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Generalized Euler transformation for summing strongly divergent Rayleigh-Schrödinger perturbation series: The Zeeman effect

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A generalized Euler transformation (GET) is introduced which provides a powerful alternative method of accurately summing strongly divergent Rayleigh-Schrödinger (RS) perturbation series when other summability methods fail or are difficult to apply. The GET is simple to implement and, unlike a number of other summation procedures, requires no *a priori* knowledge of the analytic properties of the function underlying the RS series. Application of the GET to the difficult problem of the RS weak-field ground-state eigenvalue series of the hydrogen atom in a magnetic field (quadratic Zeeman effect) yields sums of good accuracy over a very wide range of field strengths up to the most intense fields of 10^{14} G. The GET results are compared with those obtained by other summing methods.

The work of Bender and Wu[1] and of Simon[2] on the anharmonic oscillator inaugurated an era of intense interest in large-order perturbation theory; several recent reviews[3,4] of these developments are available. In this context, very high-order Rayleigh-Schrödinger (RS) perturbation series have been obtained[1,3–6] for the eigenvalues of a number of simple one-particle systems; these series are strongly divergent, at best asymptotic. Further, in the case of the widely employed RS $1/Z$ expansions of N-electron atomic isoelectronic sequences, which are known to be convergent, the radii of convergence have been shown[7] to be quite small. Since one anticipates that RS series with poor convergence properties will prove to be the rule rather than the exception, summability procedures are of utmost importance. Several powerful summation techniques exist which have been successfully applied[2–4,6,8,9] to some of these divergent series, often with results of phenomenal accuracy. These include the classical methods of Padé approximants[10] (PA's) and Borel summability[11] (BS), extrapolated PA [Ref. 4(b)] (EPA's), modified BS [Refs 3, 4(a), and 6] (MBS), and the recently introduced[3,6,9] method of order-dependent mapping (ODM). Nevertheless, each of these approaches suffers from certain drawbacks. Thus, in a number of cases, conventional PA's fail and EPA's converge very slowly, e.g., the quadratic Zeeman effect for the hydrogen atom in a magnetic field (HAMF) for intense field strengths[4(b)] of $B > 10^9$ G. Further, BS and MBS are in general difficult to implement[3,6,8(b)] and although in theory[12] applicable to the HAMF system, there are problems[4(a),6] in obtaining accurate summations for $B > 10^{10}$ G. The sophisticated ODM gives[6] impressively accurate values for the HAMF ground-state eigenvalue over a very wide range of field strengths up to $B \approx 10^{13}$ G. The success of ODM, as well as of EPA and MBS, is dependent, however, upon incorporating into the formalism quite detailed information (which in other cases may not be available) concerning the large-field asymptotic behavior of the eigenvalue or of the large-order asymptotic behavior of the RS series. In this Communication, we introduce an alternative method for accurately summing divergent RS series, namely, a generalized Euler transformation[13] (GET), which has the advantages of being extremely simple to implement and of not requiring any *a priori* knowledge of the analytic properties of the eigenvalue; further, we demonstrate the efficacy of the GET by applying it to the difficult HAMF problem.

The HAMF system is a logical candidate for testing the GET, not only because of its intractability both to variational calculations and summability methods but also because it is of great current interest[4(b),6,14,15] *per se* in atomic physics, solid-state physics, and astrophysics, particularly for intense fields; for a concise review of the physical and mathematical background, see Ref. 6. The spinless HAMF Hamiltonian (in a.u.) has the form

$$H(\gamma) = -\tfrac{1}{2}\Delta - r^{-1} + \gamma L_z + (\gamma^2/8)(x^2+y^2) \quad , \tag{1}$$

where γ is a dimensionless coupling parameter giving the strength of the magnetic field ($\gamma = 1$ corresponds to $B = 2.3505 \times 10^9$ G). For the ground-state eigenvalue, the linear term in γ makes no contribution, and the RS weak-field series can be written as

$$E(\gamma) = \sum_{j=0}^{\infty} E_j (\gamma^2/8)^j \quad , \tag{2}$$

where the E_j have been computed[5] exactly through 10th order, to 12 digits through 100th order, and more recently,[6] to 20 to 27 digits through 61st order. The formidable task of summing this series is evident when it is recalled[5] that for large j, the controlling factor in E_j is $(-1)^{j+1}(2j+\frac{1}{2})!$; for example, the conventional sum of the 33rd order RS series (2) for

TABLE I. Comparison of ground-state energy (a.u.) of the HAMF system for $0 < \gamma \leq 10$ obtained by various methods.

γ	E_{var} Ref. 4(b)	E_{EPA} Ref. 4(b)	E_{MBS} Ref. 6	E_{GET}	E_{ODM} Ref. 6
0.1	−0.497 53	−0.497 53		−0.497 526 480 401	
0.2				−0.490 381 565 035	−0.490 381 565 034 8[a]
0.5	−0.447 21	−0.447 21	−0.447 210 538 458 1	−0.447 210 538 8	−0.447 210 538 458 1
1.0	−0.331 17	−0.331 17	−0.331 168 895	−0.331 169 22	−0.331 168 896
2.0	−0.022 23	−0.022 19		−0.022 234	−0.022 213 9
3.0	0.335 47	0.3357	0.3355	0.335 390	0.335 466
4.0	0.719 20	0.7206		0.719 129	
5.0	1.119 63	1.1235	1.120	1.119 76	1.119 60
10.0				3.2564	3.2522

[a] Rounded from 22 digits.

$\gamma = 1$ is $0.115\,38 \times 10^{62}$ while the corresponding variational value[4(b)] is −0.331 17. Using the accessible[4(b)] data, i.e., 12-digit E_j through 36th order,[16] and working throughout in ordinary double-precision computer arithmetic (about 16 significant digits), we applied the GET to (2) to obtain the E_{GET} entries of Tables I and II. In Table I, E_{GET} is compared with the variational E_{var} and E_{EPA} of Čížek and Vrscay,[4(b)] and the E_{MBS} and E_{ODM} of Le Guillou and Zinn-Justin,[6] in the range $0 < \gamma \leq 10$ ($0 < B \lesssim 2 \times 10^{10}$ G). As previously mentioned, E_{EPA}, E_{MBS}, and E_{ODM} were all obtained by explicitly including in the formalism via a variety of methods the dominant elements of the analytic behavior of the eigenvalue; the E_{GET}, however, is free of such *a priori* bias. Further, it should be noted that both E_{MBS} and E_{ODM} were computed with about twice as many significant digits in the input, twice as much computer precision, and to twice as high order as E_{GET}. It is seen that E_{GET} is markedly superior to E_{EPA} and, bearing in mind the relative accuracy of the input and precision of the computer arithmetic, slightly superior to E_{MBS} and comparable to E_{ODM}. Table II collects E_{GET}, adiabatic[14] or variational[15] E_{other}, and E_{ODM} (Ref. 6) for very large γ ($5 \times 10^{10} \lesssim B \leq 10^{14}$ G) of astrophysical interest (e.g., neutron stars); the E_{MBS} have not been computed throughout this region since the method fails[6] here. As might be anticipated, E_{GET} can no longer keep pace with E_{ODM} for such larger γ due to the comparatively limited accuracy of our input data which introduces severe cancellation[17] of significant digits in the calculation of the GET expansion coefficients. Despite this handicap, E_{GET} sums (2) with promising accuracy, the deviation from E_{other} reaching a maximum of 3% in the neighborhood of $B \approx 5 \times 10^{11}$ G and diminishing to 0.6% at $B = 10^{14}$ G. The fluctuations of E_{GET} above and below E_{other} observed in Table II, and to a very slight degree in Table I, may be attributed to numerical rounding effects; as yet, there is insufficient evidence to draw any conclusions about possible bounds furnished by the GET.

TABLE II. Comparison of ground-state energy (a.u.) of the HAMF system for large γ obtained by various methods.

γ	E_{other}[a]	E_{GET}	E_{ODM}[b]
2.0×10	7.7847	7.855	7.7847[c]
1.0×10^2	$4.621\,07 \times 10$	4.48×10	4.621×10
2.0×10^2	$9.527\,30 \times 10$	9.25×10	9.5275×10[d]
3.0×10^2	$1.451\,811 \times 10^2$	1.41×10^2	$1.446\,45 \times 10^2$
1.0×10^3	$4.959\,388 \times 10^2$	4.87×10^2	4.9236×10^2
2.0×10^3	$9.906\,953\,3 \times 10^2$	9.93×10^2	9.9073×10^2
$2.127\,511 \times 10^3$	$1.075\,883\,4 \times 10^3$	1.06×10^3	
$4.255\,022 \times 10^3$	$2.161\,602\,8 \times 10^3$	2.16×10^3	
$4.255\,022 \times 10^4$	$2.269\,842 \times 10^4$	2.28×10^4	

[a] The first, second, third, and sixth entries are from Ref. 14 and the remainder from Ref. 15.

[b] Reference 6.

[c] $E_{\text{MBS}} = 7.8$.

[d] $E_{\text{MBS}} = 9.3 \times 10$.

The GET formalism may be summarized as follows. Consider any formal RS power series,

$$\mathfrak{A}(\Lambda)=\sum_{j=0}^{\infty}\mathfrak{A}_j\Lambda^j \ , \tag{3}$$

where Λ is a real natural (variable) or dummy (fixed at unity) coupling parameter, $\mathfrak{A}$ is the eigenvalue, any expectation value, the eigenvector, or an operator-valued function of Λ (e.g., the Hamiltonian), and $\mathfrak{A}_j$ is the jth-order RS expansion coefficient. As the first step of the GET, for $\Lambda > 0$ introduce the simple but nontrivial transformation,[18]

$$\mathfrak{A}(\Lambda)=A(\lambda)=\sum_{j=0}^{\infty}\alpha_j\lambda^j \ , \tag{4a}$$

$$\lambda=\Lambda^{1/2};\ \alpha_{2k}=\mathfrak{A}_k,\ \ \alpha_{2k+1}=0,\ \ k=0,1,\ldots \ . \tag{4b}$$

For example, to apply (4) to (2), we take $\Lambda=\gamma^2$. For $\Lambda<0$, (4b) is readily modified. As the next step, transform (4a) to

$$\begin{aligned}A(\lambda)&=\lambda^{-m}\lambda^m A(\lambda)=F(m,\sigma)A(\lambda)\\&=G(m,\mu)A(\lambda) \ ,\end{aligned} \tag{5}$$

where the GET operators $F(m,\sigma)$ and $G(m,\mu)$ are defined by

$$F(m,\sigma)A(\lambda)\equiv\lambda^{-m}\tilde{\lambda}^m\sum_{j=0}^{\infty}\tilde{\alpha}_j(m,\sigma)\tilde{\lambda}^j \ , \tag{6a}$$

$$G(m,\mu)A(\lambda)\equiv\lambda^{-m}\tilde{\nu}^m\sum_{j=0}^{\infty}\tilde{\beta}_j(m,\mu)\tilde{\nu}^j \ . \tag{6b}$$

In (5) we have decomposed the factor of unity in $A(\lambda)$ in order to introduce a disposable GET exponent m which can assume arbitrary real values; the GET $\tilde{\alpha}_j(m,\sigma)$, $\tilde{\lambda}$ and $\tilde{\beta}_j(m,\mu)$, $\tilde{\nu}$ are the appropriate transforms of the RS α_j, λ when λ is, respectively, natural and dummy, and the tilde denotes GET quantities throughout. The GET coupling parameters $\tilde{\lambda}$ and $\tilde{\nu}$ are homographically related to one another and to λ by

$$\lambda=\tilde{\lambda}(1+\sigma\tilde{\lambda})^{-1}=\tilde{\nu}[\mu+(1-\mu)\tilde{\nu}]^{-1} \ , \quad \sigma=1-\mu \ , \tag{7}$$

where σ or μ is a second diposable GET real parameter. Equation (7) is defined for all λ except for the inherent GET singularity $\lambda_s=\sigma^{-1}=(1-\mu)^{-1}$. The GET expansion coefficients are given by

$$\tilde{\alpha}_j(m,\sigma)=\sum_{k=0}^{j}\begin{pmatrix}j+m-1\\ j-k\end{pmatrix}(-\sigma)^{j-k}\alpha_k \ , \tag{8a}$$

$$\tilde{\beta}_j(m,\mu)=\mu^{-(j+m)}\sum_{k=0}^{j}\begin{pmatrix}j+m-1\\ j-k\end{pmatrix}(\mu-1)^{j-k}\alpha_k \ . \tag{8b}$$

Note that if the RS series (3) is given through nth order, the GET series (6) are known through $(2n+1)$th order.

One gains insight into the analytic properties of the GET by introducing the tth-order GET approximant for the general case of natural λ,

$$F^{(t)}(m,\sigma)A(\lambda)\equiv\lambda^{-m}\tilde{\lambda}^m\sum_{j=0}^{t}\tilde{\alpha}_j(m,\sigma)\tilde{\lambda}^j \ . \tag{9}$$

Equation (9) can be written in the alternative λ form,

$$F^{(t)}(m,\sigma)A(\lambda)=\tilde{\Omega}^{(t)}(\lambda)/(1-\sigma\lambda)^{t+m} \ , \tag{10}$$

where $\tilde{\Omega}^{(t)}(\lambda)$ is a polynomial of tth degree in λ,

$$\tilde{\Omega}^{(t)}(\lambda)=\sum_{j=0}^{t}\tilde{\omega}_j(t+m,\sigma)\lambda^j \ , \tag{11a}$$

$$\tilde{\omega}_j(t+m,\sigma)=\sum_{k=0}^{j}\begin{pmatrix}t+m\\ j-k\end{pmatrix}(-\sigma)^{j-k}\alpha_k \ . \tag{11b}$$

For arbitrary m and σ, it follows from (10) and (11) that

$$A(\lambda)-F^{(t)}(m,\sigma)A(\lambda)=O(\lambda^{t+1}) \ , \tag{12}$$

thus exhibiting a fundamental property of the GET. Further, one can read off directly from (10) the nature of the GET singularity λ_s as a function of the exponent m: For $m=0,\pm1,\pm2,\ldots$, and $t+m>0$, (10) is meromorphic and λ_s is a pole of order $t+m$, whereas, for $m=$ noninteger, (10) is a multivalued function and λ_s is a branch point of index $-(t+m)$. The extension of m to nonintegral values is nontrivial as it completely changes the character of the GET approximant and enhances its capacity to simulate or reproduce the leading singularities of $A(\lambda)$; this can be demonstrated analytically in simple cases and has been verified numerically for the divergent series considered.

Finally, the GET gains enormously in power by applying it in a reiterative manner; thus, for natural λ, by indexing m, σ, $\tilde{\alpha}_j$, and $\tilde{\lambda}$ suitably, we can write for f successive applications,

$$A(\lambda)=\prod_{e=1}^{f}F(m_e,\sigma_e)A(\lambda) \ , \tag{13}$$

$$\tilde{\lambda}_{e-1}=\tilde{\lambda}_e(1+\sigma_e\tilde{\lambda}_e)^{-1},\ \ \tilde{\lambda}_0=\lambda \ , \tag{14}$$

where the $\tilde{\alpha}_j^{(e)}(m_e,\sigma_e)$ are computed from the $\tilde{\alpha}_k^{(e-1)}(m_{e-1},\sigma_{e-1})$ via (8a) with $\tilde{\alpha}_k^{(0)}=\alpha_k$. Similar results hold for dummy λ. The determination of the GET parameters was reduced to a routine numerical procedure, the criterion being rapidity of convergence. The most effective choice of the σ_e was found to be

$$\sigma_e=-2^{e-1}\lambda_c^{-1},\ \ e=1,2,\ldots,f \ , \tag{15}$$

where λ_c is a selected value of λ (normally 1.0 or 2.0) used to test convergence. This, in turn, led to simple determination of the m_e where, for the series considered, m_1 is a noninteger in the range $-2 < m_1 < 0$, and the m_e, $e = 2, 3, \ldots, f$, are negative integers satisfying $m_e < m_{e-1}$. The resultant $\tilde{\alpha}_j^{(f)}$, derived for a *fixed* value of λ_c, were then used to sum $A(\lambda)$ via (13) over a wide range of λ values. Each successive GET cycle greatly increases the accuracy of the results but, in practice, double-precision computer arithmetic limits one to a maximum of $f = 5$ before rounding effects predominate. It will be noted that the entire GET process is algebraic requiring but modest computational effort, indeed, even less than for PA.

We now touch upon the relationship between the GET and ODM. Qualitatively, the principal distinction between these methods lies in their selection of the mapping functions which transform the original RS series (3) in powers of Λ into another series in powers of, say, $\tilde{\lambda}$. In ODM, this mapping function is selected so as to mirror the supposedly known analytic properties of the function underlying the RS series. In the GET, however, Λ is always transformed with two prespecified mappings, first with (4b), and then with (7), where the latter is rendered more flexible with the adjustable exponent m introduced in (5); still greater flexibility is then achieved via the reiterative procedure of (13).

It is also of interest to note that several apparently unrelated previous transformations are special cases of the GET. These transformations, which have been widely used in attempting to improve the convergence of low-order RS series for atomic and molecular properties, can be recovered by omitting[18] (4) (thus taking $\lambda = \Lambda$, $\alpha_k = \mathfrak{a}_k$), considering only a single GET cycle, and restricting m to certain integral values. For example, $F(1, \sigma)$ or $G(1, \mu)$ corresponds to the classical ET.[19] For dummy λ, $G(-1, \mu)$ is equivalent to the Feenberg-Goldhammer[20] transformation[21] (FGT) for the RS series of the Hamiltonian and eigenvalue; here, μ scales the zero-order Hamiltonian. Similarly, for RS $1/Z$ expansions of atomic isoelectronic sequences, $F(-2, \sigma)$ generates the screening transformation[7,22] (ST) of the eigenvalue series; here, σ is a nuclear screening parameter, $\lambda = Z^{-1}$, and $\tilde{\lambda} = (Z - \sigma)^{-1}$. Both the FGT (Ref. 20) and ST (Ref. 22) were derived by heuristically repartitioning the Hamiltonian without noting that the resulting transformations were either the ET or minor variants thereof. The above analysis has the pleasing feature of unifying the theory and providing a firmer mathematical foundation for the FGT and ST.

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[1]C. M. Bender and T. T. Wu, Phys. Rev. Lett. 21, 406 (1968); Phys. Rev. 184, 1231 (1969).

[2]B. Simon, Ann. Phys. (N.Y.) 58, 76 (1970).

[3]J. Zinn-Justin, Phys. Rep. 70, 109 (1981).

[4](a) B. Simon, Int. J. Quantum Chem. 21, 3 (1982); (b) J. Čížek and E. R. Vrscay, *ibid.* 21, 27 (1982); (c) other papers in this review issue.

[5]J. E. Avron, B. G. Adams, J. Čížek, M. Clay, M. L. Glasser, P. Otto, J. Paldus, and E. Vrscay, Phys. Rev. Lett. 43, 691 (1979), and references cited therein.

[6]J. C. Le Guillou and J. Zinn-Justin, CEN-Saclay Report No. DPhT/39 (unpublished); we received this report after the calculations reported herein were completed.

[7]J. N. Silverman, Phys. Rev. A 23, 441 (1981), and references cited therein.

[8](a) J. J. Loeffel, A. Martin, B. Simon, and A. S. Wightman, Phys. Lett. 30B, 656 (1969); (b) S. Graffi, V. Grecchi, and B. Simon, *ibid.* 32B, 631 (1970).

[9]R. Seznec and J. Zinn-Justin, J. Math. Phys. 20, 1398 (1979).

[10]G. A. Baker, Jr., *Essentials of Padé Approximants* (Academic, New York, 1975).

[11](a) G. H. Hardy, *Divergent Series* (Oxford University Press, Oxford, 1973); (b) K. Knopp, *Theory and Applications of Infinite Series* (Blackie, London, 1949), Chaps. XIII and XIV.

[12]J. Avron, I. Herbst, and B. Simon, Phys. Lett. 62A, 214 (1977); Commun. Math. Phys. 79, 529 (1981).

[13]Various generalizations of the classical Euler transformation (ET) have long been in use; see, e.g., P. M. Morse and H. Feshback, *Methods of Theoretical Physics, Part I* (McGraw-Hill, New York, 1953), pp. 394–398, and K. Bhattacharyya, Int. J. Quantum Chem. 22, 307 (1982) for recent applications. The GET presented here differs in several fundamental aspects from the earlier treatments.

[14]J. Simola and J. Virtamo, J. Phys. B 11, 3309 (1978).

[15]M. S. Kaschiev, S. I. Vinitsky, and F. R. Vukajlović, Phys. Rev. A 22, 557 (1980).

[16]To our knowledge, these are the most accurate high-order E_j which have actually been published.

[17]For a similar loss of accuracy due to 12-digit input coefficients, see the PA-BS calculations of Ref. 8(b).

[18]It is well known that many summation methods achieve convergence by suitably averaging divergent terms; cf. Ref. 11 for extensive discussions of arithmetic and other means. The heuristic justification for the transformation of (4) is that it facilitates the GET averaging process of (8) by introducing vanishing terms. For the series considered, we have numerically verified that the *omission* of (4) decreases the accuracy of the GET by several orders of magnitude.

[19]The so-called (E,q) method of Ref. 11(a).

[20]E. Feenberg, Ann. Phys. (N.Y.) 3, 292 (1958), and references cited therein.

[21]S. Wilson and M. F. Guest, J. Phys. B 14, 1709 (1981), and references cited therein.

[22]A. Dalgarno and A. L. Stewart, Proc. R. Soc. London, Ser. A 257, 534 (1960).