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New hybrid non-linear transformations of divergent perturbation series for quadratic Zeeman effects

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Abstract. The problem of hydrogen atoms in an external uniform magnetic field (quadratic Zeeman effect) is studied by means of perturbation theory. The power series for the ground-state energy in terms of magnetic-field strength B is divergent. Nevertheless, it is possible to induce convergence of this divergent series by applying various non-linear transformations, such as those of Shanks (e), Levin (t, u, v) as well as the present (ω) algorithm. These transformations of originally divergent perturbation series yield new sequences, which then converge. The induced convergence is, however, quite slow. A new hybrid Shanks-Levin non-linear transform is devised here for accelerating these slowly converging series and sequences. Significant improvement in the convergence rate is obtained. Agreement with the exact results is excellent.

The quadratic Zeeman effect, which is associated with the hydrogen atom in a uniform magnetic field, represents one of the fundamental non-separable two-dimensional problems of quantum mechanics (Ruderman 1975). A large number of methods have been used to compute the energy values of many low-lying states as functions of magnetic-field strength B (Garstang 1977, Avron *et al* 1979, Wunner *et al* 1983, Delande and Gay 1981, Clark and Taylor 1982, Cižek and Vrscay 1982). Among the most versatile are the variants of the Padé-Borel summability methods recently studied in details by Popov and Weinberg (1982) as well as by Le Guillou and Zinn-Justin (1983). However, to date the most extensive is the work of Rösner *et al* (1984) who obtained highly accurate energies from the Schrödinger variational principle. Alternative variational estimates of the exact energies can also be found from a matrix diagonalisation of the Hamiltonian in a complete Sturmian basis representation of the SO(4, 2) Lie algebra (Čižek and Vrscay 1977, Gerry and Laub 1982).

The Rayleigh-Schrödinger quantum mechanical perturbation theory represents a quite natural starting point for studying the energy spectra of an atom interacting with external static fields. Powerful algorithms have been developed for fast computation of arbitrary orders in several perturbation series (Avron *et al* 1979, Adams *et al* 1980, Vrscay 1985). With these algorithms at hand, the relevant perturbation series could be readily summed up to an arbitrary order for a given value of the external magnetic-field strength B. This cannot be accomplished, however, since addition of partial sums yields divergent results. This problem is said to be in the class of asymptotic perturbation series (Reed and Simon 1978).

The summability problem of diverging series or sequences plays an important role in rigorous calculus (Knopp 1947, Hardy 1956). There are many techniques for

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accelerating slowly converging series or even inducing convergence of some diverging expansions (Wimp 1981, Brezinski 1977). Some of these accelerators have been shown (Brezinski 1977) to be much more efficient than various Padé-type generalisations of the continued fractions which, nevertheless, received most attention in physics (Baker and Gammel 1970). In particular, the u-transform of Levin (1973) has emerged from the considerable mathematical research literature (Brezinski 1977, Blakemore *et al* 1976, Fessler *et al* 1983, Smith and Ford 1979, 1982) as one of the most useful methods but, with few exceptions (Thakkar 1978, Tanner and Thakkar 1982, Weniger *et al* 1986, Belkić and Taylor 1986, 1987, Belkić 1988), has remained virtually unexplored by physicists. It is, however, important to examine the usefulness of the non-linear Levin-type algorithms for the quantum mechanical asymptotic perturbation theories, for which the usual Padé approximant is known to be insufficient. The purpose of such an examination, which is presently carried out for the Zeeman effect as an important first illustration, is to render the perturbation theory into a practical tool for computation of atomic spectra. This systematic theory is, however, useless without suitable accelerators due to its slow convergence and/or marked divergence.

Let $\{A_n\}$ be a sequence of partial sums which converges to its limit A. Further, let F be a transformation which maps $\{A_n\}$ into another sequence $\{B_n\}$. Thus, mapping F will represent an accelerator, i.e. sequence $\{B_n\}$ converges to A faster than $\{A_n\}$ if the following necessary and sufficient condition is fulfilled: $(B_n - B)/(A_n - A) \to 0$, as $n \to \infty$. Here it is assumed that the new sequence $\{B_n\}$ also converges to the same limit $B = A$. Transformation F will be non-linear if its coefficients depend upon A, e.g. the so-called e-algorithm of Shanks (1955), who employed operators e_k to convert sequence $\{A_n\}$ into $\{B_n\}$, i.e. $e_k(A_n) = B_{k,n} (n \geq 0, n \geq k)$. The general term in the kth-order transform $B_{k,n}$ of A_n can efficiently be computed from the recursive ε-algorithm of Wynn (1956), i.e. $e_s(A_m) = \varepsilon_{2s}^{(m)}$, where

$$\varepsilon_{s+1}^{(m)} = \varepsilon_{s-1}^{(m+1)} + 1/(\varepsilon_s^{(m+1)} - \varepsilon_s^{(m)}) \qquad m, s \geq 0 \tag{1}$$

with $\varepsilon_{-1}^{(m)} = 0$, $\varepsilon_0^{(m)} = A_m$, $\varepsilon_{2s+1}^{(m)} = 1/e_s(\Delta A_m)$ and Δ is the forward difference operator: $\Delta x_j = x_{j+1} - x_j$. In applications, we shall employ the diagonal Shanks e_d-transform which is defined by $e_d(A_n) = B_{n,n}$.

When $\{A_n\}$ is the sequence of partial sums of a power series, the two-dimensional array $\varepsilon_{2s}^{(m)}$ yields the upper half of the well known Padé table. The present computation is concerned with the partial sums of power series expansions, and we shall employ Wynn's ε-algorithm (1), which is known to be stable (Wynn 1966, Blakemore *et al* 1976). Also presently studied are the non-linear Levin t, u and v transforms.

We shall hereafter be dealing with partial sums $A_n = \sum_{j=1}^{n} a_j$ of a given infinite series $\sum_{j=1}^{\infty} a_j$, where $n \geq 1$ and $A_n \to A$ as $n \to \infty$. It is assumed that sequence $\{A_n\}$ ($n \geq 1$) exhibits prohibitively slow convergence, which prevents any useful addition of partial sums in searching for the limiting value A. Straightforward addition of a_n can also lead to significant loss of accuracy due to the accumulation of round-off errors, especially for alternating series. Furthermore, the original sequence $\{A_n\}$ could be divergent, as is usually the case in quantum mechanics, and the concept of 'antilimit' should be invoked along the lines of the work of Shanks (1955). Therefore, an alternative method is sought for extracting the correct limiting value A. To achieve this goal, consider the following model sequence for $\{A_n\}$:

$$A_q = X_{k,n} + R_q \sum_{i=0}^{k-1} C_{in}/q^i \qquad q \geq n + k, k > 1 \tag{2}$$

where C_{in} are unknown coefficients and R_n is a non-zero 'estimate' of the remainder $A_n - A$. The standard application of the Vandermonde determinants will eliminate C from system (2) of $k+1$ linear equations with the final result:

$$x_k(A_n) = X_{k,n} = \left(\sum_{j=0}^{k} C_j^{kn} \frac{A_{n+j}}{R_{n+j}}\right)\left(\sum_{j=0}^{k} C_j^{kn} \frac{1}{R_{n+j}}\right)^{-1} \tag{3}$$

where $C_j^{kn} = (-k)_j[(n+j)/(n+k)]^{k-1}/j!$ and $(x)_n$ is the Pochhammer symbol, i.e. $(x)_n = x(x+1)(x+2)\ldots(x+n-1)$. The approximation to the limit A, based upon inclusion of n terms, is $X_{n,1} = x_d(A_n)$. Transforms $x_d(A_{2n})$ and $e_d(A_n)$ are not strictly analogous to each other because they contain different number of terms A_n. However, scaling $A_n \to A_{n+1}$ implies that both $x_d(A_{2n})$ and $e'_d(A_n)$ depend upon the same $2n+1$ terms $A_1, A_2, \ldots, A_{2n+1}$, where $e'_d(A_{n+1}) = e_d(A'_n)$ and $A'_i = A_{i+1} (i \geqslant 0)$. This enables direct comparisons between the numerical results obtained by means of the $x_d(A_{2n})$ and $e'_d(A_n)$ transformations. The remainder R_q is an adjustable function which, however, should fulfil the requirement $R \propto A_q - A$ up to a constant factor, which cancels in the quotient of (3). In this way, transformation $x_k(A_n)$ will represent an accelerator method for sequence $\{A_n\}$. It is seen from (3) that the general term $X_{k,n}$ of the new sequence is a weighted combination of the original A. Hence non-linear transformations are obtained from (3) by choosing the remainder R_n to be dependent upon $a_n (= A_n - A_{n-1} = \Delta A_{n-1})$.

Levin's (1973) three non-linear t, u and v transformations can all be obtained from (3) by choosing remainder R_q to be equal to a_q, qa_q and $a_q a_{q+1}/\Delta a_q$, respectively. Thus

$$t_k(A_n) = T_{k,n} = \left(\sum_{j=0}^{k} C_j^{kn} \frac{A_{n+j}}{a_{n+j}}\right)\left(\sum_{j=0}^{k} C_j^{kn} \frac{1}{a_{n+j}}\right)^{-1} \tag{4}$$

$$u_k(A_n) = U_{k,n} = \left(\sum_{j=0}^{k} C_j^{kn} \frac{A_{n+j}}{(n+j)a_{n+j}}\right)\left(\sum_{j=0}^{k} C_j^{kn} \frac{1}{(n+j)a_{n+j}}\right)^{-1} \tag{5}$$

$$v_k(A_n) = V_{k,n} = \left(\sum_{j=0}^{k} C_j^{kn} \frac{A_{n+j}}{a_{n+j}^{-1} - a_{n+j+1}^{-1}}\right)\left(\sum_{j=0}^{k} C_j^{kn} \frac{1}{a_{n+j}^{-1} - a_{n+j+1}^{-1}}\right)^{-1}. \tag{6}$$

Motivation for these selections is best seen by assuming that the Shanks e_k-transformation of the kth order is a good approximation to the limiting value. For example, the use of operator e_1 i.e. $e_1(A_q) = A_q - a_q a_{q+1}/\Delta a_q$ implies that $R_q = A_q - A = A_q - e_1(A_q) = a_q a_{q+1}/\Delta a_q$, which is the remainder of the v-transformation (6).

We shall presently improve the remainder estimate R_q by using the second-order Shanks operator, i.e. $e_2(A_q) = A_q - D_q - D'_q$, where $D_q = a_{q+1}/\Delta a_{q+1}$, $D'_q = a'_q a'_{q+1}/(a'_{q+1}a''_q - a''_{q+1}a'_q)$, $a'_q = a_q a_{q+2} - a_{q+1}^2$ and $a''_q = \Delta a_{q+1} - \Delta a_q$. Hence, choosing $R_q = A_q - A = A_q - e_2(A_q) = D_q + D'_q$ we presently obtain a new non-linear algorithm which is henceforth called the ω-transformation, i.e.

$$\omega_k(A_n) = \Omega_{k,n} = \left(\sum_{j=0}^{k} C_j^{kn} \frac{A_{n+j}}{D_{n+j} + D'_{n+j}}\right)\left(\sum_{j=0}^{k} C_j^{kn} \frac{1}{D_{n+j} + D'_{n+j}}\right)^{-1}. \tag{7}$$

In analogy to $x_d(A_n)$ we shall define $t_d(A_n)$, $u_d(A_n)$, $v_d(A_n)$ and $\omega_d(A_n)$ by $t_d(A_n) = T_{n,1}$, $u_d(A_n) = U_{n,1}$, $v_d(A_n) = V_{n,1}$ and $\omega_d(A_n) = \Omega_{n,1}$. Recursive algorithms for the t, u, v and ω transformations can all be obtained from the common equation (3) following Fessler *et al* (1983).

As an introductory illustration, let us consider the Maclaurin expansion, i.e. $I(x) = 1-1!x+2!x^2-3x^3+4!x^4-\ldots$, which is strongly divergent for every $x \neq 0$. Applying the t, u, v and ω transforms here, we have obtained a rapidly converging series, as is evident from table 1. All of these four non-linear transformations are efficient in converting divergent into convergent series for $I(1)$, and agreement with the exact result to *eight* decimal places is obtained by using only seven or eight terms. It is seen from table 1 that the present ω- and Levin v-transformations yield results which are very close to each other. The exact result $I(1) = \exp(1)E_1(1) = 0.596\,347\,361$ is available from an alternative expression in terms of exponential integral $E_1(1)$ given by Abramowitz and Stegun (1982, table 5.1). Also employed in the present computation of $I(1)$ is Wynn's ε-algorithm (1) for the computation of the diagonal Shanks e_d-transformation. This latter method is also able to induce convergence of series $I(1)$, but the exact limiting value is approached by eight terms to only two decimal places, i.e. 0.596 57 (see table 1). We shall presently attempt to enhance the rate of convergence of Shanks' sequence by submitting it to the Levin v-accelerator. The new *hybrid* Shanks-Levin non-linear transformation converges very rapidly and with inclusion of five terms reaches *nine* exact decimal places 0.596 347 361 as opposed to only two in the original Shanks sequence (see table 1). Similar conclusions are also drawn from the application of the u and ω transforms to the Shanks sequence (ε-algorithm), which is given in the seventh column of table 1. These remarkable improvements demonstrate the power of the hybrid non-linear Shanks-Levin transforms. This also indicates that

Table 1. Non-linear transformation of the Maclaurin expansion $I(x) = 1-1!x+2!x^2-3!x^3+4!x^4-\ldots$ at $x=1$. The kth partial sum is labelled by A_k with the convention $A_0 = 0$. The results of the Levin t-, u- and v-transformations are listed in the third, fourth and fifth columns, respectively. The Shanks transformation yields the sequence shown in the seventh column. The sequences in the sixth and eighth columns are due to the present ω- and hybrid-transformations, respectively. The data of our hybrid method resulted in the application of the Levin v-transformation to the Shanks sequence of the seventh column. The Shanks sequence is generated recursively by means of the ε-algorithm (1). As to the t, u, v, ω, as well as hybrid, transforms, explicit formulae (4)-(6) and their recursive analogues are presently found to yield the same result. In the actual computation of the hybrid Shanks-Levin array, the Shanks sequence is taken in double precision (32 digits), and not in the form of rounded numbers of the seventh column. Moreover, the seventh column contains only the first few elements as an illustration. To obtain the hybrid Shanks-Levin array in a general case, our program automatically generates the Shanks sequence of the required size for a given set of partial sums. The exact result $I(1) = \exp(1)$ $E_1(1) = 0.596\,347\,361$ is available from the exponential integral $E_1(1)$ as given by Levin (1973) and Abramowitz and Stegun (1982, table 5.1).

k	A_k	$t_d(A_{2k-2})$	$u_d(A_{2k-2})$	$v_d(A_{2k-2})$	$\omega_d(A_{2k-2})$	$e_d'(A_{k-1})$	Hybrid $(e-v)$
Exact: 0.596 347 361							
1	1.0						
2	0.0	0.615 384 6	0.571 428 6	0.600 000 0	0.597 561 0	0.666 666 7	0.597 302 2
3	2.0	0.596 139 0	0.595 362 8	0.595 940 3	0.596 157 5	0.615 384 6	0.596 353 3
4	−4.0	0.596 330 6	0.596 399 2	0.596 344 7	0.596 357 6	0.602 739 7	0.596 347 35
5	20.0	0.596 349 4	0.596 346 1	0.596 348 8	0.596 348 9	0.598 802 4	0.596 347 361
6	−100.0	0.596 347 2	0.596 347 28	0.596 347 2	0.596 347 2	0.597 383 4	
7	620.0	0.596 347 37	0.596 347 38	0.596 347 37	0.596 347 37	0.596 816 6	
8	−4420.0	0.596 347 362	0.596 347 360	0.596 347 362	0.596 347 362	0.596 572 1	

the original Shanks array inherently contains the exact answer in the first several terms, but is not efficient enough in making this fact transparent.

Finally, we shall return to the Zeeman effect, whose perturbation series of the ground-state energy is given by

$$E(\text{au}) = -\tfrac{1}{2} + \sum_{n=1}^{\infty} E^{(n)}(\gamma^2/8)^n. \tag{8}$$

Here, γ is the coupling constant which is, with the adoption of atomic units, equal to the magnetic-field strength B. Expansion coefficients $E^{(n)}$ have been computed to within twelve decimal places of accuracy by means of the large-order perturbation theory and the SO(4, 2) Lie algebra (Čižek and Vrscay 1977, 1982). The infinite series in (8) is markedly divergent. Direct application of Shanks e_d-transform to the original Zeeman perturbation sequence produces slowly convergent series for larger values of γ (see table 2(b)). The same is true for the Levin-type t-, u-, v- and ω-transforms. However, substantial improvement in the convergence rate is presently obtained by employing our hybrid Shanks–Levin algorithm, where the Shanks array $e_d(A_k)$ is submitted to the Levin v-transform (see tables 2(a, b)). The case with much larger values of γ covering the magnetic fields, which is of utmost importance in astrophysics (Garstang 1977, Le Guillou and Zinn-Justin 1983), has not yet been studied but certainly merits a careful investigation by hybrid-type non-linear transformations. In a test run, we have verified that the present method is also useful in other divergent quantum mechanical perturbation series (anharmonic oscillator, Stark effect, charmonium model potential, etc). The results of such a study, together with many other model sequences and series, will be reported shortly.

In conclusion, we have demonstrated that the divergent perturbation series can successfully be treated by means of the new hybrid non-linear transformations of Shanks–Levin type. These transforms are very efficient in mapping the slowly converging series into series which rapidly converge, and/or converting the divergent into convergent sequences of various functions and numbers. Universal methods for accelerating a wide general class of sequences cannot exist. Hence, it is natural to devise certain new *hybrid* transforms by *combining* the accelerators which are expedient for various types of convergence. Our investigation of the divergent series in the case of the Zeeman effect clearly illustrates that the new non-linear hybrid Shanks–Levin type transforms represent substantial improvements over both the Shanks and Levin accelerators considered separately. The hybrid Shanks–Levin non-linear accelerators significantly enhance the rate of convergence of slowly converging sequences and series. A sample of markedly diverging power series which we have investigated here is efficiently 'summed' up beyond their radius of convergence (analytic continuation). Various other combinations are possible, yielding different hybrid accelerators. For example, one could employ the Levin v-transform twice (or even more), i.e. in the first step, a given diverging series is mapped into rational approximations by means of the Levin v-transformation. This resulting sequence of v-transforms, however, may be slowly converging and, as such, could, in the second step, again be submitted to the v-algorithm of Levin. A similar procedure could be done with Levin's u- or with Brezinski's θ-transforms. Thorough numerical investigation is, however, required to select those hybrid accelerators which are useful for detailed applications in various areas of atomic and molecular physics, e.g. evaluation of multicentre integrals (Weniger *et al* 1986, Belkić and Taylor 1986, Belkić 1988), the partial wave treatment of electron–atom collisions (Whelan and Piraux 1987), etc. Further work is required to

Table 2. The Zeeman perturbation series for the ground-state energy of atomic hydrogen: $E(\text{a.u}) = -\frac{1}{2} + \sum_{n=1}^{\infty} E^{(n)}(\gamma^2/8)^n$. For details about the Shanks (e) and hybrid Shanks–Levin (e-v) transformations, see table 1. Exact results are obtained from the Schrödinger extremum variational principle by Rösner *et al* (1984) with uncertainty as to the sixth decimal place.

γ	Exact (Rösner *et al* 1984)	k	$e_d(A_k)$	k	$e_d(A_k)$	k	Hybrid (e-v)
(*a*)							
0.1	−0.497 527	1	−0.497 526	9	−0.497 526	1	−0.497 526
		2	−0.497 526	10	−0.497 526	2	−0.497 526
		3	−0.497 526	11	−0.497 526	3	−0.497 526
		4	−0.497 526	12	−0.497 526		
		5	−0.497 526	13	−0.497 526		
		6	−0.497 526	14	−0.497 526		
		7	−0.497 526	15	−0.497 526		
		8	−0.497 526	16	−0.497 526		
0.14	−0.495 198	1	−0.495 198	9	−0.495 198	1	−0.495 198
		2	−0.495 198	10	−0.495 198	2	−0.495 198
		3	−0.495 198	11	−0.495 198	3	−0.495 198
		4	−0.495 198	12	−0.495 198		
		5	−0.495 198	13	−0.495 198		
		6	−0.495 198	14	−0.495 198		
		7	−0.495 198	15	−0.495 198		
		8	−0.495 198	16	−0.495 198		
0.2	−0.490 382	1	−0.490 376	9	−0.490 382	1	−0.490 382
		2	−0.490 381	10	−0.490 382	2	−0.490 382
		3	−0.490 382	11	−0.490 382	3	−0.490 382
		4	−0.490 382	12	−0.490 382		
		5	−0.490 382	13	−0.490 382		
		6	−0.490 382	14	−0.490 382		
		7	−0.490 382	15	−0.490 382		
		8	−0.490 382	16	−0.490 382		
0.3	−0.479 187	1	−0.479 103	9	−0.479 187	1	−0.479 187
		2	−0.479 177	10	−0.479 187	2	−0.479 187
		3	−0.479 185	11	−0.479 187	3	−0.479 187
		4	−0.479 186	12	−0.479 187		
		5	−0.479 186	13	−0.479 187		
		6	−0.479 186	14	−0.479 187		
		7	−0.479 187	15	−0.479 187		
		8	−0.479 187	16	−0.479 187		
(*b*)							
0.4	−0.464 606	1	−0.464 152	9	−0.464 605	1	−0.464 605
		2	−0.464 516	10	−0.464 605	2	−0.464 605
		3	−0.464 579	11	−0.464 605	3	−0.464 605
		4	−0.464 596	12	−0.464 605		
		5	−0.464 601	13	−0.464 605		
		6	−0.464 603	14	−0.464 605		
		7	−0.464 604	15	−0.464 605		
		8	−0.464 605	16	−0.464 605		
0.5	−0.447 21†	1	−0.445 728	9	−0.447 206	1	−0.447 210
		2	−0.446 809	10	−0.447 207	2	−0.447 211
		3	−0.447 062	11	−0.447 208	3	−0.447 211
		4	−0.447 144	12	−0.447 209		
		5	−0.447 176	13	−0.447 209		

Table 2. (continued)

γ	Exact (Rösner *et al* 1984)	k	$e_d(A_k)$	k	$e_d(A_k)$	k	Hybrid $(e\text{-}v)$
		6	−0.447 191	14	−0.447 209		
		7	−0.447 199	15	−0.447 210		
		8	−0.447 203	16	−0.447 210		
0.6	−0.427 463	1	−0.423 869	9	−0.427 431	1	−0.427 461
		2	−0.426 256	10	−0.427 439	2	−0.427 462
		3	−0.426 936	11	−0.427 445	3	−0.427 462
		4	−0.427 192	12	−0.427 449		
		5	−0.427 307	13	−0.427 452		
		6	−0.427 366	14	−0.427 454		
		7	−0.427 399	15	−0.427 456		
		8	−0.427 419	16	−0.427 457		
1.0	−0.331 169	1	−0.301 237	9	−0.329 450	1	−0.331 146
		2	−0.315 773	10	−0.329 736	2	−0.331 169
		3	−0.321 825	11	−0.329 956	3	−0.331 169
		4	−0.324 906	12	−0.330 129		
		5	−0.326 682	13	−0.330 268		
		6	−0.327 798	14	−0.330 382		
		7	−0.328 544	15	−0.330 481		
		8	−0.329 068	16	−0.330 589		

† Exact result at $\gamma = 0.5$ is that of Čižek and Vrscay (1982). Their Padé-Thiele extrapolation procedure also significantly improves the original Padé sequence.

establish the convergence criteria and to precisely assess the domain of validity of the hybrid non-linear transformations.

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