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Comparison within the algebraic approximation of configuration interaction and many-body perturbation theory for the Be ground state

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Calculations of the electronic energy of the Be-atom ground state are performed using a configuration-interaction technique and a nondegenerate formulation of diagrammatic many-body perturbation theory. Both methods are applied within the algebraic approximation defined by three finite-basis sets. One of the basis sets contains only *s* functions, and it defines an algebraic problem without degeneracies where agreement between the two methods is excellent. The other two basis sets, although more complete, both contain *p* functions, and they define algebraic problems involving a near degeneracy where agreement between the two methods is found to be less satisfactory. It is concluded that either a degenerate formulation of perturbation theory is required, or certain diagrams in the model perturbative scheme need to be summed to high order through denominator shifts in order to properly handle the nondynamic-correlation effect found in the Be atom.

I. INTRODUCTION

The determination of the electronic structure of an atom or molecule involves solving for an appropriate eigenvalue and eigenfunction of a semibounded self-adjoint Hamiltonian operator $\mathcal{H}$ in Hilbert space. A tractable scheme for treating such equations is the algebraic approximation in which eigenfunctions are parametrized by expansion in a finite set of functions. This procedure transforms differential equations into algebraic equations that need to be solved to find expansion coefficients. Use of the algebraic approximation induces a restriction on the domain of the operator $\mathcal{H}$ to a particular finite-dimensional subspace S of Hilbert space. For an N-electron system, the algebraic approximation may be implemented by defining a suitable orthonormal basis set containing $M(>N)$ one-electron spin orbitals and constructing all unique N-electron determinants that can be formed using the M one-electron functions. The number of unique determinants that can be formed is $\eta = \binom{M}{N}$, and η is the dimension of the subspace S spanned by the set of determinants. The algebraic approximation restricts the domain of $\mathcal{H}$ to this η-dimensional subspace. Even the exact solution to this restricted problem is only an approximation to the solution of the original problem. The quality of the approximation depends on the extent of "completeness" relative to the full Hilbert space of the η-dimensional subspace, which in turn is strongly dependent on the size and composition of the one-electron spin orbitals chosen as the expansion functions.

A given choice of basis functions defines a particular algebraic approximation. In principle, the exact solution to this restricted algebraic problem may be obtained by using a full configuration-interaction technique that includes all possible N-electron determinants (i.e., including all single, double, etc., and N-tuple excitations from a reference configuration). The exact solution to the algebraic problem may also be obtained, in principle, using appropriate convergent perturbation theory techniques in which all terms in the perturbative series are treated exactly. In practice, usually, neither the configuration-interaction nor the perturbation theory can be utilized without introducing further approximations and truncations.

The purpose of this work is to present a comparison of results obtained using configuration-interaction[1] and many-body perturbation theory,[2] where each of these methods is applied to the Be ground state within the same basis set. The Be atom is chosen because both methods can be applied to this system, and a large basis set has been determined.[1] There have been numerous previous calculations of the Be atom ground-state energy[3-13]; none of these is relevant to the specific objective of the present work.

Details of the theoretical approaches have been fully described previously[1,2,14]: the reader is referred to these earlier papers for all pertinent definitions. Section II of the present work contains the numerical results on the Be atom. A comparison of the results is given in Sec. III followed by a short discussion in Sec. IV.

II. CORRELATION ENERGIES OF THE Be ATOM

A. Basis sets

The Slater basis functions used in this work are given in Table I. These functions are the *s*, *p*, and *d* functions used in the previous Be atom work[1] except that a $3d(\zeta=16.0)$ function has been dropped from the previous set to facilitate current computer limitations. These functions are used to form three basis sets: one using only the ten *s* functions, a second using the ten *s* and nine *p* functions, and a third using all *s*, *p*, and *d* functions. The matrix Hartree-Fock reference energy obtained with this basis set is −14.57302 hartree.

TABLE I. Basis-set parameters of Slater orbitals for the Be atom (orbital exponents in bohr^{-1}).

10*s*		9*p*		7*d*	
1*s*	3.437	2*p*	1.036	3*d*	1.6
1*s*	6.225	2*p*	2.9	3*d*	7.1
2*s*	0.869	3*p*	2.1	4*d*	1.74
2*s*	7.45	3*p*	14.9	4*d*	16.0
3*s*	1.08	4*p*	5.0	5*d*	2.55
3*s*	1.776	4*p*	14.0	5*d*	16.0
3*s*	8.8	5*p*	14.0	6*d*	16.0
4*s*	2.7	6*p*	2.8		
4*s*	16.0	6*p*	14.0		
5*s*	2.2				

B. Results of configuration-interaction calculations

The correlation energy has been computed using a variety of trial wave functions. One of these choices consists of the matrix Hartree-Fock single determinant as a reference state plus all possible configurations that are doubly excited relative to the reference state. The corresponding energy is designated ΔE_D. Another choice consists of the reference state plus all singly and doubly excited states: the energy is ΔE_{SD}. The numerical results are presented in Table II for the three choices of basis set. In addition, for the *spd* basis, a further calculation was performed using a natural orbital scheme, described previously,[1] which included 511 configurations including a selection of single, double, triple, and quadruple excitations from the reference natural orbital: this energy is ΔE_{SDTQ}. Finally, an extrapolation procedure[1] was used to obtain an extrapolated "full CI" energy, ΔE_{extrap}.

The calculated energies have been split into energy increments in Table III to indicate their source. After the double excitations, the triple and quadruple excitations are next in importance but an order of magnitude smaller than the double-excitation contribution. The single excitations are still another order of magnitude smaller. For correlation purposes, the *p* functions are the most important. Of course, the *p* subspace includes the nondynamical correlation effect[15] arising from the near degeneracy of the $1s^22s^2$ and $1s^22p^2$ configurations in Be. However, the energy increment corresponding to the lowest $1s^22p^2$ configuration is −0.044 hartree.[16] Thus the residual increment from double excitations in the *p* subspace is about −0.021 hartree which is larger than the *s* or *d* contributions.

C. Results of perturbation calculations

The components of the perturbation expansions for the correlation energy of Be are presented in Table IV. Two different reference Hamiltonians are used[2] to generate perturbation series: model and shifted. The relative importance of the various diagrammatic contributions is evident.

The convergence of the perturbation series is displayed in Table V as a function of the number of interacting bodies through third order. The addition of *d* functions is rather ineffective in the

TABLE II. Correlation energies from configuration interaction calculations for Be (energy in hartree).

Basis set	10*s*	10*s* + 9*p*	10*s* + 9*p* + 7*d*
ΔE_D	−0.01863	−0.08401	−0.08779
ΔE_{SD}	−0.01869	−0.08457	−0.08837
ΔE_{SDTQ}			−0.09239
ΔE_{extrap}			−0.09243

TABLE III. Energy increments from configuration interaction calculations for Be (energy in hartree).

Source of increment[a]	s	p	d	spd
Doubles[b]	−0.01863	−0.06538	−0.00378	−0.08779
Singles[c]	−0.00006	−0.00050	−0.00002	−0.00058
Triples + quadruples[d]				−0.00402

[a] Column headings indicate the group of basis functions from which the energy increment is obtained. For instance, p represents $E(sp)-E(s)$, and $E(sp)$ is the energy obtained with the sp basis.

[b] Correlation energy corresponding to ΔE_D.

[c] Correlation energy corresponding to $\Delta E_{SD}-\Delta E_D$.

[d] Correlation energy corresponding to $\Delta E_{SDTQ}-\Delta E_{SD}$.

shifted scheme but has a sizable effect on the two-body terms in the model scheme. The distribution of two-body energy contributions among the electron pairs in Be is shown in Table VI. The effect of the d functions is strong for E_2 both in the model and shifted scheme and for the restricted third-order energy in the model scheme. As is seen in Table V, the d functions are rather ineffective for the total two-body restricted third-order energies in the shifted scheme. However, this ineffectiveness can be seen from Table VI to arise from a cancellation due to a positive contribution to the $2s^2$ pair in the third-order (shifted) energy.

To give another representation of the source of the correlation energy contributions, a second-order energy increment is defined using the previous[2] notation:

$$\epsilon_{ij}(ab) = \langle ij|O|ab\rangle\langle ab|O|ij\rangle/D_{ijab}. \tag{1}$$

The second-order energy is therefore a sum of these increments

$$E_2 = \sum_{i<j}\sum_{a<b}\epsilon_{ij}(ab). \tag{2}$$

The energy increments are plotted in Fig. 1 for the model scheme as a function of the unoccupied orbitals (a, b) for each occupied pair (i, j). The unoccupied orbitals are arranged in order of increasing orbital energy as indicated in Fig. 2. The contributions to the core arise predominantly from the orbitals 4–6 of the unoccupied list. The core-valence contributions are an order of mag-

TABLE IV. Components of the perturbation expansions for Be.[a]

Basis set	$10s$		$10s+9p$		$10s+9p+7d$	
$\mathcal{H}_0$	model	shifted	model	shifted	model	shifted
			Intrapair energies (two–body)			
E_2^2	−0.01590	−0.01736	−0.06425	−0.09347	−0.07195	−0.10272
E_3^2(pp)	+0.00170	+0.00125	+0.01689	+0.02136	+0.02153	+0.03112
E_3^2(hp)	−0.00552	−0.00240	−0.04404	−0.01977	−0.04708	−0.02032
E_3^2(hh)	+0.00168	0.0	+0.01233	0.0	+0.01316	0.0
		Interpair interactions between pairs having a common hole state (three–body)				
E_3^3(hp)	−0.00014	−0.00016	+0.00044	+0.00108	+0.00044	+0.00109
E_3^3(hh)	+0.00009	+0.00010	+0.00007	+0.00006	+0.00007	+0.00006
		Interpair interactions between pairs having no common hole states (four–body)				
E_3^4(hh)	+0.00001	+0.00002	+0.00003	+0.00005	+0.00003	+0.00005
Overlap Δ_{II}	+0.00216	+0.00352	+0.02829	+0.13549	+0.03033	+0.13944

[a] Energy terms are labeled with subscripts to denote order and superscripts to denote number of interacting bodies. The parenthetical description indicates the nature of the diagram from which the energy is calculated: h ≡ hole, p ≡ particle. Energies are in hartree.

TABLE V. Convergence of the perturbative series with increasing number of interacting bodies for the correlation energy of Be (energy in hartrees).

Basis set		10*s*	10*s* + 9*p*	10*s* + 9*p* + 7*d*
E_2+E_3 model	two–body	−0.01805	−0.07907	−0.08434
	three–body	−0.00005	+0.00051	+0.00051
	four–body	+0.00001	+0.00003	+0.00003
E_2+E_3 shifted	two–body	−0.01851	−0.09187	−0.09192
	three–body	−0.00006	+0.00114	+0.00115
	four–body	+0.00002	+0.00005	+0.00005

nitude smaller but arise predominantly from orbitals 3–5. The valence contributions arise from the lowest unoccupied orbitals and principally from the lowest unoccupied *p* orbital, as would be expected since this is the orbital responsible for the nondynamic correlation effect.[15]

A summary of the various perturbative correlation energy contributions is given in Table VII. Also included are the [2/1] Padé approximants $E[2/1]$ and the many-body perturbative upper bounds E_{var}. For the *spd* basis, the contributions arising from quadruple excitations in fourth order in the model scheme[17] are presented in Table VIII. The unlinked diagrams contribute about −2 mhartree while the linked diagrams contribute about +1 mhartree.

III. COMPARISON OF METHODS

The total energies calculated for the Be atom are summarized in Table IX. In addition, the matrix Hartree-Fock reference energy, the estimated nonrelativistic energy eigenvalue[1] for Be, and the estimated correlation energy for Be are presented.

A direct comparison of the configuration-interaction and perturbation theory results is given in Table X. Using a given basis set defines a particular eigenvalue problem within the algebraic approximation. For the full *spd* basis set, E_{extrap} is taken to be a good estimate of the exact eigenvalue of the corresponding algebraic problem. For the *s* and *sp* basis sets, E_{SD} is used for comparison purposes. A further comparison is presented in Table XI which gives an indication of the quality of the various algebraic approximations relative to the estimated correct nonrelativistic results[1] for the Be atom.

The most obvious feature of Tables X and XI is that the second-order energy results are in poor agreement for both the model and shifted scheme. The full third-order results are much better be-

TABLE VI. Two–body pair energies for the Be atom (energies in hartrees).

Basis set		10*s*	10*s* + 9*p*	10*s* + 9*p* + 7*d*
E_2 model	$1s^2$	−0.01247	−0.03492	−0.03844
	$1s$-$2s$	−0.00108	−0.00488	−0.00529
	$2s^2$	−0.00236	−0.02445	−0.02822
	total	−0.01591	−0.06425	−0.07195
E_2 shifted	$1s^2$	−0.01305	−0.03661	−0.04028
	$1s$-$2s$	−0.00118	−0.00545	−0.00589
	$2s^2$	−0.00313	−0.05141	−0.05656
	total	−0.01736	−0.09347	−0.10272
$E_2+E_3^{\text{2-body}}$ shifted	$1s^2$	−0.01374	−0.03788	−0.04096
	$1s$-$2s$	−0.00119	−0.00555	−0.00592
	$2s^2$	−0.00312	−0.03565	−0.03746
	total	−0.01805	−0.07907	−0.08434
$E_2+E_3^{\text{2-body}}$ shifted	$1s^2$	−0.01383	−0.03808	−0.04111
	$1s$-$2s$	−0.00120	−0.00567	−0.00604
	$2s^2$	−0.00348	−0.04812	−0.04477
	total	−0.01851	−0.09187	−0.09192

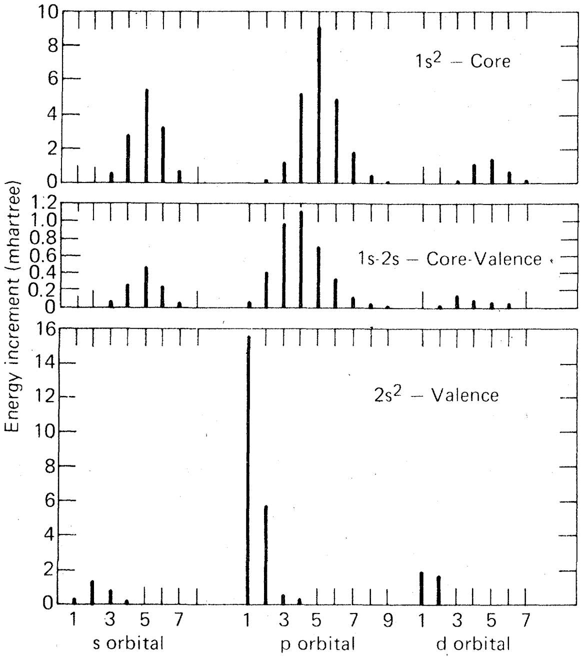

FIG. 1. Energy increments to the second-order energy in the model perturbative scheme as a function of the unoccupied orbitals.

haved as are the [2/1] Padé approximants and the optimized upper bounds. For the s basis, all of the third-order results tend to be in reasonable corresponding agreement.

One measure of the convergence of the perturbation series is obtained by comparing the extent of agreement between corresponding results obtained in the model and shifted scheme. This is because the converged result should be invariant to changes in the unperturbed Hamiltonian. For the sp and spd basis sets, the best agreement is found for the $E_{\mathrm{var}}(\gamma_{\mathrm{opt}})$ which signifies that these are perhaps the most reliable of the perturbative results. If so, then the remaining third-order results in the model scheme would be judged more reliable than the shifted results.

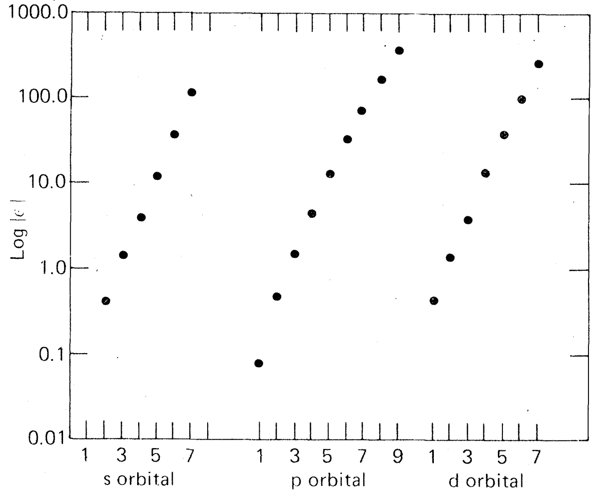

FIG. 2. Logarithm of the absolute value of the orbital energy of the unoccupied orbitals.

A second measure of the convergence of the perturbative expansions is to compare the extent of agreement between the two third-order results, E_2+E_3 and $E[2/1]$, within a given perturbative scheme. The converged result should be independent of whether a Taylor series or Padé approximant representation of the energy is employed. From this point of view, the shifted scheme shows reasonable convergence. In this regard, it is interesting to note that previous perturbative calculations for Be by Kelly[12] and by Kaldor[13] had achieved excellent correlation energies using shifted denominator techniques corresponding to the shifted scheme of the present work.

Another feature of interest is that for the s basis, all of the third-order perturbative results are in much better agreement with the s basis configuration-interaction values than are the corresponding

TABLE VII. Perturbative correlation energies, the [2/1] Padé approximants and the many-body perturbative upper bounds for Be (energies in hartrees).

Basis set	10s		10s + 9p		10s + 9p + 7d	
$\mathcal{H}_0$	model	shifted	model	shifted	model	shifted
E_2	−0.01591	−0.01736	−0.06425	−0.09347	−0.07195	−0.10272
$E_2+E_3^{2\text{-body}}$ shifted	−0.01805	−0.01851	−0.07907	−0.09187	−0.08434	−0.09192
E_2+E_3	−0.01808	−0.01855	−0.07853	−0.09068	−0.08380	−0.09072
$E[2/1]$	−0.01843	−0.01864	−0.08261	−0.09076	−0.08613	−0.09198
$E_{\mathrm{var}}(\gamma = 1)$	−0.01804	−0.01849	−0.07637	−0.07986	−0.08133	−0.07962
γ_{opt}	1.15517	1.06969	1.23065	0.87118	1.14924	0.81290
$E_{\mathrm{var}}(\gamma_{\mathrm{opt}})$	−0.01837	−0.01857	−0.07907	−0.08143	−0.08268	−0.08350

TABLE VIII. Fourth–order quadruple excitation contributions in the model perturbative scheme for Be using the *spd* basis (energy in hartree).

Source		Energy
Linked diagrams	$E_4(A_Q)$	−0.00041
	$E_4(B_Q+C_Q)$	−0.00087
	$E_4(D_Q+E_Q)$	+0.00041
	$E_4(F_Q+G_Q)$	+0.00190
Unlinked diagrams	$E_4(q_1+q_2)$	−0.00218
Total linked and unlinked diagrams		−0.00115
Total linked diagrams		+0.00104

results for the *sp* and *spd* basis sets. This is apparently a ramification of the absence of any near-degeneracy effect when the domain of the Hamiltonian is restricted to the subspace spanned by *s* functions. In this case, the strictly nondegenerate formulation[2] of perturbation theory is being applied to a strictly nondegenerate algebraic problem and the perturbative results to third order are in rather good agreement with the configuration interaction results. This is the situation that has been observed in several previous comparisons[2,18,19] involving strictly nondegenerate ground states of atoms and molecules.

When the domain of the Hamiltonian is allowed to include the subspace spanned by the *p* functions (as is the case for the *sp* and *spd* basis sets), then the near-degeneracy problem is present. As a measure of the magnitude of this difficulty, the normalized configuration-interaction coefficient of the $1s^22p^2$ configuration is[16] −0.2949 while the $1s^22s^2$ configuration has a coefficient of[16] 0.9533. Together these two configurations account for 0.9957 of the unit normalization integral for the full Be atom wave function.[1,16] Application of nondegenerate perturbation theory to this near-degenerate problem gives the somewhat degraded results indicated in Tables X and XI. A similar degradation for Be can be seen from a comparison of perturbative results for Be and Ne.[20]

IV. DISCUSSION

Because of the near-degeneracy of the $1s^22s^2$ and $1s^22p^2$ configurations for the Be atom, this is a severe test of the nondegenerate perturbation theory. It is an appropriate choice of system for

TABLE IX. Comparison of total energies for the Be atom (energy in hartree).

Basis	10*s* E_s	10*s* + 9*p* E_{sp}	10*s* + 9*p* + 7*d* E_{spd}
Configuration interaction			
E_D	−14.59165	−14.65703	−14.66081
E_{SD}	−14.59171	−14.65759	−14.66139
E_{extrap}			−14.66545
Perturbation theory—model scheme			
E_2	−14.58893	−14.63727	−14.64497
E_2+E_3	−14.59110	−14.65155	−14.65682
$E[2/1]$	−14.59145	−14.65563	−14.65915
$E_{\text{var}}(\gamma_{\text{opt}})$	−14.59139	−14.65209	−14.65570
Perturbation theory—shifted scheme			
E_2	−14.59038	−14.66649	−14.67574
E_2+E_3	−14.59157	−14.66370	−14.66374
$E[2/1]$	−14.59166	−14.66378	−14.66500
$E_{\text{var}}(\gamma_{\text{opt}})$	−14.59159	−14.65445	−14.65652

$E_{\text{SCF}}{}^{a} = -14.57302$ $E_{\text{nr}}{}^{b} = 14.66736$ $E_{\text{corr}}{}^{c} = -0.09434$

[a] E_{SCF} is the matrix Hartree–Fock reference energy.
[b] E_{nr} is the estimated nonrelativistic energy eigenvalue for Be from Ref. 1.
[c] $E_{\text{corr}} = E_{\text{nr}} - E_{\text{SCF}}$.

TABLE X. Comparison of calculated correlation energies with the estimated solution to the problem defined by the algebraic approximation.[a]

Basis	$10s$ $100(E-E_{SCF})/E_{SD}$	$10s+9p$ $100(E-E_{SCF})/E_{SD}$	$10s+9p+7d$ $100(E-E_{SCF})/E_{extrap}$
Configuration interaction			
E_D	99.7	99.3	95.0
E_{SD}	100.0	100.0	95.6
E_{extrap}			100.0
Perturbation theory—model scheme			
E_2	85.1	76.0	77.8
E_2+E_3	96.7	92.9	90.7
$E[2/1]$	98.6	97.7	93.2
$E_{var}(\gamma_{opt})$	98.3	93.5	89.5
Perturbation theory—shifted scheme			
E_2	92.9	110.5	111.1
E_2+E_3	99.3	107.2	98.1
$E[2/1]$	99.7	107.3	99.5
$E_{var}(\gamma_{opt})$	99.4	96.3	90.3

[a] Tabulated values are percentages: E_{SCF}, E_{SD}, and E_{extrap} are given in Table IX.

demonstrating the inherent limitation of a nondegenerate formulation of perturbation theory for applications involving a near degeneracy. The comparison of results in Table XI is particularly interesting in this regard since it exhibits excellent agreement between all of the third-order perturbative results and the configuration-interaction values for the nondegenerate algebraic problem defined by the s-orbital basis. Concurrently, it exhibits the degradation of this agreement especially for the model perturbative scheme when the near degeneracy is introduced into the algebraic problem by the inclusion of p functions in the basis set. Clearly a remedy for this problem is to take specific account of the $1s^22p^2$ configuration by using a degenerate formulation of perturbation theory, particularly when the model scheme is used to define the perturbative expansion.

It should be noted that the shifted third-order perturbative energies are in quite good agreement with the non relativistic energy eigenvalue for Be: E_2+E_3 and $E[2/1]$ in the shifted scheme give 96.2% and 97.5% of E_{corr}, respectively, while the extrapolated full configuration-interaction result

TABLE XI. Comparison of calculated correlation energies with the estimated correlation energy of the Be atom given as percentages of E_{corr}.[a]

Configuration interaction			
E_D	19.7	89.1	93.1
E_{SD}	19.8	89.6	93.7
E_{extrap}			98.0
Perturbation theory—model scheme			
E_2	16.9	68.1	76.3
E_2+E_3	19.2	83.2	88.8
$E[2/1]$	19.5	87.6	91.3
$E_{var}(\gamma_{opt})$	19.5	83.8	87.6
Perturbation theory—shifted scheme			
E_2	18.4	99.1	108.9
E_2+E_3	19.7	96.1	96.2
$E[2/1]$	19.8	96.2	97.5
$E_{var}(\gamma_{opt})$	19.7	86.3	88.5

[a] Tabulated values correspond to $100(E-E_{SCF})/E_{corr}$ where $E_{SCF}=-14.57302$ hartree and $E_{corr}=-0.09434$ hartree from Ref. 1.

gives 98.0%. One interpretation[21] of the significance of denominator shifts that are used in the shifted perturbation scheme is that they provide a means for summing certain diagrams in the model scheme to infinite order. In this sense, the shifted third-order result represents a compromise which includes all of the diagrammatic contributions through third order in the model scheme plus a selection of additional diagrams summed to infinite order. This interpretation allows for the conjecture that, although the third-order calculation in the model scheme is not sufficient to handle the near-degeneracy problem in Be, this difficulty can be overcome by including certain higher-order diagrammatic terms.

The use of a shifted zero-order Hamiltonian seems to lead to a more rapidly convergent perturbation series for the correlation energy. The shifted perturbation scheme has previously been found to converge more rapidly for the LiH and BH molecules.[18] This is due to the presence of low-lying virtual orbitals in these species. The small positive single-particle energies lead to denominators in the perturbation expansion based on the Hartree-Fock model operator which are very large. The use of the shifted zero-order operator appears to avoid this problem.

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[1] C. F. Bunge, Phys. Rev. A 14, 1965 (1976).

[2] S. Wilson and D. M. Silver, Phys. Rev. A 14, 1949 (1976).

[3] R. E. Watson, Phys. Rev. 119, 170 (1960).

[4] R. K. Nesbet, Phys. Rev. 155, 51 (1967).

[5] F. W. Byron and C. J. Joachain, Phys. Rev. 157, 7 (1967).

[6] C. F. Bunge, Phys. Rev. 168, 92 (1968).

[7] K. J. Miller and K. Ruedenberg, J. Chem. Phys. 48, 3414 (1968).

[8] J. S. Sims and S. Hagstrom, Phys. Rev. A 4, 908 (1971).

[9] J. Paldus and J. Cizek, in *Energy Structure and Reactivity*, edited by D. W. Smith and W. B. McRae (Wiley, New York, 1973), p. 198.

[10] E. Kansa, Phys. Rev. A 9, 1555 (1974).

[11] C. F. Fischer and K. M. S. Saxena, Phys. Rev. A 9, 1498 (1974).

[12] H. P. Kelly, Phys. Rev. 131, 684 (1963); Phys. Rev. B 136, 896 (1964).

[13] U. Kaldor, Phys. Rev. A 7, 427 (1973).

[14] D. M. Silver, Comput. Phys. Commun. 14, 71, 81 (1978); S. Wilson, Comput. Phys. Commun. 14, 91 (1978).

[15] D. F. Tuan and O. Sinanoğlu, J. Chem. Phys. 41, 2677 (1964).

[16] C. F. Bunge, At. Data Nucl. Data Tables 18, 293 (1976).

[17] S. Wilson and D. M. Silver, Molec. Phys. 36, 1539 (1978).

[18] S. Wilson and D. M. Silver, J. Chem. Phys. 66, 5400 (1977).

[19] S. Wilson and D. M. Silver, J. Chem. Phys. 67, 1689 (1977); S. Wilson, D. M. Silver, and R. J. Bartlett, Molec. Phys. 33, 1177 (1977); R. J. Bartlett, S. Wilson, and D. M. Silver, Intl. J. Quantum Chem. 12, 737 (1977); H. J. Silverstone, D. P. Carroll, and D. M. Silver, J. Chem. Phys. 68, 616 (1978).

[20] T. P. Eggarter and E. Eggarter, J. Phys. B 11, 1157, 2069, 2969 (1978).

[21] H. P. Kelly, Ad. Chem. Phys. 14, 129 (1969).