S2-level calculations

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I.

At the S2-level the computations are simple and fast. The basic equation to be solved is given in our paper in operator form as

$$0 = \langle 0| \Big\{ \mathbf{V_{02}} + \big[\mathbf{S_2}, \mathbf{V_{00}}\big] + \big[\mathbf{S_2}, (\mathbf{H_0} + \mathbf{U_0})\big] + \big[\mathbf{S_3}, \mathbf{V_{10}}\big] + \big[\mathbf{S_4}, \mathbf{V_{20}}\big] + \frac{1}{2}\Big[\mathbf{S_2}, \big[\mathbf{S_2}, \mathbf{V_{20}}\big]\Big] \Big\} |2p2h\rangle \, .$$

At the S_2-level we set $\mathbf{S_3} = \mathbf{S_4} = 0$. Then, taking the matrix elements yields:

$$\begin{aligned}
\langle p_1p_2|Z|h_1h_2\rangle \;=\; & \frac{-1}{e_{p_1} + e_{p_2} - e_{h_1} - e_{h_2}} \big\{ \langle p_1p_2|V|h_1h_2\rangle \\
& + \sum_{p_3 \le p_4} \langle p_3p_4|Z|h_1h_2\rangle\langle p_3p_4|V|p_1p_2\rangle + \sum_{h_3 \le h_4} \langle h_3h_4|V|h_1h_2\rangle\langle p_1p_2|Z|h_3h_4\rangle \\
& + \sum_{p_3,h_3} \langle p_3\bar{h}_3|V|p_1\bar{h}_1\rangle\langle p_3\bar{h}_3|Z|h_2\bar{p}_2\rangle + \sum_{p_3,h_3} \langle p_3\bar{h}_3|V|p_2\bar{h}_2\rangle\langle p_3\bar{h}_3|Z|h_1\bar{p}_1\rangle \\
& - \sum_{p_3,h_3} \langle p_3\bar{h}_3|V|p_1\bar{h}_2\rangle\langle p_3\bar{h}_3|Z|h_1\bar{p}_2\rangle - \sum_{p_3,h_3} \langle p_3\bar{h}_3|V|p_2\bar{h}_1\rangle\langle p_3\bar{h}_3|Z|h_2\bar{p}_1\rangle \\
& + \sum_{p_3 \le p_4} \sum_{h_3 \le h_4} \langle p_3p_4|Z|h_1h_2\rangle\langle p_1p_2|Z|h_3h_4\rangle\langle p_3p_4|V|h_3h_4\rangle \\
& + \sum_{p_3,h_3} \sum_{p_4,h_4} \langle p_3\bar{h}_3|Z|h_1\bar{p}_1\rangle\langle p_4\bar{h}_4|Z|h_2\bar{p}_2\rangle\langle p_4\bar{h}_4|V|h_3\bar{p}_3\rangle \\
& - \sum_{p_3,h_3} \sum_{p_4,h_4} \langle p_3\bar{h}_3|Z|h_2\bar{p}_1\rangle\langle p_4\bar{h}_4|Z|h_1\bar{p}_2\rangle\langle p_4\bar{h}_4|V|h_3\bar{p}_3\rangle \Big\} \, .
\end{aligned}$$

The mean field equation in m-representation takes the form:

$$\begin{aligned}
\langle h_1|H^{sp}|h_2\rangle &= e_{h_1}\delta_{h_1,h_2} = \langle h_1|H1|h_2\rangle + \frac{1}{2}\sum_{p_1,p_2,h_3} \langle p_1p_2|Z|h_1h_3\rangle\langle p_1p_2|V|h_2h_3\rangle \\
\langle p_1|H^{sp}|p_2\rangle &= e_{p_1}\delta_{p_1,p_2} = \langle p_1|H1|p_2\rangle - \frac{1}{2}\sum_{h_1,h_2,p_3} \langle p_1p_3|Z|h_1h_2\rangle\langle p_2p_3|V|h_1h_2\rangle \\
\langle p_1|H^{sp}|h_1\rangle &= 0 = \langle p_1|H1|h_1\rangle + \frac{1}{2}\sum_{p_2,p_3,h_3} \langle p_2p_3|Z|h_1h_3\rangle\langle p_2p_3|V|p_1h_3\rangle - \frac{1}{2}\sum_{h_2,p_3,h_3} \langle p_3p_1|Z|h_2h_3\rangle\langle h_2h_3|V|p_3h_1\rangle \\
&\quad + \sum_{p_2,h_2} \langle p_1p_2|Z|h_1h_2\rangle\langle p_2|H1|h_2\rangle \, .
\end{aligned}$$

Here the one-body part of the hamiltonian is called:

$$\langle h_1|H1|h_2\rangle = \langle h_1|T|h_2\rangle + \sum_h \langle h_1\bar{h}_2|V|h\bar{h}\rangle \, .$$

We compute the correlations in angular-momentum coupling. This can be performed either in particle-particle(pp) coupling or in particle-hole(ph) coupling. Either way, some re-coupling is required since those terms indicated in ph-notation require ph-coupling whereas the other terms require pp-coupling. The particle energies are given as the diagonal terms of the effective single-particle hamiltonian:

$$e_i = \langle i|V^{sp}|i\rangle \, .$$

We also define the always positive "quasi-particle"-energies:

$$\epsilon_{p(h)} = \begin{cases} e_p & for \quad particles \\ -e_h & for \quad holes \end{cases}$$

This procedure essentially provides a G-matrix calculation inside a finite nucleus.
We compute the amplitudes Z in ph-coupling as:

$$\langle p_1\bar{h}_1|Z^\lambda|h_2\bar{p}_2\rangle \;=\; \frac{-1}{e_{p_1}+e_{p_2}-e_{h_1}-e_{h_2}}\left\{\langle p_1\bar{h}_1|V^\lambda|h_2\bar{p}_2\rangle + \langle p_1\bar{h}_1|V^{\lambda,corr}|h_2\bar{p}_2\rangle\right\}.$$

The correction has three contributions: (c1,c2,c3)

$$\begin{aligned}\langle p_1\bar{h}_1|V^{\lambda,c1}|h_2\bar{p}_2\rangle \;&=\sum_{p_3h_3}\langle p_1\bar{h}_1|Z^\lambda|h_3\bar{p}_3\rangle\langle h_3\bar{p}_3|V^\lambda|h_2\bar{p}_2\rangle \\ &+\sum_{p_3h_3}\langle p_2\bar{h}_2|Z^\lambda|h_3\bar{p}_3\rangle\langle h_3\bar{p}_3|V^\lambda|h_1\bar{p}_1\rangle \\ &+\sum_{p_3h_3,p_4h_4}\langle p_1\bar{h}_1|Z^\lambda|h_3\bar{p}_3\rangle\langle h_3\bar{p}_3|V^\lambda|p_4\bar{h}_4\rangle\langle p_2\bar{h}_2|Z^\lambda|h_4\bar{p}_4\rangle\end{aligned}$$

and

$$\langle p_1\bar{h}_1|V^{\lambda,c2}|h_2\bar{p}_2\rangle \;=\sum_\ell(2\ell+1)\begin{Bmatrix} p_1 & h_1 & \ell \\ h_2 & p_2 & \lambda\end{Bmatrix}\langle p_1\bar{h}_2|V^{\ell,c2}|h_1\bar{p}_2\rangle$$

with

$$\begin{aligned}\langle p_1\bar{h}_2|V^{\ell,c2}|h_1\bar{p}_2\rangle \;&=\sum_{p_3h_3}\langle p_1\bar{h}_2|Z^\ell|h_3\bar{p}_3\rangle\langle h_3\bar{p}_3|V^\ell|h_1\bar{p}_2\rangle \\ &+\sum_{p_3h_3}\langle p_2\bar{h}_1|Z^\ell|h_3\bar{p}_3\rangle\langle h_3\bar{p}_3|V^\ell|h_2\bar{p}_1\rangle \\ &+\sum_{p_3h_3,p_4h_4}\langle p_1\bar{h}_2|Z^\ell|h_3\bar{p}_3\rangle\langle h_3\bar{p}_3|V^\ell|p_4\bar{h}_4\rangle\langle p_2\bar{h}_1|Z^\ell|h_4\bar{p}_4\rangle\end{aligned}$$

Finally:

$$\langle p_1\bar{h}_1|V^{\lambda,c3}|h_2\bar{p}_2\rangle \;=\sum_K(-)^{K+1}(2K+1)\begin{Bmatrix} p_1 & p_2 & K \\ p_1 & h_1 & \lambda\end{Bmatrix}\langle p_1p_2|V^{K,c3}|h_1h_2\rangle$$

with

$$\begin{aligned}\langle p_1p_2|V^{K,c3}|h_1h_2\rangle \;&=\sum_{p_3\le p_4}\frac{1}{1+\delta_{p_3,p_4}}\langle p_3p_4|V^K|p_1p_2\rangle\langle p_3p_4|Z^K|h_1h_2\rangle \\ &+\sum_{h_3\le h_4}\frac{1}{1+\delta_{h_3,h_4}}\langle h_3h_4|V^K|h_1h_2\rangle\langle p_1p_2|Z^K|h_3h_4\rangle \\ &+\sum_{h_3\le h_4,p_3\le p_4}\frac{1}{1+\delta_{h_3,h_4}}\frac{1}{1+\delta_{p_3,p_4}}\langle p_3p_4|Z^K|h_1h_2\rangle\langle p_3p_4|V^K|h_3h_4\rangle\langle p_1p_2|Z^K|h_1h_2\rangle\end{aligned}$$

The single particle energies can be computed in p-p-coupling as:

$$\begin{aligned}e_{p,p'} &= \langle p|T|p'\rangle+\sum_{K,h}\frac{(2K+1)}{(2j_p+1)}\langle p\ h|V^K|p'\ h\rangle \\ &+\sum_{K,p_2,h_2\le h_3}\frac{(2K+1)}{(2j_p+1)}\langle pp_2|Z^K|h_2h_3\rangle\langle p'p_2|V^K|h_2h_3\rangle\frac{1}{1+\delta_{h_2,h_3}}\end{aligned}$$

and

$$e_{h,h'} = \langle h|T|h'\rangle + \sum_{K,h_3} \frac{(2K+1)}{(2j_h+1)} \langle h\ h_3|V^K|h'\ h_3\rangle$$
$$- \sum_{K,p_2\le p_3,h_2} \frac{(2K+1)}{(2j_h+1)} \langle p_2p_3|Z^K|hh_2\rangle\langle p_2p_3|V^K|h'h_2\rangle \frac{1}{1+\delta_{p_2,p_3}}$$

In our programs they are computed in p-h-coupling. These numbers have been checked against the expression given here.

The binding energy is computed as:

$$\langle H\rangle = \langle 0|\mathbf{H_S}(1+\tilde{\mathbf{S}}^\dagger)|0\rangle$$

where

$$\mathbf{H_S} = e^{\mathbf{S}}\mathbf{H}e^{-\mathbf{S}}$$

If the CCE has been solved without any truncations, i.e. satisfying the generating equations for all $\mathbf{S}_n$, then the binding energy is exactly given by

$$\langle H\rangle = \langle 0|\mathbf{H_S}|0\rangle$$

If we now truncate and use only $\mathbf{S}_2$, we obtain

$$\langle H\rangle = \langle 0|\mathbf{H}|0\rangle + \langle 0|\mathbf{S_2H}|0\rangle$$

It has been customary to quote this value as the result of the $\mathbf{S}_2$-calculation. Thus we use the expression

$$E_b = \sum_h (2j_h+1)\langle h|T|h\rangle + \frac{1}{2}\sum_{K,h_1,h_2}(2K+1)\langle h_1\ h_2|V^K|h_1\ h_2\rangle$$
$$+\frac{1}{2}\sum_{K,p_2\le p_3}\sum_{h_1,h_2}(2K+1)\langle p_2p_3|Z^K|h_1h_2\rangle\langle p_2p_3|V^K|h_1h_2\rangle\frac{1}{1+\delta_{p_2,p_3}}$$

This value is not necessarily an upper bound to the binding energy. If, however, we treat this as a variational problem, such expectation value, if computed without approximations, must give an upper bound independent of truncations in $\mathbf{S_n}$. In that case we must compute the expectation value precisely, in particular we must include contributions from $\tilde{\mathbf{S}}_n$ with $n \ge 3$. While $\mathbf{S_2}$ has been adjusted such that $\langle \mathbf{H_S}\ \tilde{\mathbf{S}}_\mathbf{2}\rangle = 0$ this is not the case for all other $\tilde{\mathbf{S}}_\mathbf{n}$. In a reasonable approximation we can compute

$$\langle H\rangle = \langle 0|\mathbf{H_S}|0\rangle + \langle 0|\mathbf{H_S}\tilde{\mathbf{S}}_\mathbf{4}^\dagger)|0\rangle$$

We can approximate

$$\mathbf{S_4}^\dagger = \frac{1}{2}\mathbf{S_2}^\dagger\mathbf{S_2}^\dagger$$

This allows us to approximate

$$\langle H\rangle = \langle 0|\mathbf{H}|0\rangle + \langle 0|\mathbf{S_2H}|0\rangle + \frac{1}{2}\langle 0|\mathbf{S_2HS_2}^\dagger\mathbf{S_2}^\dagger|0\rangle$$

The binding energies quoted here have not been obtained using the variational approach. Thus, the values given here are not upper bounds to the true binding energy, even leaving open the possibility that the S4-level results give less binding than the S3-level results.

Our calculations are influenced by three parameters as our wave functions are expanded into harmonic oscillator functions: the HO-length parameter b_{ho}, the maximum n_{max}, and the maximum ℓ_{max} of our basis. To examine the convergence according to all parameters we have made a series of tests. Table I shows the dependence of the result on the length parameter chosen. These calculations were done for ^{4}He using the Argonne V-8' potential without the Coulomb interaction. All calculations in Table I were done with an $\ell_{max} = 18$

Table I

Binding energy (Kinetic energy) in MeV		
b_{ho}	$n_{max} = 25$	$n_{max} = 30$
$0.6[fm]$	-16.94(41.45)	-16.97(41.33)
$0.7[fm]$	-16.99(41.24)	-16.96(41.30)
$0.8[fm]$	-17.01(41.15)	-16.97(41.29)
$0.9[fm]$	-16.99(41.16)	-17.01(41.14)
$1.0[fm]$	-16.98(41.09)	-17.00(41.14)
$1.1[fm]$	-16.96(41.01)	-17.00(41.03)

Table II shows similar results for ^{12}C and ^{16}O this time using the Argonne V8' potential including the Coulomb interaction. These were done with fixed $n_{max} = 30$ and $\ell_{max} = 18$.

Table II

Binding energy (Kinetic energy) in MeV		
b_{ho}	^{12}C	^{16}O
$0.6[fm]$	-24.12(161.45)	
$0.7[fm]$	-25.18(157.05)	-55.49(226.38)
$0.8[fm]$	-25.43(155.80)	-55.98(224.25)
$0.9[fm]$	-25.51(155.35)	-55.77(225.05)
$1.0[fm]$	-25.54(155.02)	-55.99(223.82)
$1.1[fm]$	-25.54(154.64)	-55.92(223.70)
$1.2[fm]$	-25.52(154.20)	-55.56(224.52)

We expect that as the length parameter gets too small, the Harmonic Oscillator expansion can no longer reproduce the long range tails of the wave functions leading to reduced binding. On the other hand, if the length parameter gets too large, the finite basis can no longer provide the high Fourier components in the correlations, again leading to reduced binding.

Table III shows computations to test the convergence with respect to ℓ_{max}, using the Argonne V-18 interaction.

Table III

Binding energy in MeV			
n,ℓ	^{16}O	^{12}C	^{4}He
n=25,$\ell = 12$	-50.482	-22.769	-16.102
n=25,$\ell = 14$	-54.972	-25.137	
n=25,$\ell = 16$	-57.241	-26.391	-16.381
n=25,$\ell = 18$	-57.285	-26.588	-16.392

The results shown in these three tables indicate that our calculations i are converged with respect to the choice of all three parameters. In fact the results are quite stable even for a substantial increase in the length parameter. This gives us confidence that these computations can be extended to larger nuclei such as ^{40}Ca or even heavier nuclei within the basis used here.

II. S3-LEVEL CORRECTIONS

The S2-level calculations are considerably under-bound when compared to the GFMC calculations. This is not a surprise; and we have to examine the S3-level corrections as the next most important contributions. Similar to our paper we make here a perturbation expansion for the corrections in the S2-equation, still assuming that $\mathbf{S_4} = 0$ and $\mathbf{S_5} = 0$:

$$\mathbf{S_3 H}_{10} \approx \frac{-1}{\epsilon_{3p3h}} \Big\{ [\mathbf{S_2}, \mathbf{H}_{01}] + \frac{1}{2} \big[\mathbf{S_2}, [\mathbf{S_2}, \mathbf{H}_{10}]\big] + [\mathbf{S_3}, \mathbf{H}_{00}] + \big[\mathbf{S_3}, [\mathbf{S_2}, \mathbf{H}_{20}]\big] \Big\} \mathbf{H}_{10}$$

In first order perturbation we leave out the two terms containing S3 on the right hand side. The second order correction is obtained by replacing the S3 on the right hand side by the expression above and again leaving out all S3 terms on the right hand side. This can be done to all orders in an iterative procedure.

We will first focus on the first-order corrections. Our calculations so far have shown that there are three significant terms. Of these, the most important correction arises from an effective quasi-particle energy. We give those in angular momentum coupling:

$$\begin{aligned}
\epsilon(p,p') = & -\frac{1}{2} \sum_{\ell,p_3,p_4,h_3} \frac{2\ell+1}{2j_p+1} \frac{\langle p\bar{p}_4 | V^\ell | p_3 \bar{h}_3 \rangle \langle p' \bar{p}_4 | V^\ell | p_3 \bar{h}_3 \rangle}{\epsilon_{p_3 h_3} + \epsilon_{p_4} + \omega} \\
& -\frac{1}{2} \sum_{\ell,p_3,p_4,h_3} \sum_{p_5,h_5} \frac{2\ell+1}{2j_p+1} \frac{\langle p\bar{p}_4 | V^\ell | p_3 \bar{h}_3 \rangle \langle p_3 \bar{h}_3 | Z^\ell h_5 \bar{p}_5 \rangle \langle p' \bar{p}_4 | V^\ell | h_5 \bar{p}_5 \rangle}{\epsilon_{p_3 h_3} + \epsilon_{p_4} + \omega} \\
& -\sum_K
\end{aligned}$$

and

$$\begin{aligned}
\epsilon(h,h') = & -\frac{1}{2} \sum_{\ell,p_3,h_4,h_3} \frac{2\ell+1}{2j_p+1} \frac{\langle h_4 \bar{h} | V^\ell | p_3 \bar{h}_3 \rangle \langle h_4 \bar{h}' | V^\ell | p_3 \bar{h}_3 \rangle}{\epsilon_{p_3 h_3} + \epsilon_{h_4} + \omega} \\
& -\frac{1}{2} \sum_{\ell,p_3,h_4,h_3} \sum_{p_5,h_5} \frac{2\ell+1}{2j_p+1} \frac{\langle h_4 \bar{h} | V^\ell | p_3 \bar{h}_3 \rangle \langle p_3 \bar{h}_3 | Z^\ell | h_5 \bar{p}_5 \rangle \langle h_4 \bar{h}' | V^\ell | h_5 \bar{p}_5 \rangle}{\epsilon_{p_3 h_3} + \epsilon_{h_4} + \omega} \\
& -\sum_K
\end{aligned}$$

Here ω is the sum of the other three single particle energies not appearing in this equation. These terms are well known and important contributions to the single particle energies which we name QPE.

It should be pointed out that the quasi-particle energies appearing in the denominator do not contain the correction itself. To treat the quasi-particle energies in a self-consistent way enters only when we also include all higher clusters S_n with $n \geq 4$.

The boost in binding due to this quasi-particle energy correction is demonstrated in the second line of table IV. However, we find this correction to be huge and leading to complete over-binding particularly in ^{4}He as well as to rather unstable results. The reason is the bare interaction in the two-particle state. We re-normalize this interaction by including S3 of equation (2.1) on the right hand side and iterating this equation to convergence. This results in a much more reasonable correction which we call Re-normalized Quasi-Particle Energy(RQPE). The effect on the binding energy is shown in line 4 of table IV. Iterating this equation to all orders does not take us out of the S3-framework.

The other two significant contributions are called "f3b" and "f3c" for historical reasons. For these corrections we give only the leading term here, the others can be worked out in a similar fashion. These terms require some re-coupling and thus their calculation is more time-consuming.

The f3b-correction is given in our catalog of terms by the equations (121)→(124) and (132)→(133). The f3c-corrections are listed in our catalog (160)→(164) and (169)→(172). In both cases we have to include all the exchanges. In most cases these two terms have an opposite effect and somewhat cancel each other so that the most important correction remains the quasi-particle energy correction. in table IV the columns three and four indicate the effect of these terms on the binding energy.

The S3 correlations also affect the mean field.

Table IV

Binding energy in MeV			
	^{4}He	^{12}C	^{16}O
S2	-17.01	-25.54	-57.51
S2+QPE	-55.63	-87.72	
S2+RQPE	-29.	-61.61	-110.35
S2+RQPE+f3b			
S2+RQPE+f3b+f3c	-26.56		
full S3	-26.21	-51.87	-92.21
GFMC	-25.93	-80.0	

Here again, the calculations for ^{4}He were made with the Argonne-V8' interaction without the Coulomb part ($b_{ho} = 0.9$ fm), whereas the ^{12}C and ^{16}O calculations were made with the V8' interaction ($b_{ho} = 1.0$ fm).

III. S4-LEVEL CORRECTIONS

Since we found that the main mechanism of increasing the binding from S3-clusters is by changing the single particle energies, we make the approximation that also for S4-clusters the main effect is via single particle energies. Thus we have focussed on getting those contributions that modify the single particle energies as complete as possible. We have also included those contractions that can be added to individual matrix elements in the S2 and S3 contributions.

The contributions to the hole energies from term (VI) and (IX) are computed according to:

$$\begin{aligned}\Delta\epsilon(p_1,p_6,\omega) = \Delta e(p_1,p_6,\omega) = &+d(p_5,p_4,\omega)\langle p_5\bar{p}_4|V|p_6\bar{p}_1\rangle \\ &-d(h_6,h_3,\omega)\langle h_6\bar{h}_3|V|p_1\bar{p}_6\rangle\end{aligned}$$

This term together with the equivalent term for hole orbits correct the single-particle potential for fractional occupation of the natural orbits.

These are somewhat compensated by

$$\begin{aligned}\Delta\epsilon(p_1,p_6,\omega)=\Delta e(p_1,p_6,\omega)=&+d(p_5,p_4,\omega)\langle p_5p_1|V|h_3h_4\rangle\langle h_3h_4|Z|p_4p_6\rangle\\&+d(h_6,h_3,\omega)\langle p_1\bar{h}_6|V|h_4\bar{p}_4\rangle\langle h_4\bar{p}_4|Z|p_6\bar{h}_3\rangle\end{aligned}$$

In addition we have the terms

$$\begin{aligned}\Delta\epsilon(p_1,p_6,\omega)=\Delta e(p_1,p_6,\omega)=&+\langle p_1\bar{h}_6|Z|h_3\bar{p}_3\rangle\frac{\langle p_3\bar{h}_3|V|h_4\bar{p}_4\rangle}{\epsilon_{p_3h_3}+\epsilon_{p_4h_4}+\omega}\langle p_4\bar{h}_4|V|p_5\bar{h}_6\rangle\\&+\langle p_1p_5|Z|h_3h_4\rangle\frac{\langle p_3p_4|V|h_3h_4\rangle}{\epsilon_{p_3h_3}+\epsilon_{p_4h_4}+\omega}\langle p_3p_4|V|p_5p_6\rangle\end{aligned}$$

For hole states we have similar terms, but we need to include the extra negative sign for the QPE.

$$\begin{aligned}\Delta\epsilon(h_1,h_5,\omega)=-\Delta e(h_1,h_5,\omega)=&-d(p_5,p_4,\omega)\langle p_5\bar{p}_4|V|h_5\bar{h}_1\rangle\\&+d(h_6,h_3,\omega)\langle h_6\bar{h}_3|V|h_1\bar{h}_5\rangle\end{aligned}$$

These are compensated by

$$\begin{aligned}\Delta\epsilon(h_1,h_5,\omega)=-\Delta e(h_1,h_5,\omega)=&+d(p_5,p_4,\omega)\langle p_5\bar{h}_5|V|h_6\bar{p}_6\rangle\langle h_6\bar{p}_6|Z|p_4\bar{h}_1\rangle\\&+d(h_6,h_3,\omega)\langle h_6h_5|V|p_6p_5\rangle\langle p_6p_5|Z|h_3h_1\rangle\end{aligned}$$

In addition we have the terms

$$\begin{aligned}\Delta\epsilon(h_1,h_5,\omega)=-\Delta e(h_1,h_5,\omega)=&+\langle p_5\bar{h}_1|Z|h_3\bar{p}_3\rangle\frac{\langle h_3\bar{p}_3|V|p_4\bar{h}_4\rangle}{\epsilon_{p_3h_3}+\epsilon_{p_4h_4}+\omega}\langle p_4\bar{h}_4|V|p_5\bar{h}_5\rangle\\&+\langle h_1h_6|Z|p_3p_4\rangle\frac{\langle p_3p_4|V|h_3h_4\rangle}{\epsilon_{p_3h_3}+\epsilon_{p_4h_4}+\omega}\langle h_3h_4|V|h_5h_6\rangle\end{aligned}$$

Our calculations using the Argonne V8' interaction appear to give reliable results, whereas our calculations using Argonne-V18 seem to have still some problems. In order to not confuse the issue of interaction and coupled cluster approximation, we have made the comparison to GFMC with the Argonne-V8' interaction. The Kamada-test case was made using the V8' interaction without the Coulomb interaction. We have included our result for that case as well in table V, labelled "He-4-Kam".

Table V

Comparison of CCE-results with GFMC

Binding energy in MeV				
Nucleus	S2-level	S3-level	S4-level	GFMC
^{4}He-Kam	-17.01	-26.21	-26.17	-25.93
^{4}He(V-8')	-16.39	-25.48	-25.27	-25.14
^{6}n(V-8')		-31.35	-32.02	-31.99
^{8}n(V-8')		-39.35	-39.17	-39.73
^{8}He(V-8')		-17.71	(-19.3*)	-23.7
^{12}C(V-8')	-25.54	-51.87	-55.42	-80.00
^{14}C(V-8')	-40.70	-69.64	(-78.24 *)	
^{14}O(V-8')	-35.54	-63.28	(-68.8 *)	
^{16}O(V-8')	-57.51	-92.21	-100.7	
^{22}O(V-8')	-59.23	(-103.7*)		
^{28}Si(V-8')	-66.8	(-134.2 *)		
^{30}S(V-8')	-70.3			
^{32}S(V-8')	-105.54	(-243.25 *)		
^{40}Ca(V-8')	-289.4	(-354.21 *)		

Note: ($*$) implies that computation has not yet fully converged.

IV. CONCLUSIONS

The systematic studies show convergence in the three parameters that affect the calculation namely n_{max}, ℓ_{max}, and the length parameter b_{ho}.

The comparison of the final results up to S4 with the GFMC results find reasonable agreement for the three lightest systems: ^{4}He, ^{6}n, and ^{8}n. However, quite disconcerting are the discrepancies found in ^{8}He and ^{12}C. In ^{8}He the calculations miss by 4.8 MeV and in ^{12}C it misses by 25 MeV. However, for ^{16}O the computed binding is quite reasonable again. The situation that this problem does not show in the ^{6}n comparison seems to indicate that the problem is in the p-n channel of the interaction. Also, since it is a huge discrepancy it is likely to be in the tensor interaction.