Supplementary Material for "Weight-dependent local density-functional approximations for ensembles"

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CONSTRUCTION OF THE DENSITY-FUNCTIONAL APPROXIMATIONS

The density-functional approximations designed in this manuscript are based on highly-accurate energies for the ground state ($I = 0$), the first singly-excited state ($I = 1$), and the first doubly-excited state ($I = 2$) of the (spin-polarized) two-electron ringium system. We refer the interested reader to Refs. 1–3 for more details about this paradigm.

The reduced (i.e. per electron) HF energy for these three states is:

$$\epsilon_{\rm HF}^{(0)}(n) = \frac{\pi^2}{8} n^2 + n, \tag{1a}$$

$$\epsilon_{\rm HF}^{(1)}(n) = \frac{\pi^2}{2} n^2 + \frac{4}{3} n, \tag{1b}$$

$$\epsilon_{\rm HF}^{(2)}(n) = \frac{9\pi^2}{8} n^2 + \frac{23}{15} n. \tag{1c}$$

All these states have the same (uniform) density $n = 2/(2\pi R)$ where R is the radius of the ring on which the electrons are confined.

The total energy of the ground and doubly-excited states are given by the two lowest eigenvalues of the Hamiltonian $\boldsymbol{H}$ with elements

$$\begin{aligned} H_{ij} &= \int_0^\pi \left[\frac{\psi_i(\omega)}{R} \frac{\psi_j(\omega)}{R} + \frac{\psi_i(\omega)\psi_j(\omega)}{2R\sin(\omega/2)} \right] d\omega \\ &= \frac{\sqrt{\pi}}{2R} \left[\frac{\Gamma\left(\frac{i+j}{2}\right)}{\Gamma\left(\frac{i+j+1}{2}\right)} + \frac{ij}{4R} \frac{\Gamma\left(\frac{i+j-1}{2}\right)}{\Gamma\left(\frac{i+j+2}{2}\right)} \right], \end{aligned} \tag{2}$$

where $\omega = \theta_1 - \theta_2$ is the interelectronic angle, $\Gamma(x)$ is the Gamma function,[4] and

$$\psi_i(\omega) = \sin(\omega/2) \sin^{i-1}(\omega/2), \quad i = 1, \ldots, M \tag{3}$$

are (non-orthogonal) explicitly-correlated basis functions with overlap matrix elements

$$S_{ij} = \int_0^\pi \psi_i(\omega)\psi_j(\omega) d\omega = \sqrt{\pi} \frac{\Gamma\left(\frac{i+j+1}{2}\right)}{\Gamma\left(\frac{i+j+2}{2}\right)}. \tag{4}$$

Thanks to this explicitly-correlated basis, the convergence rate of the energy is exponential with respect to M. Therefore, high accuracy is reached with a very small number of basis functions.

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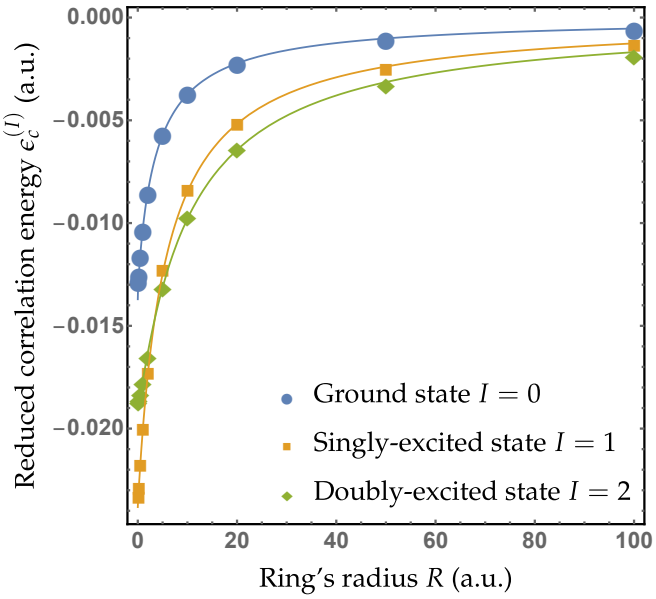

FIG. 1. Reduced (i.e., per electron) correlation energy $\epsilon_{\rm c}^{(I)}$ [see Eq. (8)] as a function of $R = 1/(\pi n)$ for the ground state ($I = 0$), the first singly-excited state ($I = 1$), and the first doubly-excited state ($I = 2$) of the (spin-polarized) two-electron ringium system. The data gathered in Table I are also reported.

Here, we typically use $M = 10$. For the singly-excited state, one has to modify the basis functions as

$$\psi_i(\omega) = \cos(\omega/2) \sin^{i-1}(\omega/2), \tag{5}$$

and its energy is obtained by the lowest root of the Hamiltonian in this basis, and the matrix elements reads

$$H_{ij} = \frac{\sqrt{\pi}}{4R} \left[\frac{\Gamma\left(\frac{i+j}{2}\right)}{\Gamma\left(\frac{i+j+1}{3}\right)} + \frac{3ij + i + j - 1}{4R} \frac{\Gamma\left(\frac{i+j-1}{2}\right)}{\Gamma\left(\frac{i+j+4}{2}\right)} \right], \tag{6}$$

$$S_{ij} = \frac{\sqrt{\pi}}{2} \frac{\Gamma\left(\frac{i+j+1}{2}\right)}{\Gamma\left(\frac{i+j+4}{2}\right)}. \tag{7}$$

The numerical values of the correlation energy for various R are reported in Table I for the three states of interest.

Based on these highly-accurate calculations, one can write down, for each state, an accurate analytical expression of the reduced correlation energy[2,5] via the following Padé approximant

$$\epsilon_{\rm c}^{(I)}(n) = \frac{a_1^{(I)} n}{n + a_2^{(I)} \sqrt{n} + a_3^{(I)}}, \tag{8}$$

TABLE I. $-\epsilon_c^{(I)}$ as a function of the radius of the ring R for the ground state ($I = 0$), the first singly-excited state ($I = 1$), and the first doubly-excited state ($I = 2$) of the (spin-polarized) two-electron ringium system.

State	I	Ring's radius $R = 1/(\pi n)$										
		0	1/10	1/5	1/2	1	2	5	10	20	50	100
Ground state	0	0.013708	0.012859	0.012525	0.011620	0.010374	0.008558	0.005673	0.003697	0.002226	0.001046	0.000567
Singly-excited state	1	0.0238184	0.023392	0.022979	0.021817	0.020109	0.017371	0.012359	0.008436	0.005257	0.002546	0.001399
Doubly-excited state	2	0.018715	0.018653	0.018576	0.018300	0.017743	0.016491	0.013145	0.009670	0.006365	0.003231	0.001816

where $a_2^{(I)}$ and $a_3^{(I)}$ are state-specific fitting parameters, which are provided in Table I of the manuscript. The value of $a_1^{(I)}$ is obtained via the exact high-density expansion of the correlation energy.[2,5] Equation (8) is depicted in Fig. 1 for each state alongside the data gathered in Table I.

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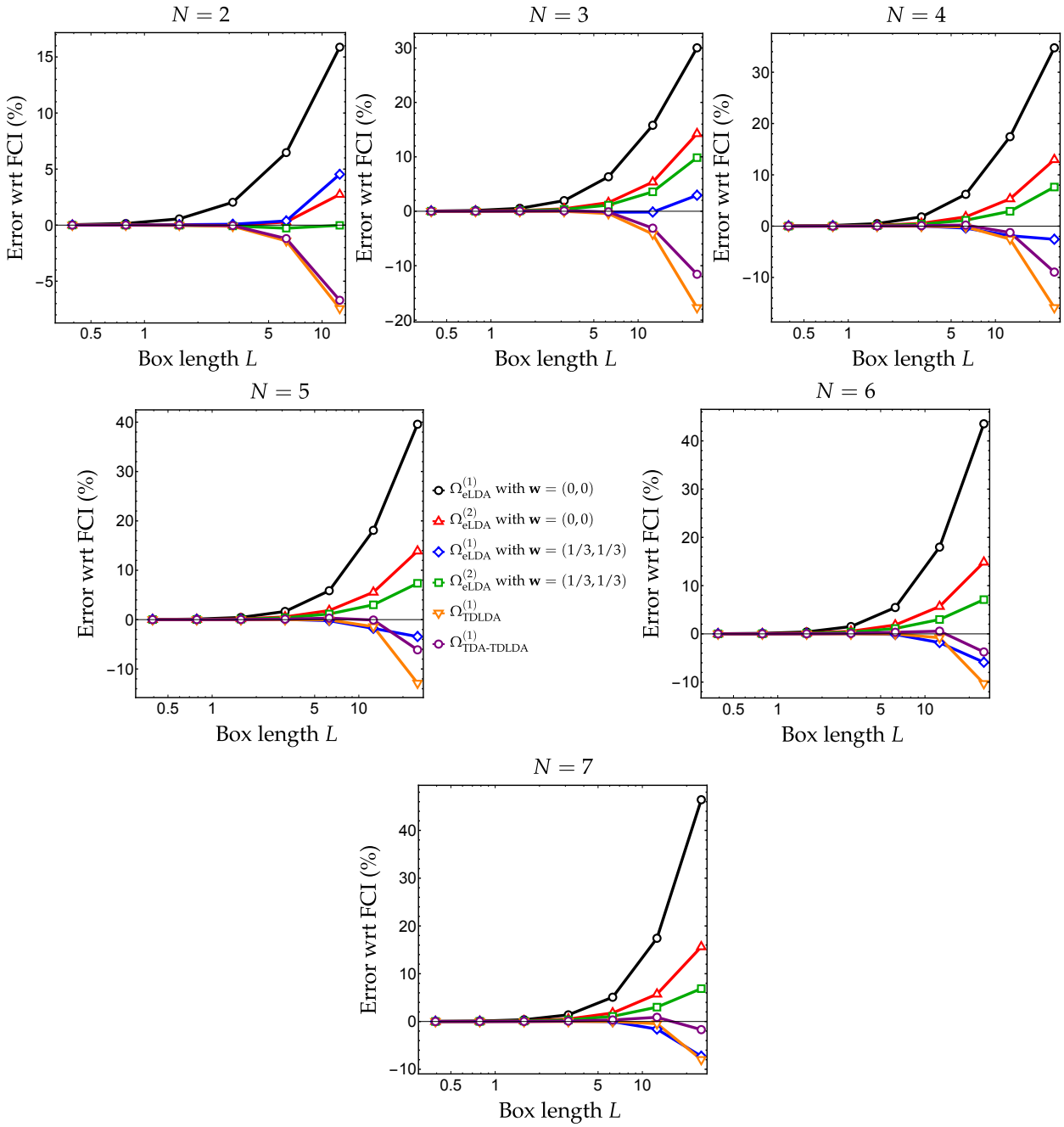

FIG. 2. Error with respect to FCI in single and double excitation energies of N-boxium as a function of the box length L for various methods. See main text for additional details.

TABLE II. Deviation from the FCI quantities (in hartree) of the individual energies, $E^{(I)}$, and the corresponding excitation energies, $\Omega^{(I)}$, for the ground ($I = 0$), singly-excited ($I = 1$) and doubly-excited ($I = 2$) states of 2-boxium (i.e., $N = 2$ electrons in a box of length L). The values of the ensemble correlation derivative $\Upsilon_c^{(I)}$ are also reported.

			2-boxium with a box of length L						
Method	$\boldsymbol{w}$	State	$\pi/8$	$\pi/4$	$\pi/2$	π	2π	4π	8π
FCI		$E^{(0)}$	168.1946	44.0662	12.0035	3.4747	1.0896	0.3719	0.1367
		$E^{(1)}$	330.2471	85.0890	22.5112	6.2247	1.8355	0.5845	0.2006
		$E^{(2)}$	809.9972	204.9840	52.4777	13.7252	3.7248	1.0696	0.3300
		$\Omega^{(1)}$	162.0525	41.0228	10.5078	2.7500	0.7458	0.2125	0.0639
		$\Omega^{(2)}$	641.8026	160.9177	40.4743	10.2505	2.6352	0.6977	0.1933
			Deviation from FCI						
CIS		$\Omega^{(1)}$	0.0104	0.0102	0.0099	0.0092	0.0077	0.0051	0.0022
TDHF		$\Omega^{(1)}$	0.0019	0.0021	0.0023	0.0027	0.0029	0.0023	0.0011
TDA-TDLDA		$\Omega^{(1)}$	0.0099	0.0088	0.0058	−0.0041	−0.0316	−0.0467	
TDLDA		$\Omega^{(1)}$	0.0015	0.0006	−0.0018	−0.0106	−0.0370	−0.0518	
KS-eLDA	$(0, 0)$	$E^{(0)}$	−0.0397	−0.0391	−0.0380	−0.0361	−0.0323	−0.0236	
		$E^{(1)}$	0.0215	0.0213	0.0210	0.0200	0.0159	0.0102	
		$E^{(2)}$	−0.0426	−0.0425	−0.0419	−0.0387	−0.0250	−0.0045	
		$\Omega^{(1)}$	0.0612	0.0604	0.0590	0.0561	0.0483	0.0337	
		$\Omega^{(2)}$	−0.0029	−0.0034	−0.0039	−0.0025	0.0074	0.0191	
		$\Upsilon_c^{(0)}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
		$\Upsilon_c^{(1)}$	0.0064	0.0056	0.0043	0.0022	−0.0007	−0.0037	
		$\Upsilon_c^{(2)}$	0.0159	0.0147	0.0126	0.0093	0.0046	−0.0009	
KS-eLDA	$(1/3, 1/3)$	$E^{(0)}$	0.0031	0.0036	0.0044	0.0054	0.0042	−0.0025	
		$E^{(1)}$	0.0090	0.0087	0.0083	0.0076	0.0070	0.0071	
		$E^{(2)}$	−0.0005	−0.0009	−0.0015	−0.0023	−0.0030	−0.0026	
		$\Omega^{(1)}$	0.0058	0.0052	0.0039	0.0022	0.0028	0.0096	
		$\Omega^{(2)}$	−0.0036	−0.0045	−0.0058	−0.0077	−0.0072	0.0000	
		$\Upsilon_c^{(0)}$	−0.0074	−0.0067	−0.0055	−0.0036	−0.0010	0.0019	
		$\Upsilon_c^{(1)}$	−0.0010	−0.0011	−0.0014	−0.0017	−0.0021	−0.0022	
		$\Upsilon_c^{(2)}$	0.0084	0.0079	0.0069	0.0053	0.0031	0.0003	

TABLE III. Deviation from the FCI quantities (in hartree) of the individual energies, $E^{(I)}$, and the corresponding excitation energies, $\Omega^{(I)}$, for the ground ($I = 0$), singly-excited ($I = 1$) and doubly-excited ($I = 2$) states of 3-boxium (i.e., $N = 3$ electrons in a box of length L). The values of the ensemble correlation derivative $\Upsilon_c^{(I)}$ are also reported.

			3-boxium with a box of length L						
Method	$\boldsymbol{w}$	State	$\pi/8$	$\pi/4$	$\pi/2$	π	2π	4π	8π
FCI		$E^{(0)}$	475.6891	125.7776	34.8248	10.3536	3.3766	1.2126	0.4721
		$E^{(1)}$	702.8330	183.3370	49.5922	14.2255	4.4269	1.5105	0.5606
		$E^{(2)}$	1379.3128	353.5967	92.7398	25.3135	7.3546	2.3203	0.7990
		$\Omega^{(1)}$	227.1438	57.5594	14.7674	3.8720	1.0504	0.2979	0.0885
		$\Omega^{(2)}$	903.6236	227.8191	57.9150	14.9599	3.9780	1.1077	0.3269
			Deviation from FCI						
TDA-TDLDA		$\Omega^{(1)}$	0.0162	0.0157	0.0146	0.0110	−0.0049	−0.0344	−0.0378
TDLDA		$\Omega^{(1)}$	0.0262	0.0264	0.0264	0.0269	0.0273	0.0206	−0.0116
KS-eLDA	$(0, 0)$	$E^{(0)}$	−0.0481	−0.0478	−0.0473	−0.0463	−0.0446	−0.0387	−0.0257
		$E^{(1)}$	0.0343	0.0336	0.0321	0.0292	0.0220	0.0084	0.0008
		$E^{(2)}$	0.0277	0.0267	0.0247	0.0216	0.0187	0.0208	0.0209
		$\Omega^{(1)}$	0.0824	0.0814	0.0794	0.0755	0.0666	0.0471	0.0266
		$\Omega^{(2)}$	0.0759	0.0745	0.0720	0.0679	0.0633	0.0595	0.0467
		$\Upsilon_c^{(0)}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		$\Upsilon_c^{(1)}$	0.0100	0.0092	0.0077	0.0051	0.0012	−0.0034	−0.0072
		$\Upsilon_c^{(2)}$	0.0244	0.0231	0.0208	0.0168	0.0108	0.0029	−0.0050
KS-eLDA	$(1/3, 1/3)$	$E^{(0)}$	0.0078	0.0080	0.0082	0.0085	0.0081	0.0024	−0.0022
		$E^{(1)}$	0.0172	0.0162	0.0144	0.0112	0.0064	0.0019	0.0004
		$E^{(2)}$	0.0645	0.0636	0.0621	0.0590	0.0530	0.0420	0.0300
		$\Omega^{(1)}$	0.0094	0.0083	0.0062	0.0027	−0.0018	−0.0004	0.0026
		$\Omega^{(2)}$	0.0567	0.0557	0.0539	0.0506	0.0449	0.0397	0.0323
		$\Upsilon_c^{(0)}$	−0.0115	−0.0107	−0.0094	−0.0072	−0.0038	0.0005	0.0045
		$\Upsilon_c^{(1)}$	−0.0015	−0.0016	−0.0018	−0.0022	−0.0028	−0.0033	−0.0032
		$\Upsilon_c^{(2)}$	0.0129	0.0123	0.0113	0.0094	0.0066	0.0028	−0.0013

TABLE IV. Deviation from the FCI quantities (in hartree) of the individual energies, $E^{(I)}$, and the corresponding excitation energies, $\Omega^{(I)}$, for the ground ($I = 0$), singly-excited ($I = 1$) and doubly-excited ($I = 2$) states of 4-boxium (i.e., $N = 4$ electrons in a box of length L). The values of the ensemble correlation derivative $\Upsilon_c^{(I)}$ are also reported.

			4-boxium with a box of length L						
Method	$\boldsymbol{w}$	State	$\pi/8$	$\pi/4$	$\pi/2$	π	2π	4π	8π
FCI		$E^{(0)}$	1020.3778	270.0849	74.9426	22.3790	7.3595	2.6798	1.0633
		$E^{(1)}$	1312.2776	344.0184	93.8936	27.3398	8.7021	3.0600	1.1764
		$E^{(2)}$	2183.4399	563.5949	149.6753	41.7213	12.5052	4.1033	1.4749
		$\Omega^{(1)}$	291.8998	73.9335	18.9510	4.9608	1.3426	0.3802	0.1131
		$\Omega^{(2)}$	1163.0621	293.5099	74.7326	19.3423	5.1457	1.4235	0.4116
			Deviation from FCI						
TDA-TDLDA		$\Omega^{(1)}$	0.0203	0.0201	0.0195	0.0181	0.0106	−0.0178	−0.0369
TDLDA		$\Omega^{(1)}$	0.0008	0.0007	0.0004	−0.0006	−0.0074	−0.0360	−0.0653
KS-eLDA	$(0, 0)$	$E^{(0)}$	−0.0541	−0.0539	−0.0537	−0.0534	−0.0529	−0.0504	−0.0386
		$E^{(1)}$	0.0413	0.0406	0.0390	0.0362	0.0304	0.0159	0.0008
		$E^{(2)}$	0.0642	0.0622	0.0586	0.0517	0.0399	0.0254	0.0149
		$\Omega^{(1)}$	0.0954	0.0945	0.0927	0.0896	0.0833	0.0663	0.0394
		$\Omega^{(2)}$	0.1182	0.1162	0.1123	0.1051	0.0928	0.0758	0.0534
		$\Upsilon_c^{(0)}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		$\Upsilon_c^{(1)}$	0.0136	0.0127	0.0111	0.0083	0.0038	−0.0022	−0.0080
		$\Upsilon_c^{(2)}$	0.0330	0.0316	0.0291	0.0248	0.0178	0.0080	−0.0028
KS-eLDA	$(1/3, 1/3)$	$E^{(0)}$	0.0085	0.0085	0.0084	0.0082	0.0072	0.0021	−0.0015
		$E^{(1)}$	0.0164	0.0152	0.0129	0.0087	0.0020	−0.0050	−0.0044
		$E^{(2)}$	0.0936	0.0917	0.0880	0.0807	0.0664	0.0434	0.0300
		$\Omega^{(1)}$	0.0079	0.0067	0.0045	0.0006	−0.0051	−0.0071	−0.0029
		$\Omega^{(2)}$	0.0851	0.0832	0.0796	0.0725	0.0593	0.0413	0.0315
		$\Upsilon_c^{(0)}$	−0.0155	−0.0148	−0.0134	−0.0110	−0.0071	−0.0017	0.0040
		$\Upsilon_c^{(1)}$	−0.0020	−0.0021	−0.0023	−0.0027	−0.0034	−0.0042	−0.0044
		$\Upsilon_c^{(2)}$	0.0175	0.0168	0.0157	0.0137	0.0105	0.0059	0.0004

TABLE V. Deviation from the FCI quantities (in hartree) of the individual energies, $E^{(I)}$, and the corresponding excitation energies, $\Omega^{(I)}$, for the ground ($I = 0$), singly-excited ($I = 1$) and doubly-excited ($I = 2$) states of 5-boxium (i.e., $N = 5$ electrons in a box of length L). The values of the ensemble correlation derivative $\Upsilon_c^{(I)}$ are also reported.

			5-boxium with a box of length L						
Method	$\boldsymbol{w}$	State	$\pi/8$	$\pi/4$	$\pi/2$	π	2π	4π	8π
FCI		$E^{(0)}$	1867.6344	493.6760	136.7020	40.7244	13.3763	4.8811	1.9492
		$E^{(1)}$	2224.11488	583.8981	159.7957	46.7553	15.0029	5.3399	2.0855
		$E^{(2)}$	3289.2022	852.4249	228.0415	64.3597	19.6613	6.6206	2.4547
		$\Omega^{(1)}$	356.4804	90.2221	23.0937	6.0308	1.6266	0.4588	0.1363
		$\Omega^{(2)}$	1421.56773	358.7489	91.3395	23.6352	6.2850	1.7395	0.5055
			Deviation from FCI						
TDA-TDLDA		$\Omega^{(1)}$	0.0230	0.0230	0.0228	0.0223	0.0192	−0.0015	−0.0309
TDLDA		$\Omega^{(1)}$	0.0005	0.0005	0.0004	0.0000	−0.0033	−0.0248	−0.0650
KS-eLDA	$(0, 0)$	$E^{(0)}$	−0.0587	−0.0586	−0.0587	−0.0588	−0.0591	−0.0590	−0.0506
		$E^{(1)}$	0.0457	0.0450	0.0435	0.0409	0.0362	0.0241	0.0033
		$E^{(2)}$	0.0861	0.0838	0.0793	0.0712	0.0571	0.0377	0.0196
		$\Omega^{(1)}$	0.1044	0.1036	0.1022	0.0997	0.0953	0.0830	0.0540
		$\Omega^{(2)}$	0.1447	0.1424	0.1380	0.1300	0.1162	0.0966	0.0703
		$\Upsilon_c^{(0)}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		$\Upsilon_c^{(1)}$	0.0172	0.0163	0.0147	0.0117	0.0067	−0.0004	−0.0080
		$\Upsilon_c^{(2)}$	0.0416	0.0402	0.0376	0.0329	0.0253	0.0140	0.0005
KS-eLDA	$(1/3, 1/3)$	$E^{(0)}$	0.0070	0.0070	0.0068	0.0063	0.0053	0.0015	−0.0049
		$E^{(1)}$	0.0162	0.0151	0.0128	0.0086	0.0018	−0.0066	−0.0095
		$E^{(2)}$	0.1080	0.1056	0.1011	0.0925	0.0772	0.0538	0.0325
		$\Omega^{(1)}$	0.0092	0.0081	0.0060	0.0022	−0.0035	−0.0081	−0.0047
		$\Omega^{(2)}$	0.1010	0.0986	0.0943	0.0862	0.0719	0.0523	0.0373
		$\Upsilon_c^{(0)}$	−0.0196	−0.0188	−0.0174	−0.0148	−0.0106	−0.0044	0.0029
		$\Upsilon_c^{(1)}$	−0.0024	−0.0025	−0.0027	−0.0032	−0.0040	−0.0050	−0.0056
		$\Upsilon_c^{(2)}$	0.0220	0.0213	0.0201	0.0180	0.0146	0.0093	0.0027

TABLE VI. Deviation from the FCI quantities (in hartree) of the individual energies, $E^{(I)}$, and the corresponding excitation energies, $\Omega^{(I)}$, for the ground ($I = 0$), singly-excited ($I = 1$) and doubly-excited ($I = 2$) states of 6-boxium (i.e., $N = 6$ electrons in a box of length L). The values of the ensemble correlation derivative $\Upsilon_c^{(I)}$ are also reported.

			6-boxium with a box of length L						
Method	$\boldsymbol{w}$	State	$\pi/8$	$\pi/4$	$\pi/2$	π	2π	4π	8π
FCI		$E^{(0)}$	3082.5386	813.0910	224.3734	66.5257	21.7454	7.9136	3.1633
		$E^{(1)}$	3503.4911	919.5487	251.5842	73.6145	23.6504	8.4487	3.3217
		$E^{(2)}$	4762.0921	1236.8257	332.1993	94.3988	29.1455	9.9582	3.7572
		$\Omega^{(1)}$	420.9525	106.4577	27.2108	7.0888	1.9050	0.5351	0.1583
		$\Omega^{(2)}$	1679.5536	423.7347	107.8259	27.8731	7.4001	2.0446	0.5938
			Deviation from FCI						
TDA-TDLDA		$\Omega^{(1)}$	0.0249	0.0248	0.0250	0.0250	0.0242	0.0114	−0.0223
TDLDA		$\Omega^{(1)}$	0.0002	0.0000	0.0002	0.0000	−0.0016	−0.0162	−0.0612
KS-eLDA	$(0, 0)$	$E^{(0)}$	−0.0626	−0.0627	−0.0628	−0.0632	−0.0641	−0.0654	−0.0612
		$E^{(1)}$	0.0486	0.0477	0.0465	0.0440	0.0400	0.0308	0.0078
		$E^{(2)}$	0.1017	0.0992	0.0946	0.0862	0.0718	0.0507	0.0271
		$\Omega^{(1)}$	0.1112	0.1104	0.1093	0.1072	0.1041	0.0962	0.0690
		$\Omega^{(2)}$	0.1643	0.1619	0.1575	0.1494	0.1358	0.1162	0.0884
		$\Upsilon_c^{(0)}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		$\Upsilon_c^{(1)}$	0.0208	0.0199	0.0182	0.0151	0.0098	0.0018	−0.0075
		$\Upsilon_c^{(2)}$	0.0503	0.0488	0.0460	0.0412	0.0330	0.0205	0.0046
KS-eLDA	$(1/3, 1/3)$	$E^{(0)}$	0.0046	0.0045	0.0043	0.0039	0.0031	0.0006	−0.0067
		$E^{(1)}$	0.0157	0.0144	0.0123	0.0080	0.0009	−0.0091	−0.0160
		$E^{(2)}$	0.1167	0.1142	0.1095	0.1007	0.0853	0.0616	0.0355
		$\Omega^{(1)}$	0.0112	0.0099	0.0080	0.0041	−0.0022	−0.0097	−0.0093
		$\Omega^{(2)}$	0.1121	0.1097	0.1051	0.0968	0.0822	0.0610	0.0423
		$\Upsilon_c^{(0)}$	−0.0237	−0.0229	−0.0214	−0.0188	−0.0142	−0.0073	0.0013
		$\Upsilon_c^{(1)}$	−0.0029	−0.0030	−0.0032	−0.0037	−0.0045	−0.0057	−0.0066
		$\Upsilon_c^{(2)}$	0.0266	0.0259	0.0246	0.0224	0.0187	0.0130	0.0053

TABLE VII. Deviation from the FCI quantities (in hartree) of the individual energies, $E^{(I)}$, and the corresponding excitation energies, $\Omega^{(I)}$, for the ground ($I = 0$), singly-excited ($I = 1$) and doubly-excited ($I = 2$) states of 7-boxium (i.e., $N = 7$ electrons in a box of length L). The values of the ensemble correlation derivative $\Upsilon_c^{(I)}$ are also reported.

			7-boxium with a box of length L						
Method	$\boldsymbol{w}$	State	$\pi/8$	$\pi/4$	$\pi/2$	π	2π	4π	8π
FCI		$E^{(0)}$	4729.98018	1244.7753	342.1796	100.8943	32.7728	11.8683	4.7359
		$E^{(1)}$	5215.3307	1367.4316	373.4897	109.0326	34.9524	12.4779	4.9156
		$E^{(2)}$	6667.18516	1733.3319	466.4133	132.9686	41.2715	14.2096	5.4146
		$\Omega^{(1)}$	485.3505	122.6563	31.3101	8.1382	2.1796	0.6096	0.1797
		$\Omega^{(2)}$	1937.2050	488.5566	124.2336	32.0743	8.4987	2.3413	0.6787
			Deviation from FCI						
TDA-TDLDA		$\Omega^{(1)}$	0.0262	0.0264	0.0264	0.0269	0.0273	0.0206	−0.0116
TDLDA		$\Omega^{(1)}$	0.0000	0.0001	0.0000	−0.0001	−0.0009	−0.0107	−0.0539
KS-eLDA	$(0, 0)$	$E^{(0)}$	−0.0664	−0.0666	−0.0667	−0.0672	−0.0684	−0.0707	−0.0702
		$E^{(1)}$	0.0502	0.0495	0.0482	0.0459	0.0423	0.0355	0.0131
		$E^{(2)}$	0.1122	0.1104	0.1061	0.0979	0.0836	0.0635	0.0360
		$\Omega^{(1)}$	0.1165	0.1161	0.1149	0.1131	0.1108	0.1062	0.0834
		$\Omega^{(2)}$	0.1785	0.1769	0.1728	0.1652	0.1520	0.1342	0.1063
		$\Upsilon_c^{(0)}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		$\Upsilon_c^{(1)}$	0.0244	0.0235	0.0218	0.0186	0.0130	0.0043	−0.0065
		$\Upsilon_c^{(2)}$	0.0589	0.0574	0.0546	0.0496	0.0410	0.0275	0.0095
KS-eLDA	$(1/3, 1/3)$	$E^{(0)}$	0.0014	0.0013	0.0012	0.0009	0.0003	−0.0013	−0.0079
		$E^{(1)}$	0.0149	0.0138	0.0115	0.0072	−0.0001	−0.0110	−0.0209
		$E^{(2)}$	0.1217	0.1198	0.1154	0.1069	0.0917	0.0691	0.0389
		$\Omega^{(1)}$	0.0135	0.0125	0.0103	0.0063	−0.0005	−0.0096	−0.0130
		$\Omega^{(2)}$	0.1203	0.1185	0.1142	0.1060	0.0914	0.0705	0.0469
		$\Upsilon_c^{(0)}$	−0.0278	−0.0270	−0.0255	−0.0227	−0.0180	−0.0105	−0.0007
		$\Upsilon_c^{(1)}$	−0.0034	−0.0034	−0.0037	−0.0041	−0.0050	−0.0063	−0.0076
		$\Upsilon_c^{(2)}$	0.0311	0.0304	0.0291	0.0268	0.0230	0.0168	0.0083