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Scaling in Second-Order Electron Correlation Calculations Using Systematic Sequences of Even-Tempered Basis Sets*

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Improved results can often be obtained from second-order Rayleigh–Schrödinger perturbation calculations of electron correlation energies using large basis sets by introducing a scaling factor in the zero-order Hamiltonian. The scaling parameter may be determined from full third-order calculations using a smaller basis set. This scaling procedure can be applied in a systematic fashion by employing a sequence of even-tempered basis sets. Calculations illustrating this approach for the beryllium atom and the neon atom are presented. The scaling procedure is also employed in conjunction with a universal systematic sequence of basis functions. Calculations illustrating this Correlation energy – Mang-body perturbation theory.

Key words: Basis set – Even-tempered basis set – Universal basis set – Correlation energy — Many-body perturbation theory.

1. Introduction

The absolute accuracy of atomic and molecular electronic structure calculations is ultimately determined by the quality of the basis set employed. The use of basis sets in molecular calculations is almost obligatory due to the impossibility of factorising the molecular field. To perform accurate calculations large basis sets

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are required. However, the use of large basis sets makes the computations time-consuming (e.g. the time required for integral evaluation depends on the fourth power of the number of basis functions while the time required for a four-index transformation depends on the fifth power). Clearly, in order to perform accurate calculations the construction of large basis sets and the development of efficient schemes for handling them are required.

In this paper three recent developments in the construction of large basis sets are combined; namely,
(i) even-tempered basis sets [1–6]
(ii) universal basis sets [7–11]
(iii) systematic sequences of basis sets [12–15].
These developments are employed in conjunction with two advances in the calculation of correlation energies:
(i) many-body perturbation theory of molecules [16–20]
(ii) scaling of the reference Hamiltonian [21–24]
It is demonstrated that by combining these concepts a potentially very efficient and accurate technique for calculating electron correlation energies can be obtained.

In the following section an outline of the scaling technique is given. Even-tempered basis sets are briefly discussed in Sect. 3 and the use of systematic sequences of even-tempered basis sets is described in Sect. 4. In Sect. 5, the use of scaling in second-order electron correlation energy calculations using a systematic sequence of even-tempered basis functions is described and illustrative calculations are presented for the beryllium atom and for the neon atom. Universal even-tempered basis sets are briefly discussed in Sect. 6 and the use of a universal systematic sequence of even-tempered basis sets is addressed in Sect. 7. The use of scaling in second-order calculations using a universal systematic sequence of even-tempered basis sets is described in Sect. 8 and some illustrative calculations are presented for radial beryllium-like ions. This is followed by the concluding remarks.

2. Scaling in Electron Correlation Calculations

The introduction of a scaling parameter in the zero-order Hamiltonian used to generate perturbative expansions goes back to the work of Feenberg and his collaborators [25]. Recently it has been shown [21] that improved results can often be obtained from second-order Rayleigh–Schrödinger perturbation studies of electron correlation energies using large basis sets by introducing a scaling parameter, μ, in the zero-order Hamiltonian, $\hat{\mathscr{H}}_0$, giving

$$\mu\hat{\mathscr{H}}_0.$$

The modified perturbation is then

$$\hat{\mathscr{H}}_1+(1-\mu)\hat{\mathscr{H}}_0$$

so that the full Hamiltonian is recovered by adding the zero-order operator and the perturbing operator. The scaled energy components, which will be distinguished by a tilde, are related to the original energy components as follows: [25–27]

$$\begin{aligned}
&\tilde{E}_0+\tilde{E}_1=E_0+E_1\\
&\tilde{E}_2=\mu^{-1}E_2\\
&\tilde{E}_3=\mu^{-2}E_3+\mu^{-2}(\mu-1)E_2\\
&\tilde{E}_4=\mu^{-3}E_4+2\mu^{-3}(\mu-1)E_3+\mu^{-3}(\mu-1)^2E_2.
\end{aligned}$$

The scaling factor may be chosen so that $\tilde{E}_3=0$; that is [26]

$$\mu=1-E_3/E_2.$$

In the scaling procedure suggested in Ref. [21], μ is determined from a full third-order energy calculation using a basis set of moderate size. This value of μ is introduced into a second-order calculation using a large basis set.

The use of the scaling technique has been demonstrated previously for the beryllium atom and for the neon atom [21, 23]. It has also been employed in the calculation of molecular polarisabilities by many-body perturbation theory [24].

The scaled second-order energy, $\mu^{-1}E_2$ is closely related to the [2/1] Padé approximant to the energy series. The [2/1] Padé approximant can be constructed from third-order calculations and, since it has the form of a geometric series, it is sometimes referred to as the "geometric approximation". However, this name does not reflect the nature of the perturbation series, since terms obtained by expanding the [2/1] Padé approximant do not correspond to higher-order terms in the perturbation expansion [22, 23].

3. Even-tempered Basis Sets

In an even-tempered basis set the orbital exponents, ζ_k, are taken to form a geometric series dependent on two parameters α and β; thus

$$\zeta_k=\alpha\beta^k \qquad k=1,2,\ldots,M.$$

The selection of orbital exponents in this fashion appears to have been first suggested in 1963 by Reeves and Harrison [1–2]. More recently, this approach has been followed by Ruedenberg and his coworkers [3–6] who suggested the term "even-tempered" to describe these basis sets.

An even-tempered basis set cannot become linearly dependent since in practice the parameter β always remains greater than one. The value of the overlap integral between two normalised Gaussian or Slater functions depends only on the ratio of the exponents and thus, for a given symmetry, the elements of the overlap matrix are constant along diagonal lines. This suggests that even-tempered basis sets span the Hilbert space evenly.

4. Systematic Sequences of Even-Tempered Basis Sets

Feller and Ruedenberg [12] and Schmidt and Ruedenberg [13] have devised schemes for systematically extending basis sets of the even-tempered type. They applied their scheme to a number of atomic systems using the Hartree–Fock model and sets of Gaussian primitive functions. The present author [14] has examined this technique for atomic calculations which take account of electron correlation by means of the many-body perturbation theory. The systematic approach enables the convergence of the calculations with respect to the size of the basis set to be examined and the basis set limit estimated. It is also possible to derive empirical upper bounds and empirical lower bounds to the basis set limit by making assumptions about the convergence properties of the calculated energies with respect to the size of the basis set.

For an even-tempered basis set to approach a complete set as the number of functions, N, is increased it is necessary that α and β be functions of N. Since $\alpha \to 0$, $\beta \to 1$ and $\beta^N \to \infty$ as $N \to \infty$, Ruedenberg and his co-workers have suggested that the empirical forms [12, 13]

$$\ln \ln \beta = b \ln N + b'$$

$$\ln \alpha = a \ln (\beta - 1) + a'$$

be used to determine α and β for a given N. The constants a, a', b and b' may be determined by a leasted squares fit to "energy-optimised" values of the exponents for even-tempered basis sets of different sizes.

5. Scaling in Electron Correlation Energy Calculations Using a Systematic Sequence of Even-Tempered Basis Sets

In scaling the zero-order Hamiltonian in correlation calculations in the manner described in Sect. 2, it is clearly desirable that the two basis sets involved be related in a well defined fashion. The scaling technique can be applied to a series of calculations corresponding to a systematic sequence of even-tempered basis sets as described in Sects. 3 and 4.

Table 1. Values of $\mu[ns]^{-1}E_2[ms]$, $m \geq n$, for the ground state of the beryllium atom. The sequence of basis sets given by Schmidt and Ruedenberg for Be was used[a]

$[ms]$	E_2	$\mu[6s]$	$\mu[8s]$	$\mu[10s]$	$\mu[12s]$	$\mu[14s]$	$\mu[16s]$	$\mu[18s]$	$\mu[20s]$
$[6s]$	15.080	17.140							
$[8s]$	15.662	17.800	18.089						
$[10s]$	15.832	17.994	18.285	18.322					
$[12s]$	15.881	18.050	18.343	18.380	18.384				
$[14s]$	15.906	18.078	18.371	18.409	18.413	18.421			
$[16s]$	15.916	18.090	18.383	18.420	18.425	18.433	18.434		
$[18s]$	15.922	18.096	18.389	18.426	18.431	18.439	18.440	18.440	
$[20s]$	15.925	18.099	18.393	18.430	18.434	18.442	18.444	18.444	18.444

[a] All energies are in millihartree with signs reversed.

In Table 1, the result of introducing a scaling parameter into previously reported calculations [14] on the beryllium atom are shown. The sequence of Gaussian basis sets given by Schmidt and Ruedenberg [13] for Be were used to calculate the correlation energy in the "s limit" using third-order many-body perturbation theory. Eight basis sets, denoted by $[ns]$ $n = 6, 8, \ldots, 20$, were employed. The value of the scaling parameter has been determined, such that $\tilde{E}_3 = 0$, for each basis set and applied to all second-order calculations using basis sets which are at least as large. Thus $\mu[ns]^{-1}E_2[ms]$, $m \geqslant n$ denotes a scaled second-order energy in which the parameter μ is given by

$$\mu[ns] = 1 - E_3[ns]/E_2[ns].$$

Some of the results are displayed in Fig. 1. The lowest curve shows $\mu[ns]^{-1}E_2[20s]$ as a function of n, which can be seen to have converged to within 0.1 millihartree of $\mu[20s]^{-1}E_2[20s]$ when $n = 8$. The other curves shown are $\mu[6s]^{-1}E_2[ns]$, $\mu[8s]^{-1}E_2[ns]$, $\mu[10s]^{-1}E_2[ns]$. $E_2[ns]$ is also shown for comparison.

In Table 2 the results obtained by using the scaling procedure are shown for the neon atom using the $[2ns/np]$ "energy-balanced" sequence of even-tempered basis sets given by Schmidt and Ruedenberg [13]. The many-body perturbation

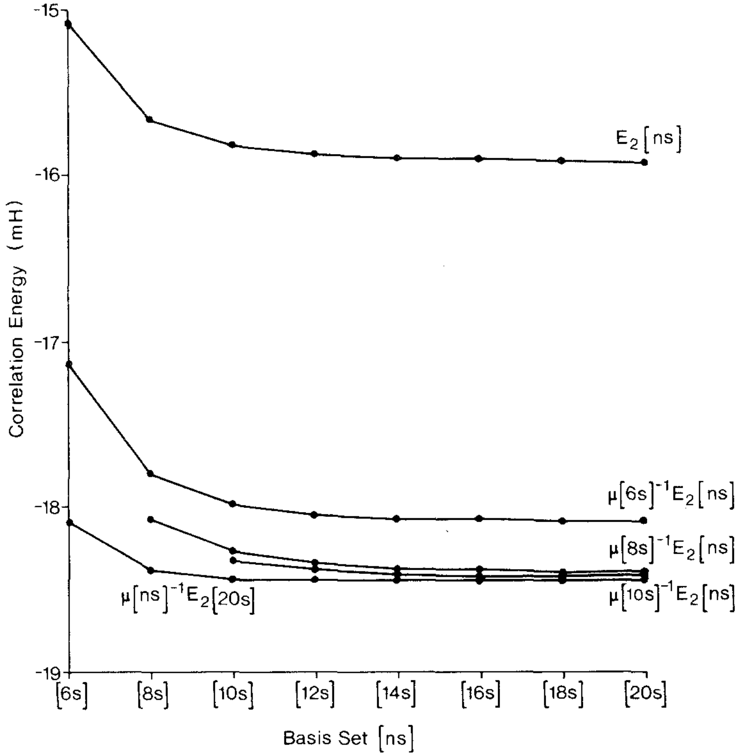

Fig. 1. Convergence of various scaled second-order energies with basis set size

Table 2. Values of $\mu[2ns/np]^{-1}E_2[2ms/mp]$, $m \geq n$, for the ground state of the neon atom. The "energy balanced" sequence of basis sets given by Schmidt and Ruedenberg for Ne was used[a]

$[2ms/mp]E_2$		$\mu[6s/3p]$	$\mu[8s/4p]$	$\mu[10s/5p]$	$\mu[12s/6p]$	$\mu[14s/7p]$	$\mu[16s/8p]$	$\mu[18s/9p]$
$[6s/3p]$	142.508	141.775						
$[8s/4p]$	170.469	169.592	167.554					
$[10s/5p]$	184.189	183.241	181.040	180.446				
$[12s/6p]$	189.122	188.149	185.888	185.278	185.080			
$[14s/7p]$	190.769	189.435	187.507	186.507	186.892	186.570		
$[16s/8p]$	191.414	190.430	188.141	187.524	187.323	187.201	187.166	
$[18s/9p]$	191.691	190.705	188.413	187.796	187.594	187.472	187.437	187.430

[a] All energies are in millihartree with signs reversed.

theory calculations using this sequence of basis sets have again been reported in Ref. [14]. It can be seen that $\mu[10s/5p]^{-1}E_2[18s/9p]$ is within 1 millihartree of $\mu[18s/9p]^{-1}E_2[18s/9p]$. Note that, unlike the calculated correlation energies for the beryllium atom, the correlation energies for the neon atom decrease in magnitude along the sequence $\mu[2ns/np]^{-1}E_2[18s/9p]$.

6. Universal Even-Tempered Basis Sets

In order to perform accurate molecular electronic structure calculations it is necessary to employ large basis sets. Large basis sets are necessarily flexible and can thus, with very little loss in accuracy, be transferred from system to system, at least for the first- and second-row of the periodic table. Such a basis set has been termed a "universal basis set" [7–11]. It is convenient to take a universal basis set to be of the even-tempered type. The advantages which result from the use of a universal even-tempered basis set have been discussed in detail previously [7–11]. The use of a universal even-tempered basis set has been demonstrated for both atoms and molecules within the matrix Hartree–Fock model and in calculations which include electron correlation effects by means of many-body perturbative techniques [7–11].

7. Systematic Sequence of Universal Even-Tempered Basis Sets

The scheme devised by Ruedenberg and his co-workers [12, 13] for systematically extending basis sets of the even-tempered type can be applied to universal even-tempered basis sets of the type described in Sect. 6. The same sequence of basis sets is used in calculations on a series of atoms irrespective of their nuclear charges. This approach has been investigated by the present author [15] by performing matrix Hartree–Fock calculations and correlation calculations for the radial beryllium-like ions Li^-, B^+, C^{2+}, N^{3+}, O^{4+}, F^{5+}, Ne^{6+}, using the basis set given by Schmidt and Ruedenberg [13] for the beryllium atom. Both the Hartree–Fock energies and the correlation energies for the neutral and positively charged species were found to converge satisfactorily with respect to the size of the basis set. On the other hand, for the Li^- ion the convergence properties with respect to

Table 3. Values of $\mu[ns]^{-1}E_2[ms]$, $m \geq n$, for beryllium-like ions. The sequence of basis sets given by Schmidt and Ruedenberg for Be was used in all calculations[a]

Li^-

$[ms]$	E_2	$\mu[6s]$	$\mu[8s]$	$\mu[10s]$	$\mu[12s]$	$\mu[14s]$	$\mu[16s]$	$\mu[18s]$	$\mu[20s]$
$[6s]$	13.302	15.302							
$[8s]$	14.084	16.201	16.444						
$[10s]$	14.435	16.605	16.854	16.995					
$[12s]$	14.716	16.928	17.182	17.325	17.347				
$[14s]$	14.939	17.185	17.442	17.588	17.610	17.859			
$[16s]$	15.123	17.397	17.658	17.805	17.827	18.080	18.191		
$[18s]$	15.279	17.576	17.839	17.988	18.010	18.265	18.378	18.477	
$[20s]$	15.411	17.727	17.993	18.143	18.166	18.423	18.537	18.637	18.603

B^+

$[ms]$	E_2	$\mu[6s]$	$\mu[8s]$	$\mu[10s]$	$\mu[12s]$	$\mu[14s]$	$\mu[16s]$	$\mu[18s]$	$\mu[20s]$
$[6s]$	15.585	17.435							
$[8s]$	15.522	17.365	17.250						
$[10s]$	15.744	17.613	17.497	17.581					
$[12s]$	15.780	17.653	17.536	17.621	17.622				
$[14s]$	15.796	17.671	17.554	17.639	17.640	17.639			
$[16s]$	15.809	17.685	17.568	17.653	17.654	17.652	17.665		
$[18s]$	15.815	17.692	17.575	17.660	17.661	17.659	17.662	17.662	
$[20s]$	15.818	17.696	17.578	17.663	17.664	17.663	17.666	17.666	17.666

C^{2+}

$[ms]$	E_2	$\mu[6s]$	$\mu[8s]$	$\mu[10s]$	$\mu[12s]$	$\mu[14s]$	$\mu[16s]$	$\mu[18s]$	$\mu[20s]$
$[6s]$	14.551	15.687							
$[8s]$	15.748	16.978	17.238						
$[10s]$	15.660	16.883	17.142	17.101					
$[12s]$	15.743	16.972	17.232	17.191	17.213				
$[14s]$	15.772	17.003	17.264	17.223	17.244	17.244			
$[16s]$	15.780	17.012	17.272	17.231	17.253	17.253	17.251		
$[18s]$	15.787	17.019	17.280	17.239	17.260	17.260	17.259	17.259	
$[20s]$	15.790	17.023	17.284	17.243	17.264	17.264	17.263	17.263	17.263

N^{3+}

$[ms]$	E_2	$\mu[6s]$	$\mu[8s]$	$\mu[10s]$	$\mu[12s]$	$\mu[14s]$	$\mu[16s]$	$\mu[18s]$	$\mu[20s]$
$[6s]$	15.480	16.653							
$[8s]$	15.419	16.587	16.579						
$[10s]$	15.690	16.879	16.871	16.900					
$[12s]$	15.745	16.937	16.929	16.959	16.971				
$[14s]$	15.756	16.950	16.941	16.971	16.983	16.980			
$[16s]$	15.774	16.969	16.961	16.991	17.003	16.999	17.003		
$[18s]$	15.780	16.975	16.967	16.997	17.009	17.006	17.009	17.009	
$[20s]$	15.784	16.979	16.971	17.001	17.013	17.009	17.013	17.013	17.013

Table 3 (cont.)

O^{4+}

[*ms*]	E_2	μ[6*s*]	μ[8*s*]	μ[10*s*]	μ[12*s*]	μ[14*s*]	μ[16*s*]	μ[18*s*]	μ[20*s*]
[6*s*]	16.029	17.193							
[8*s*]	15.339	16.453	16.308						
[10*s*]	15.729	16.872	16.722	16.786					
[12*s*]	15.716	16.858	16.709	16.772	16.759				
[14*s*]	15.765	16.911	16.761	16.824	16.811	16.820			
[16*s*]	15.774	16.920	16.770	16.833	16.820	16.829	16.828		
[18*s*]	15.780	16.927	16.777	16.841	16.827	16.836	16.835	16.835	
[20*s*]	15.785	16.932	16.782	16.845	16.832	16.841	16.840	16.840	16.840

F^{5+}

[*ms*]	E_2	μ[6*s*]	μ[8*s*]	μ[10*s*]	μ[12*s*]	μ[14*s*]	μ[16*s*]	μ[18*s*]	μ[20*s*]
[6*s*]	15.290	16.192							
[8*s*]	15.606	16.527	16.515						
[10*s*]	15.636	16.559	16.547	16.541					
[12*s*]	15.742	16.670	16.658	16.652	16.662				
[14*s*]	15.765	16.690	16.683	16.677	16.686	16.688			
[16*s*]	15.775	16.706	16.694	16.688	16.697	16.700	16.699		
[18*s*]	15.785	16.716	16.704	16.698	16.707	16.710	16.709	16.710	
[20*s*]	15.788	16.720	16.707	16.701	16.711	16.713	16.713	16.713	16.713

Ne^{6+}

[*ms*]	E_2	μ[6*s*]	μ[8*s*]	μ[10*s*]	μ[12*s*]	μ[14*s*]	μ[16*s*]	μ[18*s*]	μ[20*s*]
[6*s*]	14.372	15.055							
[8*s*]	15.700	16.446	16.539						
[10*s*]	15.611	16.353	16.446	16.408					
[12*s*]	15.759	16.507	16.601	16.563	16.583				
[14*s*]	15.759	16.508	16.602	16.563	16.584	16.579			
[16*s*]	15.783	16.533	16.626	16.588	16.608	16.604	16.607		
[18*s*]	15.788	16.538	16.632	16.593	16.614	16.609	16.612	16.612	
[20*s*]	15.792	16.543	16.636	16.598	16.618	16.614	16.617	16.616	16.616

[a] All energies are in millihartree with signs reversed.

basis set size were observed to be somewhat worse than that for the neutral and positively charged species.

8. Scaling in Electron Correlation Calculations Using a Systematic Sequence of Universal Even-Tempered Basis Sets

Clearly the procedure for using scaling of the zero-order Hamiltonian in conjunction with a systematic sequence of basis sets, as outlined in Sect. 5, can be carried out for a universal sequence of even-tempered basis sets of the form described in Sects. 6 and 7. In Table 3 the results of a series of calculations using the scaling technique and a sequence of universal even-tempered basis sets for the

Table 4. Demonstration of improved convergence of scaled second-order energies[a]

Ion	Δ_1[b]	Δ_2[c]
Li^-	0.88	3.30
B^+	0.03	0.23
C^{2+}	0.24	1.58
N^{3+}	0.03	0.36
O^{4+}	0.10	0.35
F^{5+}	0.01	0.52
N^{6+}	0.07	1.56

[a] In millihartree.

[b] $\Delta_1 = |\mu[6s]^{-1}E_2[20s] - \mu[20s]^{-1}E_2[20s]|$.

[c] $\Delta_2 = |E_2[20s] - \mu[20s]^{-1}E_2[20s]|$.

radial beryllium-like ions Li^-, B^+, C^{2+}, N^{3+}, O^{4+}, F^{5+}, Ne^{6+} are presented. The sequence of even-tempered basis sets given by Schmidt and Ruedenberg [13] for the beryllium atom are used in all of the calculations. Eight basis sets denoted by $[ms]$ $m = 6, 8, \ldots, 20$, were used. For each basis set the values

$$\mu[ns]^{-1}E_2[ms] \qquad m \geq n$$

are given.

The improved convergence obtained by introduction of a scaling parameter in the zero-order Hamiltonian is illustrated in Table 4 where differences between $\mu[6s]^{-1}E_2[20s]$ and $\mu[20s]^{-1}E_2[20s]$, Δ_1, are compared with the differences between $E_2[20s]$ and $\mu[20s]^{-1}E_2[20s]$, Δ_2. In all cases Δ_1 is considerably smaller than Δ_2. All values of Δ_1 are less than one millihartree.

9. Concluding Remarks

In the present work we have used basis sets of Gaussian primitive functions. When the present method is applied with even-tempered exponential-type functions it will certainly lead to much higher accuracy with a comparatively modest computational effort. The use of a universal basis set negates the greater computation required to evaluate integrals over exponential functions since integrals can be stored and reused again and again.

Finally, we comment that the use of large basis sets will become increasingly tractable by use of vector processing computers [29] which can achieve considerable efficiency in matrix algebra. The use of the scaling procedure together with large universal systematic sequences of even-tempered basis sets should enable "chemical accuracy" of 1 millihartree to be approached for small molecules especially when it is noted that only a restricted four-index transformation is required [30] to obtain the integrals which arise in a second-order calculation and that it is the four-index transformation which is the most time-consuming phase of many present-day computations.

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