_0 \equiv e^3 m^2 c / \hbar^3 = 2.55 \times 10^9$ G. The fields $\mathcal{H}$ up to one half of $\mathcal{H}_0$ are detected in vicinity of some white dwarfs. Neutron stars possess fields up to $\sim 10^4 \mathcal{H}_0$. For correct interpretation of the observations results it is desirable to know the atomic hydrogen spectrum in this range of external fields. For this aim, computations based on adiabatic approach with Landau level as initial approximation were accomplished [3]. It will be shown here which part of the desired external field range could be covered with the help of the usual expansion in powers of $\mathcal{H}$, starting from the Coulomb levels of hydrogen atom. We involved in the computations many orders of perturbation theory (up to 75th order). Summation of the series was performed with the help of Borel transformation, supplemented by conformal mapping of Borel variable.

The Borel summation method was introduced into quantum field theory long enough (see e.g. [4]). It has been tested on some quantum-mechanical problems (one of many examples is described in [5]) and continues to find applications in modern works [6]. Large hopes on the possibility to advance into strong coupling region were related with Borel summation of the perturbation series. Some rather simple problems, in which details can be traced and compared with corresponding exact results, supported this optimism. For example, for the funnel potential, $V(r) = -1/r + gr$, by applying conformal mapping of the Borel variable and Padé-summation of the Borel transformant, the ground state energy at $g \to \infty$ was obtained in the form $E(g) = C g^\nu$ with $\sim 0.2 \%$ precision for index $\nu$ and $\sim 5 \%$ precision for coefficient $C$ [5]. It became clear later that such a successful summation presents a special but not the general case. One can guess that this success is a consequence of simplicity of this problem. In contrast, asymptotic behaviour of energy levels in Stark and Zeeman effects comes into action at very large external fields values. For the Stark effect it is practically impossible now to reach the region of true asymptotic by perturbation series summation. An intermediate linear asymptotic is observed instead [7, 8].

To introduce notations and scale we write down the Hamiltonian

$$ H = -\frac{1}{2} \nabla^2 - \frac{1}{r} + \frac{1}{8} g (r^2 - z^2) \equiv \hat{H}_0 + g \hat{H}_1. \quad (1) $$
Here $g \equiv \mathcal{H}^2$, and hereafter we use units $\hbar = c = m = e = 1$. In (1) we drop the elementary contribution of electron’s spin and consider only states with magnetic quantum number $m \equiv 0$. We can expand $E(g)$ as a formal series in powers of $g$:

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

Now, we have to obtain hypersusceptibilities $E_k$. We could use the moment method for this aim. This method is especially useful in the cases when variables in the Schrödinger equation cannot be separated. Obviously the Zeeman effect presents just such a problem. In the previous work [9] the moment method was applied to recurrent evaluation of hypersusceptibilities. Somewhat different version of the moment method was introduced in the work [10].

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

### Table 1

| $k$ | $E_k$ for 3s state | $E_k$ for 3d state |
|-----|-------------------|-------------------|
| 1   | 19.57851476711195477229924488394 | 5.17148523288045227700755116050 |
| 2   | -7992.558488642566993349104381687 | -1017.42588635743300665085618312 |
| 3   | 9951240.466276842310264046307800 | 738127.824738782689735936921995 |
| 4   | -2093155982.53444368634980579917 | -923576528.554411294118944208231 |
| 5   | 58826900682409.79349115290157121 | 1677908319019.727217770438272530 |
| 25  | 1.3793233851820609414463787913215 $\times 10^{94}$ | 1.0431217771758614011812311858395 $\times 10^{92}$ |
| 50  | -9.322713269889616617788676903516 $\times 10^{211}$ | -6.0721978561446884300072726553011 $\times 10^{209}$ |
| 75  | 2.805353970811704326574930831176 $\times 10^{340}$ | 1.7302552995055432680731087635037 $\times 10^{338}$ |

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

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

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1We are thankful to Prof. V. D. Ovsyannikov for drawing our attention to this mistake.
where \( a_n = (n^2/\pi)^2, \beta_{nl} = 2n - 1 + \frac{(-1)^l}{2}, \) and \( C_{nl} \) are not essential for us; one can find values of them in [9] and references therein. Eq. (3) implies that series (2) is asymptotical and the formal sum of such a series is ambiguous. But in fact the choice of the summation method is restricted: physical considerations impose analytical properties of the function \( E(g) \), which the true sum of series (2) is to reproduce. In the unphysical region, at \( g < 0 \), 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 appears. Therefore energy eigenvalue should have imaginary part at \( g < 0 \) and the function \( E(g) \) should have a cut along real negative semi-axis of \( g \) plane. Summation with the help of Borel transformation results in a function having the left cut, besides the discontinuity on this cut is a smooth function of \( g \).

The Borel transformant \( B(w) \) of function \( E(g) \) is a series with coefficients \( B_k = E_k/\Gamma(2k + b_0) \):

\[
B(w) = \sum_{k=0}^{\infty} B_k w^k,
\]

(4)

where \( b_0 \) is an arbitrary constant. The choice of \( b_0 \) can affect, in principle, on the numerical results, but changing of its value within interval \( \sim [0.5 \leq b_0 \leq 5] \) reveals weakly, so the choice of \( b_0 \) was made rather by convenience. The numerical calculations in this work were performed at \( b_0 = 3 \). The series (4) converges, as usual, within the circle \( |w| < 1/a_n \). It is easy to check that the singularity of \( B(w) \) is located at \( w = -1/a_n \), substituting asymptotical coefficients \( \tilde{E}_k \) in place of \( E_k \). Energy of the level is related with the function \( B(w) \) by an integral transform

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

(5)

For the numerical integration in the right hand side to be successful, an analytical continuation of \( B(w) \) from its convergence circle on the domain, containing the image of the entire real positive \( w \) semi-axis is required. For this aim we performed 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 should be removed to infinity. Here we used the mapping

\[
y = \frac{a_n w}{1 + a_n w}
\]

(6)

which was employed in the work [9]. As is explained in [9], 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

\[
B(w) = \sum_{m=0}^{\infty} D_m y^m, \quad D_0 = B_0, \quad D_m = \sum_{k=1}^{m} \frac{(m-1)!}{(k-1)!(m-k)!} a_k^k, \quad m \geq 1.
\]

(7)

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

\[
B(w) \approx [M/N](y) \equiv P_M(y)/Q_N(y),
\]

(8)

where \( P_M \) and \( Q_N \) are polynomials of degree \( M \) and \( N \) respectively.

We performed computations using various Padé approximants and straightforward summation of the rearranged series (7). To illustrate the influence of computational accuracy on summation results we compared ones made in double precision (16 decimal digits) with these in quadruple precision (32 decimal digits).

Some graphs of the obtained binding energy \( \mathcal{E}(\mathcal{H}) = \frac{1}{2} \mathcal{H} - E(\mathcal{H}^2) \) as a function of parameter \( \gamma \equiv n^3\mathcal{H} \) are given in Figs. 1-3. As 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. For instance in the case of $3d$ state with the help of approximants $[N/N](\gamma)$ in the range $27 \leq N \leq 32$ we get binding energies with 4 stable decimal digits at $\gamma = 4$, with 6 digits at $\gamma = 3$ and with 12 digits at $\gamma = 1$. Note that in the work [3] Padé approximants were applied immediately to summation of divergent series (2). These approximants imitate the discontinuity on the cut $g < 0$ by a set of delta-functions, and it is a very rough approximation. At the same time as a result of Borel summation the same discontinuity is represented by a smooth function of $g$. Our calculations confirmed that mapping (6) is indeed very effective: after this mapping Padé summation of the Borel transformant improves the convergence only a little and for some cases its straightforward summation appears to be sufficient – see Figs. 1-3.

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

It seems at first sight that the requirement of high precision is not necessary for the Borel transformant: all essential alternating sign coefficients $B_k$ have about the same order. But any numerical procedure of analytical continuation usually requires high precision. Turning to series rearrangement (7) we see that binomial coefficients entering the sum for $D_k$ are changing 20 orders of magnitude (in the present case). Obviously, we have enormous loss of precision performing the sum for $D_k$ in (7). Therefore, if we want to use all $B_k$ up to 75th order, the precision of $B_k$ coefficients should be better than $\sim 10^{-20}$. In our calculations, the precision of $E_k$ and, consequently, the precision of $B_k$ was $\sim 10^{-30}$, so the precision of $D_k$ was decreasing from $10^{-30}$ at $k = 0$ to about $10^{-10}$ at $k = 75$.

Let us turn now to the problem of restoring of the $E(g)$ dependence at large $g$ values. We shall focus on the ground state. First of all we note that in work [3] an interpolation expression for the ground (tightly bound) state energy was obtained. In spite of the multiple anticrossings at $\mathcal{H} \leq 300$ and of the related computations complicating, the fit of [3] provides precision within $10^{-3} \div 10^{-2}$ in the range of $\mathcal{H}$ values $0.1 \leq \mathcal{H} \leq 10^4$.

The ground level energy asymptotic at large $g$ (or, the same, at large $\mathcal{H}$) is given by

$$E(\mathcal{H}) \to \frac{1}{2} \mathcal{H} - \frac{1}{2} \ln^2 (c\mathcal{H}) + ...$$

(see, for example, [14]). Here $c$ is a dimensionless constant. First, we consider the possibility of restoring of the leading term parameters in (9) – the power index and the constant multiplier – using perturbation theory. Methods applicable to this problem are considered in [3, 4]. Note that for coming of the asymptotic into action the leading term in (9) should be large comparing with the correction term. One can look, for example, at the results of work [13] (where the values of $E(\mathcal{H})$ were obtained by variational procedure) and ensure that only if $\mathcal{H} > 10^2$ then the binding energy will make less than 20% of $\frac{1}{2} \mathcal{H}$. So, we can speculate about restoring of asymptotic parameters only if we succeeded in summation of $E(g)$ in this region of external fields. But we failed to do this having used only 75 coefficients $E_k$, so the linear asymptotic couldn’t be restored. This was confirmed in our attempts to apply methods suggested in the works [3, 4] – no plausible result was obtained. In the method of Ref. [3], parameters of asymptotic of the function $E(g)$ were linked to behaviour of coefficients $D_k$ in dependence of their number $k$ at large $k$. Namely, if $E(g) \to Cy^\nu$ at $g \to \infty$, then in our case we get similarly to [3]

$$D_k \to \frac{Ck^{\nu-1}}{a_k^\nu \Gamma(2\nu)\Gamma(2\nu + b_0)}.$$
Then it was suggested to perform the fit of $C$ and $\nu$ using known $D_k$ and their errors by means of the $\chi^2$ method. But in our case the value of $\chi^2$ in its minimum was extremely large (about $10^8$ even if we tried to fit only 5 coefficients $D_k$ at statistical error $\sigma = 10^{-10}$, and we had no reason to increase this value of $\sigma$). This result indicates that the asymptotic of $D_k$ comes into action at values of $k$ much larger than 75.

The power index in $E(g)$ asymptotic could be traced also using the method of [3]. This method concerns of taking of the limit of the expression $\frac{wB'(w)}{B(w)}$ at $w \to \infty$ (or, the same, the limit of $\frac{y(1 - y)B'(y)}{B(y)}$ at $y \to 1$), that gives exactly the value of $\nu$. But numerical calculation showed that in the region where $B(y)$ was recovered (at $y$ close to 1 we obviously should have increasing of error due to finite number of $D_k$ used) we did not get reasonable precision for the limit value.

Fig. 4 illustrates precision of the linear asymptotic. The curve plotted represents the binding energy (we used here formula (6) of Ref. [3]) divided by Landau energy versus external field. One can see that at $H \leq 100$ error of asymptotic is more than 20%, and only at $H \sim 1000$ precision reaches level of 1%. So, it appears to be impossible to obtain asymptotic parameters corresponding to Landau level for the Zeeman effect.

Now, the question arises, whether we can subtract Landau energy from $E(H)$ and trace the second term of asymptotic. But this term doesn’t work even at $H \sim 10^5$, which the graph of Fig. 5 is to explain. We plotted there the values of binding energy, and the value of its logarithmic asymptotic. We have chosen constant $c$ in such a way, that the value of logarithmic term $(1/2) \ln^2(cH)$ of the asymptotic coincides with the data of [13] at $H = 10^5$. This occurs at $c = 0.010$ and the smallness of this constant indicates that the value of $H$ is too small for speaking about asymptotic.

And one can see that asymptotic curve and curve of exact data have considerably different slopes. It means that we have to recover dependence of the energy at the values of external fields larger than $10^5$. But it is really impossible having known only 75 coefficients $E_k$. Thus, knowledge of 75 hypersusceptibilities did not allow to restore neither parameters of the Landau asymptotic nor logarithmic asymptotic of binding energy.

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Figure 1: Binding energy for 1s state in atomic units. The data evaluated in double precision (with help of Padé approximant [30/30] – solid curve, by straightforward summation – dotted curve) and in quadruple precision (with help of Padé approximant [30/30] – dashed curve). Crosses denote the data from Ref. [13].
Figure 2: Binding energy for 2s and 2p states in atomic units. Notations are the same as in Fig. 1.

Figure 3: Binding energy for 3s, 3p and 3d states in atomic units. Notations are the same as in Fig. 1.
Figure 4: Relative precision of the linear asymptotic

Figure 5: Binding energy and its asymptotic. Solid curve is plotted using Eq. (6) from Ref. [3]. Crosses denote the data from Ref. [13]. Dotted curve is the logarithmic asymptotic with $c = 0.010$.