New summation technique for rapidly divergent perturbation series. Hydrogen atom in magnetic field

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The perturbation series for the ground state energy of the hydrogen atom in the external magnetic field is summed via the sequence transformations. The formula for the large-order behavior of the partial sums of the series is derived. From this formula a new general sequence transformation is suggested. This transformation contains free parameters that can be further optimized. It is shown that if the renormalization approach is used, the optimal choice of these parameters leads to the previously suggested Weniger transformation. © 2003 American Institute of Physics. [DOI: 10.1063/1.1541119]

I. INTRODUCTION

The hydrogen atom in a constant magnetic field is an elementary but tricky problem, and great deal of effort has been devoted to the solution of this problem (see, e.g., Refs. 1–20 and references therein). It is of special interest from the point of view of the summation of the divergent perturbation series. Searching for the solution of the Schrödinger equation,

$$\left[-\frac{\nabla^2}{2} - \frac{1}{r} + \frac{B^2}{8}(x^2 + y^2)\right]\psi = E\psi,\tag{1}$$

in the form of the Rayleigh–Schrödinger perturbation series in the powers of the intensity of the constant magnetic field B

$$E = -\frac{1}{2} + \sum_{n=1}^{\infty} E_n \left(\frac{B^2}{8}\right)^n,$$
(2)

it appears that the perturbation coefficients E_n behave for large n as¹⁻⁴

$$E_n = (-1)^{n+1} \left(\frac{4}{\pi}\right)^{5/2} \left(\frac{8}{\pi^2}\right)^n \left(2n + \frac{1}{2}\right)! (1 + O(1/n)).$$
(3)

It means that the series (2) diverges for every |B| > 0. Moreover, because of the peculiar logarithmic behavior of the energy for high magnetic fields,⁵ the series is known to be one of the most difficult summable divergent series encountered in physics. Particularly, it is known² that the series is not efficiently summed by the Padé approximants, the most widely used summation technique (see, e.g., Refs. 21–23). Some time ago a new method for the summation of the divergent series, the so-called Weniger summation, was introduced.^{24,25} This method was combined with the renormalization approach²⁶ and succesfully applied to the one-dimensional anharmonic oscillators.²⁴ Since there have been only a few attempts to sum the series for the hydrogen atom in the magnetic field,^{2,6,7} we apply the Weniger summation technique to this problem to better understand its advantages and drawbacks.

The article is organized as follows. In Sec. II, the large-order behavior of the partial sums of the series (2) is derived. On the basis of this behavior a new general sequence transformation is suggested. This transformation contains free parameters that can be further optimized. In special

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962

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cases, both previously suggested Levin^{23,27,28} and Weniger,^{24,25} sequence transformations are obtained. In Sec. III, the renormalization of the energy and the coupling constant is made. In the final section, Sec. IV, discussion of the results and a few general remarks on the sequence transformations are made.

II. SEQUENCE TRANSFORMATIONS

On the basis of some heuristic arguments we suggest in this section a new sequence transformation. We shall proceed in an intuitive way and arguments given here should serve only as a basis for more rigorous treatment.

For the sake of simplicity, we replace the coefficients E_n of the series (2) by their large-order behavior (3) and consider the partial sums of such a series

$$s_m = \sum_{n=0}^m a_n \,, \tag{4}$$

where

$$a_n = C(-1)^{n+1} \left(\frac{B^2}{\pi^2}\right)^n \left(2n + \frac{1}{2}\right)!$$
(5)

and $C = (4/\pi)^{5/2}$.

Obviously, the partial sums (4) have no limit in ordinary sense and, consequently, the sum of the series $\sum a_n$ does not exist in ordinary sense. Nevertheless, we can try to give some meaning to the sum of such a series. Namely, we can try to fit the partial sums (4) to a finite number of terms. The most natural way of doing it is to write the system of l equations

$$s_m = c_0 a_m + c_1 a_{m-1} + \dots + c_{l-2} a_{m-l+2} + s, \quad m = n - l + 1, \dots, n,$$
(6)

for *l* unknown coefficients $c_0, c_1, ..., c_{l-2}$ and *s*. As discussed below, the coefficient *s* has the meaning of the generalized sum of the series. Since the index of the coefficient a_{m-l+2} has to be greater or equal to zero, and since the smallest value of *m* is n-l+1, we take *l* as the integer part of (n+3)/2.

Now, we extend the meaning of the limit to the sequence $(-1)^{n+1}(2n+\frac{1}{2})!$. Particularly, if we say that such a sequence exhibits "regular oscillations" and its generalized limit is zero, then the divergent regular oscillations $c_i a_i$ are singled out by the transformation (6) and the remaining constant term *s* approaches with increasing *n* the generalized sum of the series $\sum_{n=0}^{\infty} a_n$.

This transformation yields nothing but Padé approximants [n,n] and [n-1,n] for *n* even and odd, respectively. This is most easily seen by transforming the system of Equations (6) to the system of equations for computing the Padé approximants, [see, e.g., Eq. (3.10) in Ref. 24].

However, the Padé summation (6) does not work efficiently enough for the series with the coefficients growing like $(-1)^n(2n)!$ (see, e.g., Ref. 2), which is also our case. The transformation (6) for such a series is not able to single out all of the regular oscillations and a more efficient method has to be found.

Let us insert the explicit form of the coefficients a_n , Eq. (5), into the system of the equations for the partial sums (6). Then, this system can be rewritten into the form

$$s_{m} = C(-1)^{m+1} (2m+1/2)! (B/\pi)^{2m} \left(c_{0} + c_{1} \frac{\pi^{2}}{B^{2} (2m-\frac{1}{2})(2m-\frac{3}{2})} + c_{2} \frac{\pi^{4}}{B^{4} (2m-\frac{1}{2})(2m-\frac{3}{2})(2m-\frac{5}{2})(2m-\frac{7}{2})} + \dots \right) + s.$$
(7)

For large m, the partial sums s_m behave as

964 J. Math. Phys., Vol. 44, No. 3, March 2003

Cížek, Zamastil, and Skála

$$s_m = C(-1)^{m+1} \left(2m + \frac{1}{2} \right)! \left(\frac{B}{\pi} \right)^{2m} \left(d_0 + \frac{d_1}{m+1} + \frac{d_2}{(m+1)^2} + \dots \right) + s,$$
(8)

where the coefficients d_i can be obtained from the coefficients c_i by expanding Eq. (7) into the asymptotic series in the powers of 1/(m+1). If we fitted the partial sums s_m to the infinite number of the coefficients c_i or d_i , there would be no difference between the sequences (7) and (8). However, if we fit the partial sums s_m to a *finite* number of the coefficients c_i or d_i , the sequence transformation (8) accounts better for the large-order behavior of the partial sums s_m than the transformation (7).

On the basis of these considerations we suggest a new generalized sequence transformation

$$s_{m} = a_{m} \left(d_{0} + \frac{d_{1}}{(m+q_{1})} + \frac{d_{2}}{(m+q_{1})(m+q_{2})} + \dots + \frac{d_{l-2}}{(m+q_{1})(m+q_{2})\dots(m+q_{l-2})} \right) + s,$$

$$m = n, \dots, n+l-1,$$
(9)

where q_i , i = 1, 2, ..., l-2, are arbitrary coefficients that have to be determined from some additional requirement and *n* denotes the index of the first partial sum taken into account. In principle, it can be arbitrary; however, for fast convergence of the method it is convenient to take it close, but not necessarily equal, to zero (see below).

Equations (9) represent a system of l equations for l unknowns d_0, d_1, \dots, d_{l-2} and s. It is remarkable that, regardless of the particular form of the coefficients q_i , the system of equations (9) can be solved in the closed form, namely

$$s = s_n + \frac{\sum_{j=0}^{l-1} (-1)^j [(l-1)!/(l-1-j)!j!] \prod_{i=1}^{l-2} (j+n+q_i)(s_{j+n}-s_n)/a_{j+n}}{\sum_{i=0}^{l-1} (-1)^j [(l-1)!/(l-1-j)!j!] \prod_{i=1}^{l-2} (j+n+q_i)1/a_{j+n}}.$$
 (10)

This can be interpreted that the sum of the series is the *n*th partial sum plus a correction involving partial sums of higher order. This result, which is the main result of this article, was derived by generalizing the procedure for derivation of the Levin²³ and Weniger²⁴ transformations. In special cases $q_i = 1$ and $q_i = i$, the Levin and Weniger transformations are obtained, respectively.

III. RENORMALIZATION

In this section, the renormalization of the energy and the coupling constant is discussed.

Proceeding similarly as in Ref. 26, we make the scaling transformation $x \rightarrow (1-\kappa)x$, $y \rightarrow (1-\kappa)y$ and $z \rightarrow (1-\kappa)z$. Equation (1) then becomes

$$(1-\kappa)^{-2} \left[-\frac{\nabla^2}{2} - \frac{1-\kappa}{r} + \frac{B^2}{8} (1-\kappa)^4 (x^2 + y^2) \right] \psi = E \psi.$$
(11)

Introducing the renormalized coupling constant κ related to the coupling constant B via the equation

$$\frac{B^2}{8} = \frac{\kappa}{4(1-\kappa)^4} \tag{12}$$

and the renormalized energy E_R

$$E_R(\kappa) = (1 - \kappa)^2 E(B) \tag{13}$$

we get from Eq. (11)

TABLE I. The energies *E* obtained by the summation of the ordinary series for the hydrogen atom in the magnetic field. The sequence transformation (10) for Weniger $(q_i=i)$ and quadratic $(q_i=i^2)$ choices of the coefficients q_i and the Padé approximants are compared. Only the numbers stabilized for *l* from 70 to 79 in Eq. (10) are displayed. The constant *n* in Eq. (10) was set to zero. "-" means that no stabilization was achieved.

В	Weniger	Quadratic	Padé [39,40]	Padé [39,39]
0.6	-0.4274622877	-0.427462287	-0.4274619	-0.4274626
1.0	-0.33116	-0.331168	-0.33105	-0.33128
2.0	-	-0.0221	-0.00648	-0.03868

$$\left[-\frac{\nabla^2}{2} - \frac{1}{r} + \kappa \left(\frac{x^2 + y^2}{4} + \frac{1}{r}\right)\right] \psi = E_R \psi.$$
(14)

The advantages of the renormalization approach were discussed in detail in Refs. 24, 26, and 29–32 and can be summarized as follows. First, the originally unbounded interval of the magnetic fields $B \in (0,\infty)$ is shrunk to the interval $\kappa \in (0,1)$. Second, in contrast to the ordinary energy E, the renormalized energy E_R remains finite at the point $\kappa = 1$ corresponding to $B \rightarrow \infty$. The constant 4 in the denominator of Eq. (12) is the result of the optimization procedure suggested in Ref. 26.

The renormalized energy $E_R(\kappa)$ can be expanded into the power series in the coupling constant κ ,

$$E_{R} = -\frac{1}{2} + \sum_{n=1}^{\infty} b_{n} \kappa^{n}.$$
 (15)

Proceeding analogously to Refs. 32 and 33 we find that the coefficients b_n behave for large n as

$$\lim_{n \to \infty} \frac{b_n}{E_n} = \frac{1}{4^n}.$$
(16)

Therefore, the rate of the divergence of the coefficients b_n , although somewhat milder, is essentially the same as that of the coefficients E_n .

IV. RESULTS AND DISCUSSION

In this section, we discuss the application of the sequence transformation (10) to the series (2) and (15).

The perturbation coefficients E_n and b_n can be calculated either by using the so(4,2) algebraic formulation of the perturbation theory^{2,10} or the Bender–Wu difference equation method described in Appendix D of Ref. 2. We calculated 80 coefficients E_n and b_n in the rational form using MAPLE. The coefficients a_j in Eq. (10) were set to $a_j = E_{j+1}B^{j+1}$ or $a_j = b_{j+1}\kappa^{j+1}$ for j= 0,1,2... and the partial sums s_j were calculated via Eq. (4). The zeroth-order coefficient $-\frac{1}{2}$ was added to the sum s at the very end of calculations in both the ordinary and renormalized cases.

The results obtained with the sequence transformation (10) for different choices of the coefficients q_i are compared to those obtained via the Padé approximants in Tables I and II. We found, in agreement with the earlier observation made in the case of the sextic anharmonic oscillator,²⁴ that except for the fields smaller than $B \approx 0.2$ the Levin transformation ($q_i=1$) fails to sum the series (2). The same is true also in the renormalized case. To find the reason for this failure we replaced the actual values of the E_n coefficients by the values given by the large-order formula (3). In this case the Levin choice of the coefficients q_i yields the best results. Therefore, we believe that the reason for failure of the Levin transformation to sum the series (2) is that the large-order formula (3), and consequently also the large-order formula (8), is only asymptotic, i.e., holds only for a sufficiently large m. To remain valid for small values of m, the series (8) has to be truncated after few terms. The smaller m, the sooner the series (8) has to be truncated. Therefore, it is

TABLE II. The energies *E* obtained by the summation of the renormalized series for the hydrogen atom in the magnetic field. The sequence transformation (10) for different choices of the coefficients q_i and *n* is compared with the Padé approximants and the results obtained in Ref. 12 with completely different nonperturbative method. The displayed numbers are stabilized for *l* from 70 to 79 and for *l* from 65 to 74 for n=0 and n=5 respectively.

В	Weniger $(n=0)$	Quadratic $(n=0)$	Weniger $(n=5)$	Quadratic $(n=5)$	Padé	Ref. 12
0.6	-0.4274622877571	-0.42746228	-0.4274622877571	-0.42746228775	-0.427462	-0.42746227877
1.0	-0.331168896	-0.331168	-0.3311688967	-0.33116889	-0.331	-0.33116889
2.0	-0.022213	-0.0221	-0.022213	-0.02221	-0.02	-0.0222139
3.0	0.3354	0.335	0.33546	0.33548	0.33	0.33546
10.0	3.253	3.26	3.252	3.254	3.	3.252
20.0	7.79	7.8	7.78	7.8	7.	7.784

important for efficiency of the sequence transformation (9) that the contribution of the individual terms $d_i/[(m+q_1)(m+q_2)\cdots(m+q_i)]$ in Eq. (9) decreases for small *m* with increasing *i*. This is better accomplished by the Weniger choice $q_i = i$ than by the Levin choice $q_i = 1$. The decrease has to be moderate; if the growth of the coefficients q_i is too large (e.g., quadratic), the contribution of the terms $d_i/[(m+q_1)(m+q_2)\cdots(m+q_i)]$ in Eq. (9) is suppressed with increasing *i* not only for small *m*, but also for large *m*. Then we fit the partial sums s_m only to few constants d_i and the transformation (9) becomes inefficient again. This is well illustrated in Tables I and II. We see that if the coupling constant *B* or κ is sufficiently small, i.e., either the external magnetic field is small or the renormalization is made, the Weniger transformation becomes also unstable and the best result yields the quadratic choice $q_i = i^2$.

Further, we note that the efficiency of the Weniger sequence transformation with respect to the Padé approximants decreases with the increasing value of the coupling constant. Indeed, in the case of the ordinary series the Weniger transformation for the field B = 0.2 gives the result -0.49038156503476258477439474 which is by ten orders more accurate than the result produced by the Padé approximants. However, for B = 1.0, the Weniger transformation is only by two orders better than the Padé approximants (see Table I).

The results displayed in Table II show that the results of the summation depend slightly on the choice of n in Eq. (10). Particulary, it is seen that better results for the series (15) are achieved for n=5 than for n=0. The reason for it is the following. Due to the term 1/r in the interaction part of Eq. (14), the first few b_n coefficients in Eq. (15), and consequently also the first few partial sums s_n , behave irregularly (for detailed discussion see Ref. 32). Therefore, it is better to start with n around 5 when these irregularities do not play significant role.

As it is seen from Table II, the results obtained by the sequence transformation (10) agree with the results given in Ref. 12 obtained by a completely different nonperturbative method based on the rigorous Kato inequalities for the operators in the Hilbert space. The only disagreement is for the field B = 0.6. Since otherwise our results agree with these results, the result given in Ref. 12 for B = 0.6 contains probably a typographical error.

We also compared our method with the Borel summation and order dependent mapping (ODM) performed in Ref. 7. For this purpose we considered only the first 62 perturbation coefficients as in Ref. 7. The comparison shows that the Weniger method yields results of similar accuracy as the Borel summation up to the field strength B = 20.0. It is of the same accuracy as ODM up to the field strength B = 1.0. For larger fields, it yields worse results than ODM. However, it is due to the fact that we did not incorporate into our method behavior of the energy for very large magnetic fields.⁵ Moreover, the method given in this paper is both conceptually and technically simpler than those given in Ref. 7.

It is worth remarking the question whether the series (2) does uniquely define the energy $E = E(B^2)$. If the series (2) is the Stieltjes series, then it does (see, e.g., Refs. 21 and 22). In such a case, [n-1,n] and [n,n] Padé approximants provide monotonically decreasing upper bounds and monotonically increasing lower bounds to the exact eigenvalue. Moreover, if the coefficients of

the series do not grow more rapidly than $(-1)^n(2n)!$ (which is also our case), then the sequences [n-1,n] and [n,n] converge to the same value. We do not know the rigorous proof that the series (2) is a Stieltjes one. However, the numerical results indicate strongly that this is really the case. Particularly, if the zeroth term of the series is excluded, then [n,n] and [n-1,n] Padé approximants provide lower and upper bounds to the energy $E(B^2)$ (see Table I and Ref. 2). The renormalized series (15) is not the Stieltjes series. However, it was shown in Ref. 32 on an analogous problem of the one-dimensional anharmonic oscillator that the series (15) consists of a divergent Stieltjes part and a rapidly convergent part (the rate of the convergence is geometric).

Summarizing, we found in this article the large-order behavior of the partial sums of the strongly divergent perturbation series. On the basis of this behavior a new general sequence transformation containing free parameters that can be subject of further optimalization was suggested. This sequence transformation was applied to the problem of the hydrogen atom in the constant magnetic field. Numerical analysis shows that for small values of the coupling constant, the best choice of the parameters leads to the previously suggested Weniger transformation. Such small values of the coupling constant can be achieved even for large fields, by utilizing the idea of the renormalization. Although most of our discussion was restricted to the summation of the series for the ground state energy of the hydrogen atom in magnetic field, we believe that suggestions made in this article are of much broader importance. Particulary, they show that even violently diverging series behaving as $(-1)^n (2n)!$ can be summed to accurate and realiable results.

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