

**A time-dependent formulation of coupled cluster theory for many-fermion systems at finite temperature: Supplementary material**

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Supplementary material to accompany: “A time-dependent formulation of coupled cluster theory for many-fermion systems at finite temperature” by Alec F. White and Garnet Chan. This supplement includes the complete set of results discussed in the aforementioned manuscript.

In the following sections we show FT-CCSD results for the unpolarized UEG. Table I shows the parameters used in these calculations. Calculations were performed at reduced temperatures ( $\theta$ ) of 0.25, 0.5, and 1.

$r_s$	$L (N = 14)$	$L (N = 38)$	$L (N = 66)$	$E_F$
0.5	1.94256	2.70974	3.25722	7.36634
1.0	3.88513	5.41948	6.51445	1.84158
2.0	7.77026	10.83895	13.02889	0.46040
3.0	11.65539	16.25843	19.54334	0.20462
4.0	15.54052	21.67791	26.05779	0.11510

TABLE I. Box length ( $L$ ) and Fermi energy ( $E_F$ ) for different numbers of electrons. Lengths are in units of Bohr ( $a_0$ ) and energies are in units of Hartree ( $E_h$ ).

### I. $N = 14$ UNPOLARIZED UEG

- Results in a basis of 33 plane waves are shown in Table II
- Results in a basis of 57 plane waves are shown in Table III

### II. $N = 38$ UNPOLARIZED UEG

- Results in a basis of 33 plane waves are shown in Table IV
- Results in a basis of 57 plane waves are shown in Table V
- A comparison of  $E_{xc}$  for different numbers of grid points is given in Table VI

### III. $N = 66$ UNPOLARIZED UEG

- Results in a basis of 57 plane waves are shown in Table VII

$r_s$	$\theta$	$\mu_0$	$\Omega_0$	$E_0$	$S_0$
0.5	1.0	1.54818	-122.15842	130.34735	31.33597
0.5	0.5	5.53128	-69.89354	103.56949	26.07132
0.5	0.25	7.01354	-49.21035	81.31564	17.55904
1.0	1.0	0.38704	-30.53961	32.58684	31.33597
1.0	0.5	1.38282	-17.47338	25.89237	26.07132
1.0	0.25	1.75338	-12.30259	20.32891	17.55904
2.0	1.0	0.09676	-7.63490	8.14671	31.33597
2.0	0.5	0.34571	-4.36835	6.47309	26.07132
2.0	0.25	0.43835	-3.07565	5.08223	17.55904
3.0	1.0	0.04300	-3.39329	3.62076	31.33597
3.0	0.5	0.15365	-1.94149	2.87693	26.07132
3.0	0.25	0.19482	-1.36695	2.25877	17.55904
4.0	1.0	0.02419	-1.908738	2.03668	31.33597
4.0	0.5	0.08643	-1.09209	1.61827	26.07132
4.0	0.25	0.10959	-0.76891	1.27056	17.55904

  

$r_s$	$\theta$	$N$	$\mu_{xc}$	$\Omega$	$E_{xc}$	$S_{xc}$	$F_{xc}$
0.5	1.0	14.00001	-0.47713	-117.56365	-0.20724	-0.00792	-0.14892
0.5	0.5	14.00001	-0.53566	-65.09878	-0.25463	-0.01668	-0.19318
0.5	0.25	13.99998	-0.57186	-44.32883	-0.24517	-0.01194	-0.22318
1.0	1.0	13.99953	-0.24864	-28.21506	-0.11772	-0.01903	-0.08267
1.0	0.5	13.99348	-0.28082	-15.05476	-0.14150	-0.03577	-0.10856
1.0	0.25	13.99808	-0.29738	-9.86550	-0.13362	-0.02218	-0.12340
2.0	1.0	14.00000	-0.13241	-6.45469	-0.06942	-0.04628	-0.04811
2.0	0.5	14.00000	-0.14875	-3.15788	-0.07895	-0.07240	-0.06229
2.0	0.25	14.00001	-0.15595	-1.86073	-0.07328	-0.03568	-0.06917
3.0	1.0	14.00000	-0.09233	-2.59870	-0.05070	-0.07392	-0.03558
3.0	0.5	14.00009	-0.10240	-1.13466	-0.05433	-0.09349	-0.04477
3.0	0.25	13.99999	-0.10584	-0.55978	-0.04947	-0.02517	-0.04818
4.0	1.0	14.00000	-0.07142	-1.30984	-0.03977	-0.09672	-0.02864
4.0	0.5	14.00000	-0.07759	-0.49211	-0.04004	-0.09226	-0.03473
4.0	0.25	14.00000	-0.07832	-0.17709	-0.03536	0.02396	-0.03605

TABLE II. FT-CCSD results for the  $N = 14$  systems using a basis of 33 plane waves. The exchange correlation contributions to extensive quantities ( $E$ ,  $S$ ,  $F$ ) are given on a per-electron basis.

$r_s$	$\theta$	$\mu_0$	$\Omega_0$	$E_0$	$S_0$
0.5	1.0	0.46990	-118.49764	153.2166	35.99288
0.5	0.5	5.45425	-69.46127	106.54681	27.05512
0.5	0.25	7.01303	-49.20598	81.34203	17.57484
1.0	1.0	0.11747	-29.62441	38.30415	35.99288
1.0	0.5	1.36356	-17.36532	26.6367	27.05512
1.0	0.25	1.75326	-12.3015	20.33551	17.57484
2.0	1.0	0.02937	-7.4061	9.57604	35.99288
2.0	0.5	0.34089	-4.34133	6.65918	27.05512
2.0	0.25	0.43831	-3.07537	5.08388	17.57484
3.0	1.0	0.01305	-3.2916	4.25602	35.99288
3.0	0.5	0.15151	-1.92948	2.95963	27.05512
3.0	0.25	0.19481	-1.36683	2.25950	17.57484
4.0	1.0	0.00734	-1.85153	2.39401	35.99288
4.0	0.5	0.08522	-1.08533	1.66479	27.05512
4.0	0.25	0.10958	-0.76884	1.27097	17.57484

  

$r_s$	$\theta$	$N$	$\mu_{xc}$	$\Omega$	$E_{xc}$	$S_{xc}$	$F_{xc}$
0.5	1.0	14.00000	-0.45773	-114.05219	-0.23184	-0.01244	-0.1402
0.5	0.5	13.99993	-0.54891	-64.5881	-0.27114	-0.01909	-0.20085
0.5	0.25	14.00000	-0.58935	-44.19258	-0.25135	-0.01091	-0.23125
1.0	1.0	14.00001	0.17142	-28.75369	-0.68676	-0.49977	0.23361
1.0	0.5	14.00001	-0.23748	-15.1867	-0.22682	-0.15742	-0.08187
1.0	0.25	14.00000	-0.29087	-9.89493	-0.13026	-0.02454	-0.11897
2.0	1.0	14.00001	-0.13683	-6.20438	-0.0809	-0.06495	-0.05099
2.0	0.5	14.00000	-0.15963	-3.05991	-0.08459	-0.07163	-0.0681
2.0	0.25	14.00009	-0.16733	-1.7699	-0.07692	-0.02467	-0.07408
3.0	1.0	14.00006	-0.09723	-2.47077	-0.05866	-0.09807	-0.0386
3.0	0.5	13.99993	-0.11056	-1.06892	-0.05767	-0.08387	-0.04909
3.0	0.25	13.99998	-0.11352	-0.49904	-0.05127	0.0052	-0.05154
4.0	1.0	14.00000	-0.07576	-1.22941	-0.04543	-0.12255	-0.03132
4.0	0.5	14.00000	-0.08352	-0.44722	-0.04191	-0.06899	-0.03794
4.0	0.25	14.00000	-0.08309	-0.14126	-0.04973	0.07965	-0.05202

TABLE III. FT-CCSD results for the  $N = 14$  systems using a basis of 57 plane waves. The exchange correlation contributions to extensive quantities ( $E$ ,  $S$ ,  $F$ ) are given on a per-electron basis.

$r_s$	$\theta$	$\mu_0$	$\Omega_0$	$E_0$	$S_0$
0.5	1.0	8.68718	-428.94107	223.90749	43.81225
0.5	0.5	7.63608	-231.54239	208.79981	40.77229
0.5	0.25	7.16870	-144.28309	188.55102	32.81067
1.0	1.0	2.17179	-107.23527	55.97687	43.81225
1.0	0.5	1.90902	-57.88560	52.19995	40.77229
1.0	0.25	1.79217	-36.07077	47.13776	32.81067
2.0	1.0	0.54295	-26.80882	13.99422	43.81225
2.0	0.5	0.47725	-14.47140	13.04999	40.77229
2.0	0.25	0.44804	-9.01769	11.78444	32.81067
3.0	1.0	0.24131	-11.91503	6.21965	43.81225
3.0	0.5	0.21211	-6.43173	5.79999	40.77229
3.0	0.25	0.19913	-4.00786	5.23753	32.81067
4.0	1.0	0.13574	-6.70220	3.49855	43.81225
4.0	0.5	0.11931	-3.61785	3.2625	40.77229
4.0	0.25	0.11201	-2.25442	2.94611	32.81067

  

$r_s$	$\theta$	$N$	$\mu_{xc}$	$\Omega$	$E_{xc}$	$S_{xc}$	$F_{xc}$
0.5	1.0	38.00169	-0.74018	-414.86674	-0.39926	-0.00407	-0.36931
0.5	0.5	38.00018	-0.74708	-218.18798	-0.43968	-0.01196	-0.39562
0.5	0.25	38.00257	-0.7557	-131.76134	-0.46498	-0.02120	-0.42594
1.0	1.0	38.00033	-0.36809	-100.38888	-0.20483	-0.00919	-0.18790
1.0	0.5	38.00124	-0.36892	-51.55187	-0.22573	-0.02555	-0.20220
1.0	0.25	38.00055	-0.37117	-30.23844	-0.23622	-0.04026	-0.21768
2.0	1.0	38.00037	-0.18206	-23.56165	-0.10662	-0.02176	-0.09660
2.0	0.5	38.00060	-0.18114	-11.5615	-0.11675	-0.05295	-0.10456
2.0	0.25	38.00022	-0.18123	-6.38090	-0.1195	-0.0665	-0.11184
3.0	1.0	38.00025	-0.12033	-9.84641	-0.07322	-0.03581	-0.06589
3.0	0.5	38.00038	-0.11945	-4.60473	-0.07916	-0.07610	-0.07137
3.0	0.25	38.00232	-0.11961	-2.33038	-0.07874	-0.06399	-0.07546
4.0	1.0	38.00160	-0.08967	-5.20884	-0.05612	-0.05003	-0.05036
4.0	0.5	38.00058	-0.08923	-2.29306	-0.05949	-0.08891	-0.05437
4.0	0.25	38.00241	-0.09056	-0.95413	-0.05605	0.01002	-0.05634

TABLE IV. FT-CCSD results for the  $N = 38$  systems using a basis of 33 plane waves. The exchange correlation contributions to extensive quantities ( $E$ ,  $S$ ,  $F$ ) are given on a per-electron basis.

$r_s$	$\theta$	$\mu_0$	$\Omega_0$	$E_0$	$S_0$
0.5	1.0	3.88076	-356.43136	296.93302	68.67669
0.5	0.5	6.14411	-202.00985	249.36359	59.16029
0.5	0.25	6.93722	-138.19321	197.79797	39.30133
1.0	1.0	0.97019	-89.10784	74.23326	68.67669
1.0	0.5	1.53603	-50.50246	62.34089	59.16029
1.0	0.25	1.73431	-34.54830	49.44949	39.30133
2.0	1.0	0.24255	-22.27696	18.55831	68.67669
2.0	0.5	0.38401	-12.62562	15.58523	59.16029
2.0	0.25	0.43358	-8.63708	12.36237	39.30133
3.0	1.0	0.10780	-9.90087	8.2484	68.67669
3.0	0.5	0.17067	-5.61139	6.92677	59.16029
3.0	0.25	0.19270	-3.83870	5.49439	39.30133
4.0	1.0	0.06064	-5.56924	4.63958	68.67669
4.0	0.5	0.09600	-3.15640	3.89631	59.16029
4.0	0.25	0.10839	-2.15927	3.09059	39.30133

  

$r_s$	$\theta$	$N$	$\mu_{xc}$	$\Omega$	$E_{xc}$	$S_{xc}$	$F_{xc}$
0.5	1.0	38.00001	-0.63707	-344.35503	-0.38645	-0.00912	-0.31927
0.5	0.5	38.00000	-0.69329	-190.00102	-0.47209	-0.02574	-0.37727
0.5	0.25	38.00000	-0.75023	-126.22726	-0.49686	-0.03341	-0.43533
1.0	1.0	37.99997	-0.32506	-83.1601	-0.20791	-0.02137	-0.16854
1.0	0.5	38.00000	-0.35244	-44.72504	-0.24919	-0.05298	-0.20040
1.0	0.25	38.00000	-0.37615	-28.92465	-0.25513	-0.05859	-0.22816
2.0	1.0	38.00001	-0.16760	-19.38124	-0.11436	-0.04988	-0.09140
2.0	0.5	38.00000	-0.18038	-9.88945	-0.13198	-0.10254	-0.10837
2.0	0.25	38.00000	-0.18969	-6.01026	-0.13155	-0.09551	-0.12056
3.0	1.0	38.00000	-0.11437	-8.00621	-0.08054	-0.07837	-0.06451
3.0	0.5	38.00000	-0.12263	-3.82034	-0.08955	-0.13735	-0.07550
3.0	0.25	38.00000	-0.12932	-2.04811	-0.08718	-0.09737	-0.08220
4.0	1.0	38.00000	-0.08739	-4.16299	-0.06217	-0.10240	-0.05039
4.0	0.5	37.99992	-0.09351	-1.80022	-0.06622	-0.14602	-0.05782
4.0	0.25	38.00000	-0.09895	-0.7063	-0.05962	0.03800	-0.06071

TABLE V. FT-CCSD results for the  $N = 38$  systems using a basis of 57 plane waves. The exchange correlation contributions to extensive quantities ( $E$ ,  $S$ ,  $F$ ) are given on a per-electron basis.

$r_s$	$\theta$	$E_{\text{xc}} (n_g = 10)$	$E_{\text{xc}} (n_g = 20)$	difference	% Absolute difference
0.5	1.0	-0.38645	-0.38646	2.43E-6	0.0006
0.5	0.5	-0.47209	-0.47210	6.18E-6	0.0013
0.5	0.25	-0.49686	-0.49666	1.97E-4	0.0398
1.0	1.0	-0.20791	-0.20791	2.96E-6	0.0014
1.0	0.5	-0.24919	-0.24937	1.86E-4	0.0745
1.0	0.25	-0.25513	-0.25532	1.87E-4	0.0733
2.0	1.0	-0.11436	-0.11437	3.00E-6	0.0026
2.0	0.5	-0.13198	-0.13199	1.52E-5	0.0116
2.0	0.25	-0.13155	-0.13141	1.46E-4	0.1113
3.0	1.0	-0.08054	-0.08055	1.80E-6	0.0022
3.0	0.5	-0.08955	-0.08955	2.53E-6	0.0028
3.0	0.25	-0.08718	-0.08697	2.15E-4	0.2478
4.0	1.0	-0.06217	-0.06217	8.84E-7	0.0014
4.0	0.5	-0.06622	-0.06620	1.60E-5	0.0241
4.0	0.25	-0.05962	-0.05946	1.65E-4	0.2769

TABLE VI. Comparison of the exchange correlation energy of the  $N = 38$  system (basis of 57 plane waves) for different numbers of grid points ( $n_g = 10, 20$ ). Note that small differences can be caused by slightly different values of  $N$  in the two calculations.

$r_s$	$\theta$	$\mu_0$	$\Omega_0$	$E_0$	$S_0$
0.5	1.0	8.90882	-748.07967	396.83575	75.60521
0.5	0.5	7.85541	-406.71917	371.16323	70.43536
0.5	0.25	7.52685	-265.01795	335.80688	56.50163
1.0	1.0	2.2272	-187.01992	99.20894	75.60521
1.0	0.5	1.96385	-101.67979	92.79081	70.43536
1.0	0.25	1.88171	-66.25449	83.95172	56.50163
2.0	1.0	0.55680	-46.75498	24.80223	75.60521
2.0	0.5	0.49096	-25.41995	23.1977	70.43536
2.0	0.25	0.47043	-16.56362	20.98793	56.50163
3.0	1.0	0.24747	-20.77999	11.02322	75.60521
3.0	0.5	0.21821	-11.29775	10.31009	70.43536
3.0	0.25	0.20908	-7.36161	9.32797	56.50163
4.0	1.0	0.13920	-11.68874	6.20056	75.60521
4.0	0.5	0.12274	-6.35499	5.79943	70.43536
4.0	0.25	0.11761	-4.14091	5.24698	56.50163

  

$r_s$	$\theta$	$N$	$\mu_{xc}$	$\Omega$	$E_{xc}$	$S_{xc}$	$F_{xc}$
0.5	1.0	66.00000	-0.80649	-722.92292	-0.46032	0.28470	-2.5575
0.5	0.5	66.00000	-0.80218	-383.89332	-0.50986	-0.01453	-0.45633
0.5	0.25	66.00000	-0.78534	-245.80883	-0.54433	-0.02717	-0.49429
1.0	1.0	66.00000	-0.39987	-174.94026	-0.23701	0.27850	-0.74989
1.0	0.5	66.00002	-0.39542	-91.01573	-0.26174	-0.03030	-0.23384
1.0	0.25	66.00001	-0.38666	-57.39034	-0.27542	-0.05009	-0.25236
2.0	1.0	66.00004	-0.19717	-41.12355	-0.12357	-0.02546	-0.11184
2.0	0.5	66.00004	-0.19362	-20.62514	-0.13481	-0.06015	-0.12097
2.0	0.25	66.00000	-0.18883	-12.63275	-0.13906	-0.08506	-0.12927
3.0	1.0	66.00000	-0.13001	-17.23967	-0.08474	-0.04088	-0.07637
3.0	0.5	66.00000	-0.12732	-8.34018	-0.09123	-0.08529	-0.08251
3.0	0.25	65.99997	-0.12312	-4.99721	-0.09306	-0.11269	-0.0873
4.0	1.0	66.00000	-0.09671	-9.1598	-0.06723	-0.05604	-0.06078
4.0	0.5	65.99996	-0.09488	-4.244	-0.06817	-0.10445	-0.06216
4.0	0.25	66.00000	-0.09110	-2.48048	-0.06619	-0.13972	-0.06217

TABLE VII. FT-CCSD results for the  $N = 66$  systems using a basis of 57 plane waves. The exchange correlation contributions to extensive quantities ( $E$ ,  $S$ ,  $F$ ) are given on a per-electron basis.