Improving the convergence and estimating the accuracy of summation approximants of 1/*D* expansions for Coulombic systems

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The convergence of large-order expansions in $\delta=1/D$, where D is the dimensionality of coordinate space, for energies $E(\delta)$ of Coulomb systems is strongly affected by singularities at $\delta=1$ and $\delta=0$. Padé–Borel approximants with modifications that completely remove the singularities at $\delta=1$ and remove the dominant singularity at $\delta=0$ are demonstrated. A renormalization of the interelectron repulsion is found to move the dominant singularity of the Borel function $F(\delta)=\Sigma_j E_j'/j!$, where E_j' are the the expansion coefficients of the energy with singularity structure removed at $\delta=1$, farther from the origin and thereby accelerate summation convergence. The ground-state energies of He and H_2^+ are used as test cases. The new methods give significant improvement over previous summation methods. *Shifted* Borel summation using $F_m(\delta)=\Sigma_j E_j'/\Gamma(j+1-m)$ is considered. The standard deviation of results calculated with different values of the shift parameter m is proposed as a measure of summation accuracy. © *1998 American Institute of Physics.* [S0022-2488(98)04210-8]

I. INTRODUCTION

Large-order perturbation theory in $1/D$, where D is the dimensionality of coordinate space, was proposed by Mlodinow[1,2] as an alternative to variational methods and coupling-constant perturbation theories for solving the Schrödinger equation. This ''dimensional perturbation theory'' has some appealing features. The first-order theory gives a semiquantitative description of electron correlation[3–11] and other subtle many-body effects[12] and it is relatively easy to calculate the perturbation expansion to very high order, using recursion relations.[13,14] $1/D$ expansions have now been calculated through 30th order for two-electron atoms[15] and tenth order for three-electron atoms.[16] Large-order expansions have also been calculated for the H atom in an external field[17–21] and for the H_2^+ molecule.[19,22,23]

The expansions for energies of Coulombic systems are, in general, divergent, due to singularities in the energy function $E(\delta)$, with $\delta=1/D$ treated as a continuous complex variable. One type of singularity is a pole in $E(\delta)$ that results from the fact that for certain integer values of D the expectation value of the Coulomb potential can diverge at particle coalescences.[24] This singularity can be accurately characterized and removed either by subtraction[25] or by rescaling,[5,26] making partial sums of the expansion appear rapidly convergent at low orders. A second characteristic type of singularity is a complicated branch point or essential singularity at $\delta=0$, which leads to divergence at higher orders.[15] This singularity can in principle be explained by an instanton analysis.[27–29] The zeroth-order limit of the perturbation theory corresponds to localization at an extremum of an effective potential that is the sum of the three-dimensional Coulomb potential and a centrifugal potential that comes from the dimensional continuation of the kinetic energy operator. For applications to bound systems, one generally chooses an extremum that corresponds

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to a stable minimum. However, there typically exist sub-barrier trajectories in imaginary time that allow for tunneling out of the minimum. This causes the zeroth-order limit to be singular, with the energy expansion coefficients diverging as a factorial.

Summation methods in which the Coulombic poles are removed from $E(\delta)$ and then the remainder expansion is summed with Padé approximants or Padé–Borel approximants yield apparently convergent results at all orders.[15,30,31] Our purpose here is to refine those methods to improve the rate of convergence. Our strategy is to renormalize the Hamiltonian, by redefining the dimensional continuation in such a way that the effect of the singularity at the origin is mitigated, and to improve the techniques for modeling the singularities. In addition, we develop a method for estimating the accuracy of a given summation approximant. He and H_2^+ are used as test cases.

II. SUMMATION APPROXIMANTS

The asymptotic expansion in $1/D$ for the electronic energy of an atom or molecule has the form

$$E(\delta)\sim\delta^2\sum_{j=0}^{k} E_j\delta^j, \tag{1}$$

where $\delta=1/D$. There are various algorithms for computing the expansion coefficients E_j, but the most efficient, especially for problems with more than one degree of freedom, seems to be the matrix method of Dunn *et al.*[14] The direct evaluation of Eq. (1) at $\delta=1/3$ using partial sums, from truncation at given k, typically gives slow convergence at low orders and rapid divergence at high order.

For ground states of Coulombic systems, E has an expansion about $D=1$ in the form[24]

$$E(\delta)\sim a_{-2}(D-1)^{-2}+a_{-1}(D-1)^{-1}+\cdots . \tag{2}$$

For a one-electron atom with nuclear charge Z, the first term in Eq. (2) constitutes the exact solution, with $a_{-2}=2Z^2$. For two-electron atoms a_{-2} is equal to the ground-state energy of a two-electron Schrödinger equation in which the Coulomb potentials have been replaced with delta functions.[24,32] The exact solution for this equation was obtained by Rosenthal[33] for arbitrary Z.

To remove the effects of the poles one can either rescale the expansion,[5,26] by multiplying it by $(1-\delta)^2$, or explicitly subtract out the δ expansions of the poles.[25,30] If the residues are known exactly then subtraction works best. We consider two approaches for the case where a_{-2} is known but a_{-1} is not known: subtracting the second-order pole and rescaling to remove the first-order pole,

$$E(\delta)\sim\delta^2[a_{-2}(1-\delta)^{-2}+(1-\delta)^{-1}E'(\delta)], \tag{3a}$$

$$E'(\delta)=\sum_{j=0}^{k}\delta^jE'_j, \quad E'_j=E_j-E_{j-1}-a_{-2}, \quad E_{-1}=0, \tag{3b}$$

or subtraction of both poles,

$$E(\delta)\sim\delta^2[a_{-2}(1-\delta)^{-2}+a_{-1}(1-\delta)^{-1}+E'(\delta)], \tag{4a}$$

$$E'(\delta)=\sum_{j=0}^{k}\delta^jE'_j, \quad E'_j=E_j-(j+1)a_{-2}-a_{-1}, \tag{4b}$$

with

$$a_{-1}=\lim_{\delta\to 1}\sum_{j=0}^{k}\delta^j(E_j-E_{j-1}-a_{-2}). \tag{5}$$

Equation (5) can be evaluated using Padé summation.[30] The use of approximants based on Eqs. (4) has been called *hybrid* summation,[25] since it is the combination of an expansion about $\delta=1$ and an expansion about $\delta=0$. We will refer to the approach in Eqs. (3) as *rescaled hybrid* summation.

It is possible to obtain convergent results by summing the expansions for E' with Padé approximants or with Padé-Borel approximants. The latter give a somewhat better convergence rate. Here we employ a more general technique[28] that will be useful not just for summing the energy expansion but also for analyzing the singularity structure at $\delta=0$ and for estimating summation accuracy. Consider a function $F_m(\delta)$ with asymptotic expansion

$$F_m(\delta)\sim\sum_{j=j_0}^{k}\delta^j F_{m,j}, \quad F_{m,j}=E'_j/\Gamma(j+1-m), \tag{6}$$

where j_0 is the smallest integer greater than or equal to m. This function is related to $E'(\delta)$ by the transform

$$E'(\delta)=\sum_{j=0}^{j_0-1}E'_j\delta^j+e^{-(m-1)i\xi}\lim_{y\to\infty}\int_0^{ye^{i\xi}}x^{-m}F_m(\delta xe^{i\xi})\exp(-xe^{i\xi})dx, \tag{7}$$

with the angle ξ chosen so that $F(\delta xe^{i\xi})$ is nonsingular along the path of integration and $-\pi/2<\xi<\pi/2$. If $m=0$ then Eq. (7) is the usual Borel sum. For the function F_m in Eq. (7) we will substitute Padé approximants of the expansion in Eq. (6). For $m\neq 0$ we will refer to the summation method as *shifted* Padé–Borel summation.

III. RENORMALIZATION

A. Charge renormalization

The standard approach to analytic continuation of the Hamiltonian to arbitrary D is to continue the kinetic energy operator to D dimensions while keeping the physical, three-dimensional, definition for the potential energy operator.[32,34] If the energy is expressed in atomic units multiplied by Z^2/D^2, then the effective potential for an S state of the two-electron atom at large D is

$$V_{\text{eff}}(r_1,r_2,\theta)=V_{\text{centr}}+V_{\text{Coul}}, \tag{8}$$

$$V_{\text{centr}}=\left(\frac{1-6\delta+8\delta^2}{8\sin^2\theta}-\frac{1}{8}\right)\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right), \tag{9}$$

$$V_{\text{Coul}}=-r_1^{-1}-r_2^{-1}+\lambda\,(r_1^2+r_2^2-2r_1r_2\cos\theta)^{-1/2}. \tag{10}$$

V_{centr} is the centrifugal potential from the D-dimensional kinetic energy operator while V_{Coul} is the three-dimensional Coulomb potential, with $\lambda=1/Z$. This effective potential has a stable global minimum, with $r_1=r_2$, as long as λ is less than a critical value $\lambda_c\approx 0.8144$. For H^-, with $\lambda=1$, this symmetric extremum is a saddle point,[35,36] and if this point is used for the zeroth order of the perturbation theory, then the coefficients of the energy expansion will be complex numbers. Similarly, the symmetric large-D extrema for the H_2^+ and H_2 molecules also correspond to saddle points.[35,37,38]

A strategy for calculating $1/D$ expansions for systems that are unstable in the large-D limit was proposed in Ref. 39, using the fact that the definition of the dimensional continuation of the Hamiltonian is arbitrary as long as it gives the correct operator at $D=3$. If we renormalize the repulsive part of the Coulomb potential, by replacing it with a continuous function of δ such that the repulsion becomes weaker as δ approaches zero, it is possible to ensure that the symmetric extremum will be a minimum. This approach is closely related to the renormalized perturbation theory developed by Killingbeck for anharmonic oscillators.[40]

Charge renormalization was applied to large-order perturbation theory for H^- in Ref. 41. The parameter λ in Eq. (10) was replaced with the linear polynomial

$$\lambda(\delta)=\lambda_0+\lambda_1\delta, \quad \lambda_1=3(Z^{-1}-\lambda_0) \tag{11}$$

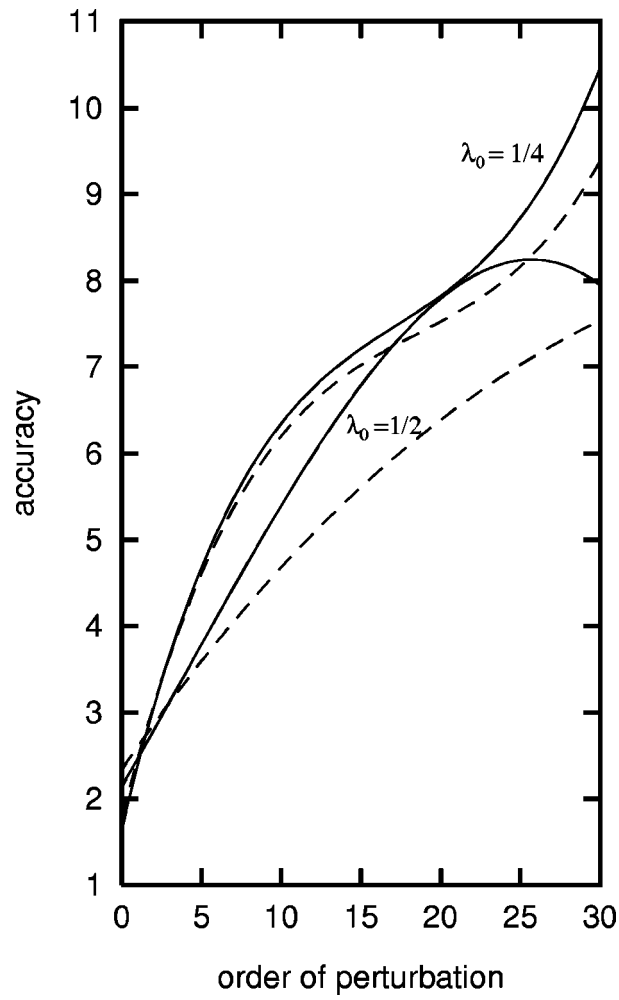

FIG. 1. Cubic polynomial fits of the number of accurate digits from summation approximants for the ground state energy of He, as a function of order, with ''accuracy'' defined as $-\log|\Delta E/E_{\text{exact}}|$, where $\Delta E = E_{\text{approx}} - E_{\text{exact}}$, with E_{exact} from Ref. 42. The dashed curves are from unshifted hybrid Padé–Borel approximants while the solid curves are from unshifted rescaled hybrid Padé–Borel approximants. Results are shown for $\lambda_0 = 1/2$ (unrenormalized) and for $\lambda_0 = 1/4$, as labeled, with $\lambda(\delta) = \lambda_0 + \lambda_1 \delta$.

with λ_0 treated as a free parameter. λ_1 is defined so that $\lambda(1/3) = 1/Z$. (This modification of λ does not affect the scale factor in the energy units. We continue to use atomic units multiplied by Z^2/D^2, where Z is independent of D.) The hybrid expansion, Eq. (4a), with Padé–Borel summation of E' gave convergent results for H^- for any value of λ_0 less than λ_c. The fastest convergence was for $\lambda_0 \approx (2Z)^{-1}$, which gave a more accurate result at given order for the ground-state energy of H^- than had been obtained[15] for the ground-state energy of He with unrenormalized λ. This rapid convergence for H^- suggests that the use of a δ-dependent potential energy operator could be used to improve the convergence even for systems that are stable at large D.

Figure 1 shows the effect on the convergence for He of setting $\lambda_0 = (2Z)^{-1}$. Since there is a fair amount of scatter in the convergence from order to order, we have plotted cubic polynomial fits to more clearly show the convergence patterns. The dashed curves correspond to hybrid approximants, based on Eq. (4a), while the solid curves correspond to rescaled hybrid approximants, based on Eq. (3a). The expansion of E' was summed with unshifted Padé–Borel approximants. We define the ''accuracy'' of a summation approximant S_k at given order k as

$$\alpha(k) = -\log_{10}|(S_k - E_{\text{exact}})/E_{\text{exact}}|, \tag{12}$$

which is a continuous measure of the number of accurate digits.

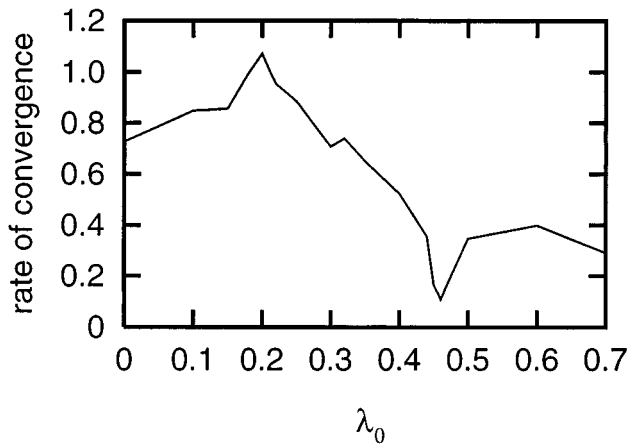

FIG. 2. The rate of convergence at low order for unshifted rescaled hybrid Padé–Borel approximants for the ground state energy of He, as a function of the renormalization parameter λ_0, using $\lambda(\delta)=\lambda_0+\lambda_1\delta$. The rate of convergence is defined here as the parameter α_1 from the three-parameter least-squares fit of the accuracy $\alpha(k)=\alpha_0+\alpha_1 k+\alpha_2 k^2+\alpha_3 k^3$ with α_0 constrained to equal the accuracy of S_0.

Several characteristic trends are evident. First, it is clear that the rescaled hybrid summation is the better of the two summation methods. It is possible to somewhat improve the accuracy of the unscaled hybrid approximants by applying Shanks extrapolation, with some subjective judgement, to the Padé-approximant sequences for a_{-1}, but the results remain less dependable than those from the rescaled hybrid method. The general shapes of the rescaled hybrid curves are representative of those over a wide range of λ_0. They begin with an almost linear increase in the number of accurate digits. Then, upon reaching an accuracy plateau of between approximately 6 and 8 digits the rate of convergence slows significantly. For $\lambda_0<0.8/Z$ there is a return to a more rapid convergence rate, beginning at around 25th order. Figure 2 shows the initial slope of $\alpha(k)$ as a function of λ_0. The increasing rate of convergence is balanced at very low order by the fact that the zeroth-order accuracy decreases for λ_0 far from the physical value. (The zeroth-order result is equal to the exact energy for $\lambda_0\approx 0.46$, which corresponds to a dip in Fig. 2.) Nevertheless, there is for the He atom a clear advantage to choosing λ_0 in the general neighborhood of $0.5/Z$.

The functional form chosen for $\lambda(\delta)$ is essentially arbitrary. In addition to the linear polynomial, Eq. (11), we have considered a quadratic polynomial,

$$\lambda(\delta)=\lambda_0+\lambda_1\delta+\lambda_2\delta^2, \tag{13}$$

$$\lambda_1=\frac{9}{2Z}-4\lambda_0-\frac{1}{2}\lambda(1), \quad \lambda_2=3\lambda_0+\frac{3}{2}\lambda(1)-\frac{9}{2Z}, \tag{14}$$

with $\lambda(1)$ and $\lambda_0=\lambda(0)$ treated as free parameters. This makes it possible to control the behavior at both of the solvable limits, $\delta=0$ and $\delta=1$. The position of the dominant singularities in the Borel function depend only on the value of λ_0. Therefore the rate of convergence of the summation approximants depends less strongly on $\lambda(1)$ than on $\lambda(0)$. We find in practice that certain choices of $\lambda(1)$ do improve the convergence at low and intermediate orders, especially for H^-, for which the linear $\lambda(\delta)$ can imply a very large value for $\lambda(1)$.

B. Effect on singularity structure

Analysis of the expansion coefficients for the ground-state energy of two-electron atoms has shown[15] that the dominant singularities of $F_0(\delta)$ (i.e., the singularities nearest to the origin of the complex δ plane) are a complex-conjugate pair of square-root branch points in the negative half-plane. Let $-\beta e^{\pm ib}$ be their locations. Then the coefficients of the asymptotic expansion in δ

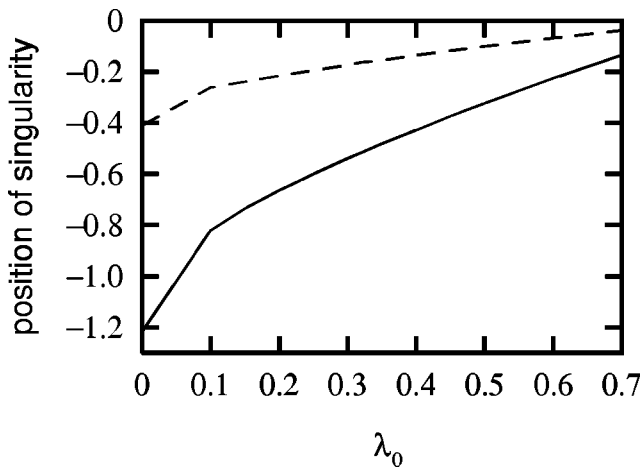

FIG. 3. Real part (solid curve) and imaginary part (dashed curve) of one of the dominant singularities in the Borel functions of the two-electron isoelectronic series, as a function of λ_0. The other dominant singularity is at the complex conjugate of this location.

of the expression $G(\delta+\beta e^{ib})^{1/2}+G^*(\delta+\beta e^{-ib})^{1/2}$, where G is a constant, will in the limit of large order be equal to the coefficients $F_{0,j}$ of the asymptotic expansion of F_0, Eq. (6). Thus, in the limit of large j we have

$$F_{0,j}\sim 2|G|\beta^{1/2}(-1)^j\,\frac{\Gamma(j-1/2)}{\Gamma(-1/2)\Gamma(j+1)}\,\beta^{-j}\,\cos\left[\left(j-\frac{1}{2}\right)b-\arg G\right]. \tag{15}$$

Now compare this to the function

$$f(\delta)=\gamma(\delta+\beta e^{ib})^{-1}+\gamma^*(\delta+\beta e^{-ib})^{-1}, \tag{16}$$

which has the expansion coefficients

$$f_j=2|\gamma|\beta^{-1}(-1)^j\beta^{-j}\,\cos[(j+1)b-\arg\,\gamma]. \tag{17}$$

If we set $\gamma=2^{-1}\pi^{-1/2}\beta^{3/2}|G|e^{i(\arg G+3b/2)}$, then $f_j\sim F_{3/2,j}$, which implies that the dominant singularities of $F_{3/2}(\delta)$ will be first-order poles at the same locations as the dominant branch points in $F_0(\delta)$.

The effect on convergence of the renormalization can be understood in terms of the effect on the locations of the dominant singularities of $F_m(\delta)$. A convenient method for determining these locations is to examine the singularities of the Padé approximants of F_m. Previously[15] we used the quadratic Padé approximants of F_0 for this purpose, noting the positions of the branch points nearest the origin. Once the branch points are approximately identified in this manner, the result can be refined by noting the positions of the corresponding poles in the linear Padé approximants of $F_{3/2}$, which stabilize somewhat faster.

We find that the positions of these singularities depend only on the value of λ_0. In general, there appear to be three distinct complex-conjugate pairs of singularities in the Borel functions. For λ_0 close to λ_c the dominant singularities are in the positive half plane, but as λ_0 decreases this pair rapidly moves away from the origin. For $\lambda_0<0.8$ the dominant singularities are the pair in the negative half plane. Figure 3 shows the real and imaginary parts of this pair. The steady movement away from the origin as λ_0 decreases is presumably related to the improvement in convergence. In the limit $\lambda_0\to 0$ the singularities in the Borel function must disappear, since $E'(\delta)$ is then nonsingular. It is interesting to note that the mechanism for this disappearance is for the prefactor multiplying the dominant singularities to go to zero, rather than for the positions of the singularities to move out to infinity. The third pair of singularities has an imaginary part of $\pm\pi$ with a small real part that depends weakly on λ_0. This is far enough from the origin that these can be expected to have no significant effect on the rate of convergence.

C. Effect on roundoff error

The recursive computation of the energy expansion coefficients E_k is somewhat unstable to roundoff error,[14,15] on account of their factorial divergence. However, in the hydrogenic limit $Z \to \infty$ (i.e., $\lambda \to 0$) the energy expansion is convergent, with only a linear increase in E_k with k. At small but nonzero λ the perturbation theory is still divergent but the growth of the expansion coefficients is nearly linear until very high order. This apparently comes about through massive cancellations of intermediate quantities that grow factorially. The result is extreme loss of precision near the hydrogenic limit.

The number of significant figures in the E_k decreases approximately linearly with k. It was stated previously[15,31] that roundoff error in the E_k becomes manifest in the S_k at about the value of k for which the precision of the E_k intersects the accuracy of the S_k. More careful analysis reveals that this rule is generally valid but somewhat conservative. The actual propagation of error in the summation approximants is complicated, with some approximants much less sensitive than others and thereby retaining their accuracy beyond the intersection. Such approximants can be identified empirically by adding to the E_k random error of a given magnitude.

For the renormalized calculations we find that the rate of precision loss depends mainly on the value of the parameter λ_0, increasing as λ_0 decreases. We have used quadruple-precision arithmetic (32 decimal digits) for computing the E_k in the calculations reported here, so that the roundoff error is always less than the convergence accuracy.

D. Renormalization for diatomic molecules

Within the Born–Oppenheimer approximation the Hamiltonian is not homogeneous, since the internuclear distance R is treated as a parameter rather than as a dynamical variable. Therefore, transformation to atomic units multiplied by D^{-2} replaces R with the D-dependent parameter $\tilde{R} = R/D^2$. In a recent study of H_2^+ it was shown that renormalization of this D dependence is a simple and effective way to improve the convergence of the $1/D$ expansion.[23] One replaces $\tilde{R}$ with

$$\tilde{R} = \frac{2(3+\beta)}{(D-1)(D+\beta)} R, \tag{18}$$

with β treated as a free parameter. (The factor of $D-1$ is included to give a reasonable $D \to 1$ limit.) An important effect of this renormalization is to ensure that the $D \to \infty$ limit corresponds to an effective potential with a single global minimum. Otherwise the molecule undergoes a symmetry breaking transition to a double-well problem as R increases, which significantly degrades the convergence of the large-order expansion. For many-electron diatomic molecules a renormalization of the interelectron repulsion, completely analogous to the procedure for atoms in Sec. III A, could be used to attenuate the effect on convergence of the interelectron repulsion in addition to the R renormalization that prevents the symmetry breaking.

IV. ESTIMATING THE ACCURACY OF THE SUMMATION APPROXIMANTS

We have calculated the summation approximants S_k using a range of integer and half-integer values for the shift parameter m in the Borel function F_m. The best results tend to correspond to $m = 0$, 1/2, 1, and 3/2, but which of these four is best at given order appears to be random. Therefore, to obtain an estimate of the accuracy of the summation at given order k we compute the standard deviation σ_k from the mean $\overline{S_k}$ of the four different S_k.

Figure 4 shows results for the He ground state energy with $\lambda_0 = 0.5/Z$. The dotted curve shows the actual accuracy of the mean. The solid curve shows $-\log_{10}|\sigma_k/\overline{S_k}|$. The largest disagreements between the actual accuracy and this estimate occurs at very high orders, where the mean tends to be significantly more accurate than the individual approximants and the estimate is too conservative.

V. DARBOUX–BOREL APPROXIMANTS

The singularity structure of the Borel function $F(\delta)$ for H_2^+ is similar to that for the two-electron atom except that the dominant singularity is typically a square-root branch point that lies

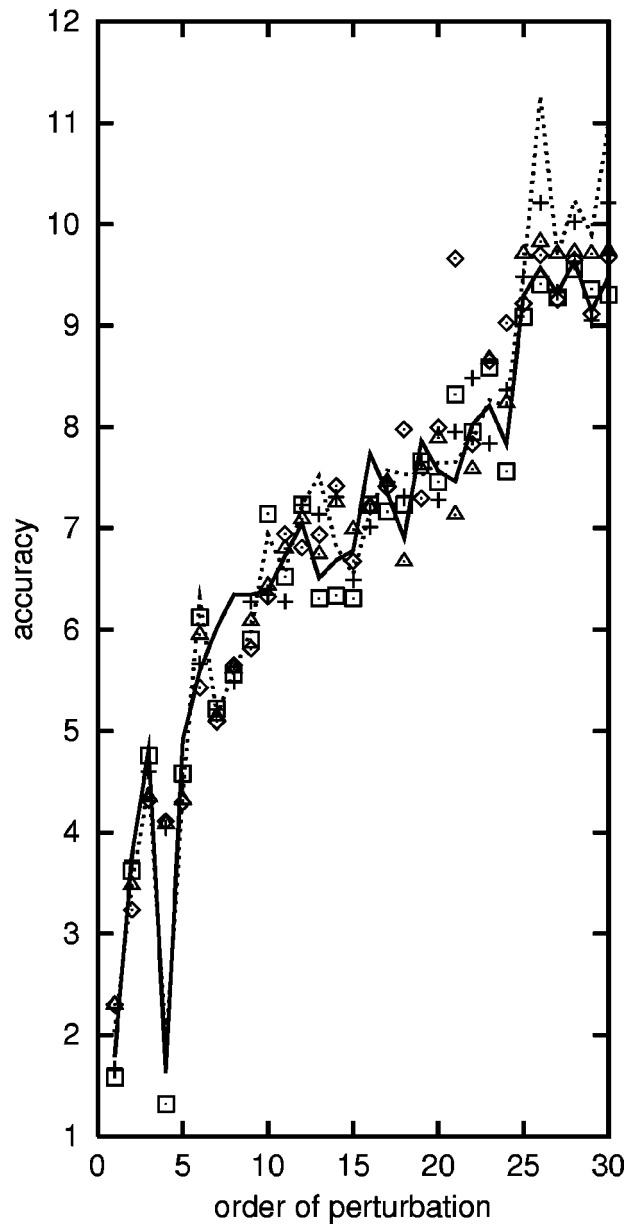

FIG. 4. Accuracy of rescaled hybrid Padé–Borel approximants for the ground state energy of He, as a function of order in the perturbation expansion. The points are determined using Borel functions F_m with the values of the shift parameter indicated as follows: $+$, $m=0$; $\square$, $m=-1/2$; $\triangle$, $m=-1$; $\diamond$, $m=-3/2$. The dotted curve shows $-\log_{10}|(\overline{S_k}-E_{\text{exact}})/E_{\text{exact}}|$, where $\overline{S_k}$ is the mean of the four summation approximants at order k. The solid curve shows $-\log_{10}|\sigma_k/\overline{S_k}|$, where σ_k is the standard deviation from the mean of the four approximants at order k.

on the negative real axis.[22,29] Because this problem is separable, in ellipsoidal coordinates, it is straightforward to derive an exact solution for the location δ_0 of the branch point.[29] Since this singularity is the nearest to the origin in the complex plane, it follows from Darboux's theorem[43] that the expression $g(\delta)(1-\delta/\delta_0)^{1/2}+h(\delta)$, where g and h are nonsingular for $|\delta|\leqslant|\delta_0|$, has the same expansion coefficients in the limit of large order as the actual expansion of F. This suggests the use of Darboux approximants,[44]

$$F_{[L,N/M]}(\delta)=\frac{R_N(\delta)}{Q_M(\delta)}(1-\delta/\delta_0)^{1/2}+\frac{P_L(\delta)}{Q_M(\delta)}, \tag{19}$$

where P_L, Q_M, and R_N are polynomials of degrees L, M, and N, respectively. These polyno-

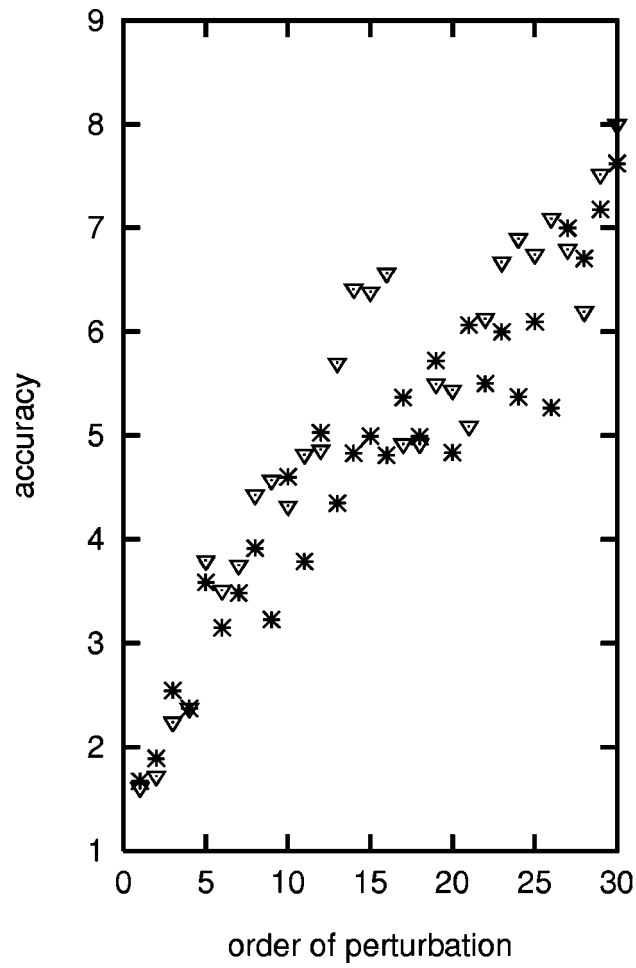

FIG. 5. Accuracy of rescaled hybrid Darboux–Borel approximants (∇) and rescaled hybrid Padé–Borel approximants (∗) for the ground state energy of H_2^+ with internuclear distance $R=2$, as a function of order in the perturbation expansion. The Borel summation is unshifted.

mials can be determined by setting $F_{[L,M/N]}$ equal to the expansion of F, expanding the square root, multiplying through by Q_M, and then solving the resulting set of linear equations.

Figure 5 compares accuracies of Darboux–Borel and Padé–Borel approximants for the ground-state energy of H_2^+. These results correspond to internuclear distance $R=2$, which is very close to the equilibrium bond length. (The renormalized D-dimensional Hamiltonian for this problem is described in Ref. 23.) There is noticeable improvement in accuracy from the Darboux approximants. This is seen as well for other values of R.

VI. DISCUSSION

Our central results are the following: (1) Summation accuracy depends significantly on removing the Coulombic poles at the $D\rightarrow 1$ limit, and rescaling removes the first-order pole more effectively than subtraction using an approximate residue. (2) Renormalization of the D-dimensional Hamiltonian, by multiplying the interelectron potential with a polynomial in δ can significantly improve the rate of convergence. (3) Comparison of results from shifted Borel transforms, given by Eqs. (6) and (7), yields a standard deviation σ_k that provides a reliable estimate of the summation accuracy at given order k. A reasonable summation procedure is to carry out a series of inexpensive moderate-order calculations using a quadratic $\lambda(\delta)$ over the full range of λ_0 values, with some arbitrary value of $\lambda(1)$, in order to determine an approximate range of λ_0 that can be expected to yield the fastest convergence. In the case of He, for example, a plot such as in Fig. 2 would suggest $0.15\leqslant\lambda_0\leqslant 0.25$. Then additional moderate-order calculations could be used to determine an optimal pair of λ_0 and $\lambda(1)$ to be used in the expensive large-order calculation.

One could smooth the convergence of the approximant sequence by using the mean $\overline{S_k}$ of various shifted approximants, eliminating $\overline{S_k}$ that have large σ_k. For example, if σ_{27} is greater than σ_{26}, as in Fig. 4, then $\overline{S_{26}}$ would be retained as the 27th-order result.

We find that the best two-parameter fit of summation accuracy versus order, for two-electron atoms and for H_2^+, is $\alpha(k)=\alpha_0+\alpha_1 k^{1/2}$. However, there appears to be a systematic deviation from this behavior, with a leveling off of accuracy at intermediate orders followed by an increase at higher orders, which led us to use cubic polynomials for the fits in Fig. 1. For He the plateau is at approximately eight significant figures. This effect was noted in Ref. 15, for unrenormalized expansions, and was attributed to the need to model more than just the dominant singularity in the Borel function. For He one obtains approximately three significant figures by explicitly including the poles at $\delta=1$, and apparently, seven figures from modeling also the dominant branch point in the Borel function. This explanation is supported by the behavior of the Darboux–Borel summation for H_2^+ in Fig. 5, which explicitly includes the square-root branch point. In that case there is rapid convergence to almost seven figures at 14th order but then it is not until 29th order that the convergence resumes. The plateau for the Padé–Borel results is less distinct, presumably because at intermediate orders the Padé approximants are still refining the description of the branch point while also attempting to decipher other singularity structure. By order 27 the Padé–Borel accuracy is about equal to the Darboux–Borel accuracy.

We have shown results only for ground states, but in general we expect similar singularity structure, and hence similar convergence behavior, for the lowest eigenstate of any given symmetry. With other excited states there are branch points in the *energy* function $E(\delta)$.[31] Although not the dominant singularities, in practice they dominate the convergence behavior until very high order. For example, it has been estimated[31] that the asymptotic behavior due to the singularity at the origin for the $1s2s\ ^1S$ state of He will not assert itself until 88th order. In that case Borel summation is not very effective, and it is more appropriate to use a summation method designed to model the apparent dominating singularities.

Recent tenth-order calculations for the three-electron atom[16] show convergence behavior almost identical to that for two-electron atoms. It remains to be seen if this will hold as well for four-electron atoms. Loeser[6] has formulated the $1/D$ expansion for S states of all atoms in the periodic table. However, with four electrons there are ten independent internal coordinates at large D but only 9 at $D=3$. Therefore it is not clear that Loeser's theory will converge to the physical solution when taken to large order. Such coordinate redundancies proliferate quadratically as the number of electrons increases. An alternative formulation that avoids this situation is ''partial'' dimensional continuation, applied recently in a study of triatomic molecular rotation spectra.[45] In that case one body-fixed axis was allowed to rotate in D dimensions while the other axis was treated as rotating about the first in only three dimensions. Some sort of related procedure could, in principle, give a D-dependent Hamiltonian with the physical number of coordinates.

Probably a more serious obstacle to applying the $1/D$ expansion to many-electron systems is the rapid increase in computational cost with increasing numbers of internal coordinates.[14] With larger systems it will be necessary to introduce approximations, such as separability assumptions[46] or basis-set truncations. The tradeoff will be between a small systematic error, from a large-order inexact theory, and a random, but possibly larger, error from truncating the exact theory at lower order.

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