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Gauge invariance of oscillator strengths in the approximate coupled cluster triples model CC3

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Abstract

The gauge invariance of the oscillator strength is examined for the lowest dipole transitions in Ne, N_2 and H_2O using the coupled cluster model hierarchy, CCS, CC2, CCSD, and CC3, and a variety of correlation consistent basis sets. The deviations between the oscillator strengths in the different gauges decrease from CCSD to CC3 (where connected triples are included) by about the same factor as they decrease from CCS to CC2 (where connected doubles are included). The deviations are very similar in CC2 and CCSD. The quality of the oscillator strengths is improved significantly at each level in coupled cluster hierarchy, also from CC2 to CCSD, where the equivalence between the oscillator strengths in the different gauges is very similar.
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1. Introduction

The positions and intensities of the bands in electronic absorption spectra are determined by the electronic excitation energies and oscillator strengths. The expression for the oscillator strength depends on the gauge of the interaction operator between the molecular system and the applied periodic field. For exact wavefunctions the oscillator strengths in the different gauges are all equivalent and give identical results [1]. For approximate wavefunctions this equivalence is, in general, lost. The extend to which the oscillator strengths differ depends on the quality of the one-electron basis set and whether the time-evolution of the approximate wavefunction satisfies Ehrenfest's equation of motion. The latter equation is not fulfilled for coupled cluster (CC) wavefunctions and the equivalence between the oscillator strengths therefore depends for CC wavefunctions not only on the quality of the one-electron basis but also on the quality of the wavefunction, i.e., on the correlation treatment.

In this Letter, we examine the equivalence of oscillator strengths in different gauges for the hierarchy of approximations CCS, CC2 [2], CCSD, and CC3 [3], which is designed for obtaining a systematically improved description of molecular response properties. In CCS all single excitations are treated, in CCSD all doubles are added and in CCSDT all triples are further added. CC2 and CC3 are approximations to CCSD and CCSDT, where, respectively, doubles and triples, are treated in an approximate fashion and where the scaling of CCSD and CCSDT is reduced.

Pedersen and Koch [4] have previously carried out an investigation of the equivalence between the oscillator strengths in different gauges for the CCS, CC2, and CCSD methods. Their conclusion based on calculations on the lowest dipole transitions for Ne, N_2, and H_2O was that the oscillator strengths in the length and velocity gauge differed by about 5% both for CC2 and CCSD while the difference was significantly larger for CCS. Our investigation shows the improvements when triples are considered. For many molecular properties the effect of triples is extremely important, for example for equilibrium geometries and atomization energies a statistical investigation on 18 molecules has shown that the mean absolute error in CCSD decreased when triples

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are considered using CCSD(T) from 0.67 to 0.09 pm for equilibrium bond lengths [5] and from 32.2 to 4.1 kJ/mol for atomization energies [6].

If the electronic excitation energy from the ground state $|0\rangle$ to an excited state $|n\rangle$ is denoted as $\omega_{0n} = E_n - E_0$, the oscillator strength in the length gauge becomes

$$f_{0n}^{r} = \frac{2\omega_{0n}}{3}\langle 0|\mathbf{r}|n\rangle\langle n|\mathbf{r}|0\rangle = \frac{2}{3}\lim_{\omega\to\omega_{0n}}(\omega-\omega_{0n})\omega\langle\langle \mathbf{r};\mathbf{r}\rangle\rangle_{\omega}, \quad (1)$$

in the velocity gauge it is

$$f_{0n}^{v} = \frac{2}{3\omega_{0n}}\langle 0|\mathbf{p}|n\rangle\langle n|\mathbf{p}|0\rangle = \frac{2}{3}\lim_{\omega\to\omega_{0n}}(\omega-\omega_{0n})\omega^{-1}\langle\langle \mathbf{p};\mathbf{p}\rangle\rangle_{\omega}, \quad (2)$$

and in the mixed length–velocity gauge it is

$$f_{0n}^{\mathrm{rv}} = -\frac{2\mathrm{i}}{3}\langle 0|\mathbf{r}|n\rangle\langle n|\mathbf{p}|0\rangle = -\frac{2\mathrm{i}}{3}\lim_{\omega\to\omega_{0n}}(\omega-\omega_{0n})\langle\langle \mathbf{r};\mathbf{p}\rangle\rangle_{\omega}, \quad (3)$$

where atomic units are used and $\mathbf{r}$ and $\mathbf{p}$ are the electronic position and momentum operators, respectively, [7]. The last equalities in Eqs. (1)–(3) express that oscillator strengths may be defined in terms of residues of linear response functions $\langle\langle \mathbf{A};\mathbf{B}\rangle\rangle_{\omega}$ [8], where the one-electron operators $\mathbf{A}$ and $\mathbf{B}$ are either $\mathbf{r}$ and $\mathbf{p}$. This last route for defining the oscillator strengths is used for most standard wave function approximations where response functions can be defined, e.g., Hartree–Fock (SCF), density functional theory (DFT) and CC [9]; in fact no alternative usually exists to this definition [10].

As pointed out above, the oscillator strength for exact wave functions is gauge invariant, i.e., the oscillator strengths in the length, the velocity and the mixed gauge are equivalent. The equivalence hinges on the fact that the linear response function for an exact state satisfies the equation of motion [11]

$$\omega\langle\langle \mathbf{A};\mathbf{B}\rangle\rangle_{\omega} = \langle\langle [\mathbf{A},H_0];\mathbf{B}\rangle\rangle_{\omega} + \langle 0|[\mathbf{A},\mathbf{B}]|0\rangle, \quad (4)$$

where H_0 is the electronic Hamiltonian for the isolated system and ω is the frequency of the applied periodic field. To obtain the equivalence, the operator identity

$$\mathbf{p} = -\mathrm{i}[\mathbf{r},H_0] \quad (5)$$

must be used. This operator identity is only fulfilled for a complete one-electron basis set.

In electronic structure calculations where finite basis sets are used the three forms for the oscillator strengths will thus not give identical results. To investigate how the equivalence between the oscillator strength depends on the completeness of the basis set, we carry out calculations using the correlation consistent basis sets of Dunning et al. [12], where a hierarchical improved description of the one-electron space is obtained by increasing the cardinal number.

The equation of motion for the linear response function, Eq. (4), is obtained from an expansion to first order in the interaction operator of Ehrenfest's theorem for a one-electron operator $\mathbf{A}$. Since Ehrenfest's theorem is used to determine the time evolution of SCF, DFT and multi-configuration SCF (MCSCF) wave functions [13], the equation of motion, Eq. (4), is satisfied for these methods and calculated oscillator strengths become gauge invariant in the limit of a complete basis set. Contrary, linear response functions for CC wave functions do not satisfy the equation of motion, Eq. (4), and CC oscillator strengths in the different gauges therefore differ even in the limit of a complete basis set [14]. Of course, if no truncation is carried out in the excitation manifold, the CC results become identical to the full configuration interaction (FCI) results and gauge invariance is obtained in the limit of a complete basis. Increasing the level in the coupled cluster hierarchy, CCS, CC2, CCSD, and CC3, gives a systematically improved description of dynamic electron correlation. The goal of this investigation is to examine if this improvement results in a similar improvement in the equivalence between the oscillator strengths in the different gauges. We also compare with the equivalence obtained for SCF wave functions where the difference between the oscillator strengths in the different gauges is solely due to approximations in the one-electron basis sets.

2. Calculational details

The oscillator strengths are calculated for the lowest allowed dipole transition for Ne, N_2, and H_2O using the CCS, CC2, CCSD, and CC3 coupled cluster models and the SCF model in the length, the velocity and the mixed length–velocity gauge. The calculations are performed using Dunning's correlation consistent basis set cc-pVXZ augmented with diffuse functions [12]. For Ne and N_2 double augmentation is used, while for H_2O single augmentation is used in accordance with the findings of Pedersen and Koch [4]. For N_2 we used the internuclear distance of 1.094339 Å. For H_2O the O–H bond length is 0.9572 Å and the H–O–H bond angle 104.52°. These geometries were also used in FCI calculations of the excitation energies [15] and in the oscillator strength gauge investigation of Pedersen and Koch [4]. The calculations are carried out using the DALTON program [16]. For the details of the implementation of the transition strengths for CCS, CC2 and CCSD see [17]. The CC3 transition strengths have recently been implemented by us [18] in the coupled-cluster code [3,19] which is part of the DALTON package [16].

3. Results

The excitation energies and the oscillator strengths in the length, velocity, and mixed gauge are given for the $1^1\Sigma_g^+ \rightarrow 1^1\Pi_u$ transition in N_2 in Table 1, for the $1^1S \rightarrow 1^1P$ transition in Ne in Table 2 and for the $1^1A_1 \rightarrow 1^1B_2$ transition in H_2O in Table 3. In addition, the tables list the differences between the length and velocity results

$$\Delta_{rv} = f_{0n}^{r} - f_{0n}^{v}, \tag{6}$$

and the excitation energy ω_{0n}. All three considered transitions are single electron replacement dominated with per cent of single replacements in the excitation vector in the CC3 calculation for the largest cardinal number of 91%, 95% and 93% for the transition in N_2, Ne and H_2O, respectively.

The absolute value of Δ_{rv} in general decreases when the cardinal number is increased. A large decrease in Δ_{rv} is in general also obtained when connected double excitations are included, i.e., going from CCS to the CC2 level, and when connected triple excitations are included, i.e., going from CCSD to the CC3 level. At the CC2 and the CCSD level the equivalence between the different gauges is very similar. The above trends are seen clearly in Fig. 1, where the difference between the oscillator strength in the length and the velocity gauge in per cent

$$\Delta_{rv}^{rel} = 100|\Delta_{rv}|/f^{rv} \tag{7}$$

is plotted as a function of the cardinal numbers for the considered wavefunction models. For the basis sets with the cardinal number $X = 5$ the relative deviation Δ_{rv}^{rel} is plotted in Fig. 2 as a function of the wavefunction for the three investigated transitions. Complete equivalence is obtained for the SCF model for all practical purposes for the three investigated transitions, while for the CC models the remaining deviations are between 5 and 25% for the CCS model, 1–6% for the CC2 and CCSD models and between 0.06 and 1% for the CC3 model.

It should be emphasized that the similar deviations from equivalence for CC2 and CCSD do not imply that the oscillator strengths in the two approximations have similar quality. Equivalence between the oscillator strengths in different gauges is a necessary condition for having a high quality wave function approximation, but only one of several. For SCF wave functions equivalence is obtained by construction for a complete one electron basis set, but the transition strengths and excitation energies obtained with this method are usually not of very high quality.

To examine the quality of the oscillator strength we examine in more detail the accuracy of the calculated excitation energies ω_{0n} and the transition strengths $I^r = \langle 0|\mathbf{r}|n\rangle\langle n|\mathbf{r}|0\rangle$ or $I^v = \langle 0|\mathbf{p}|n\rangle\langle n|\mathbf{p}|0\rangle$. In [20,21] the excitation energies for the considered transitions have been reported for the FCI model and cc-pVDZ basis sets augmented with diffuse functions. Comparison of the FCI excitation energies and the ones of the coupled cluster hierarchy CCS, CC2, CCSD, and CC3 showed

Table 1
Oscillator strength and excitation energy (ω_{0n}, in eV) for the singlet transition $1^1\Sigma_g^+ \rightarrow 1^1\Pi_u$ of N_2

Model	Basis set	f_{0n}^{r}	f_{0n}^{v}	f_{0n}^{rv}	Δ_{rv}	ω_{0n}
CC3	daDZ	0.1844	0.1806	0.1825	0.0037	12.71
	daTZ	0.2046	0.2045	0.2046	0.0002	12.87
	daQZ	0.2141	0.2147	0.2144	−0.0006	12.92
	da5Z	0.2196	0.2194	0.2195	0.0002	12.94
CCSD	daDZ	0.1671	0.1617	0.1644	0.0055	12.80
	daTZ	0.1757	0.1729	0.1743	0.0029	13.00
	daQZ	0.1794	0.1769	0.1782	0.0025	13.08
	da5Z	0.1822	0.1788	0.1805	0.0034	13.11
CC2	daDZ	0.1202	0.1144	0.1172	0.0058	12.42
	daTZ	0.1239	0.1211	0.1225	0.0028	12.58
	daQZ	0.1248	0.1230	0.1239	0.0018	12.65
	da5Z	0.1263	0.1238	0.1251	0.0025	12.69
CCS	daDZ	0.1629	0.1485	0.1556	0.0144	13.27
	daTZ	0.1662	0.1504	0.1582	0.0158	13.24
	daQZ	0.1670	0.1511	0.1589	0.0158	13.23
	da5Z	0.1675	0.1512	0.1592	0.0163	13.23
SCF	daDZ	0.1669	0.1725	0.1697	−0.0055	13.26
	daTZ	0.1702	0.1724	0.1713	−0.0022	13.22
	daQZ	0.1709	0.1717	0.1713	−0.0008	13.22
	da5Z	0.1714	0.1715	0.1715	−0.0001	13.22

The equivalence Δ_{rv} is defined in Eq. (6). Results are given for the basis set series d-aug-cc-pVXZ, with X = D, T, Q, and 5, which has been abbreviated as daDZ, daTZ, daQZ, and da5Z, respectively.

Table 2
Oscillator strength and excitation energy (ω_{0n}, in eV) for the singlet transition $1^1S \rightarrow 1^1P$ of Ne

Model	Basis set	f_{0n}^{r}	f_{0n}^{v}	f_{0n}^{rv}	Δ_{rv}	ω_{0n}
CC3	daDZ	0.1653	0.1667	0.1660	−0.0014	16.69
	daTZ	0.1696	0.1703	0.1699	−0.0007	16.70
	daQZ	0.1703	0.1702	0.1702	0.0001	16.78
	da5Z	0.1699	0.1694	0.1697	0.0005	16.81
	da6Z	0.1697	0.1690	0.1694	0.0006	16.83
CCSD	daDZ	0.1614	0.1682	0.1648	−0.0068	16.47
	daTZ	0.1657	0.1707	0.1682	−0.0050	16.61
	daQZ	0.1665	0.1704	0.1685	−0.0040	16.72
	da5Z	0.1663	0.1696	0.1679	−0.0033	16.77
	da6Z	0.1660	0.1691	0.1676	−0.0031	16.80
CC2	daDZ	0.1548	0.1569	0.1559	−0.0021	15.85
	daTZ	0.1600	0.1600	0.1600	0.0000	15.98
	daQZ	0.1607	0.1598	0.1603	0.0009	16.08
	da5Z	0.1599	0.1585	0.1592	0.0014	16.13
	da6Z	0.1594	0.1578	0.1586	0.0016	16.16
CCS	daDZ	0.1616	0.1672	0.1644	−0.0056	18.44
	daTZ	0.1668	0.1739	0.1703	−0.0071	18.38
	daQZ	0.1680	0.1758	0.1719	−0.0078	18.36
	da5Z	0.1680	0.1754	0.1717	−0.0074	18.35
	da6Z	0.1679	0.1752	0.1715	−0.0073	18.35
SCF	daDZ	0.1602	0.1640	0.1621	−0.0038	18.43
	daTZ	0.1654	0.1672	0.1663	−0.0018	18.37
	daQZ	0.1667	0.1675	0.1671	−0.0008	18.35
	da5Z	0.1666	0.1668	0.1668	−0.0002	18.35
	da6Z	0.1666	0.1666	0.1666	−0.0000	18.35

The equivalence Δ_{rv} is defined in Eq. (6). Results are given for the basis set series d-aug-cc-pVXZ, with $X = D, T, Q, 5$, and 6, which has been abbreviated as daDZ, daTZ, daQZ, da5Z, and da6Z, respectively.

Table 3
Oscillator strength and excitation energy (ω_{0n}, in eV) for the singlet transition $1^1A_1 \rightarrow 1^1B_2$ of H_2O

Model	Basis set	f_{0n}^{r}	f_{0n}^{v}	f_{0n}^{rv}	Δ_{rv}	ω_{0n}
CC3	aDZ	0.0585	0.0585	0.0585	−0.0000	7.53
	aTZ	0.0548	0.0544	0.0546	0.0004	7.62
	aQZ	0.0532	0.0526	0.0529	0.0007	7.67
	a5Z	0.0523	0.0520	0.0521	0.0003	7.69
CCSD	aDZ	0.0575	0.0608	0.0592	−0.0034	7.46
	aTZ	0.0536	0.0561	0.0549	−0.0025	7.62
	aQZ	0.0521	0.0542	0.0531	−0.0021	7.69
	a5Z	0.0511	0.0535	0.0523	−0.0024	7.72
CC2	aDZ	0.0606	0.0604	0.0605	0.0001	7.10
	aTZ	0.0575	0.0558	0.0567	0.0017	7.26
	aQZ	0.0560	0.0537	0.0548	0.0023	7.32
	a5Z	0.0547	0.0528	0.0537	0.0019	7.35
CCS	aDZ	0.0512	0.0624	0.0566	−0.0112	8.68
	aTZ	0.0488	0.0615	0.0550	−0.0127	8.70
	aQZ	0.0478	0.0611	0.0542	−0.0133	8.70
	a5Z	0.0473	0.0609	0.0538	−0.0136	8.70
SCF	aDZ	0.0498	0.0512	0.0505	−0.0014	8.64
	aTZ	0.0474	0.0478	0.0476	−0.0003	8.65
	aQZ	0.0464	0.0463	0.0464	0.0001	8.65
	a5Z	0.0459	0.0459	0.0459	−0.0000	8.65

The equivalence Δ_{rv} is defined in Eq. (6). Results are given for the basis set series aug-cc-pVXZ, with $X = D, T, Q$, and 5, which has been abbreviated as aDZ, aTZ, aQZ, and a5Z, respectively.

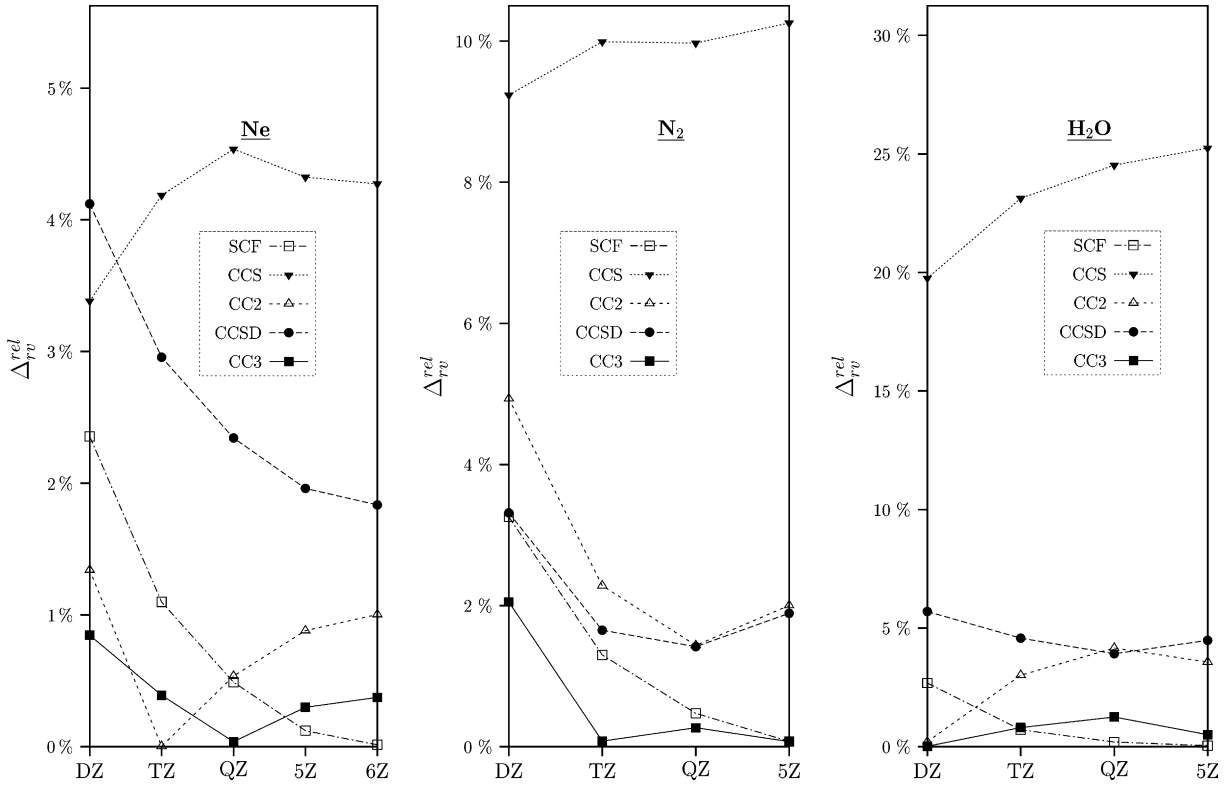


Fig. 1. The difference between the oscillator strength in the length and the velocity gauge, Δ_{rv}^{rel}, in per cent (see Eq. (7)) for Ne, N_2 and H_2O.

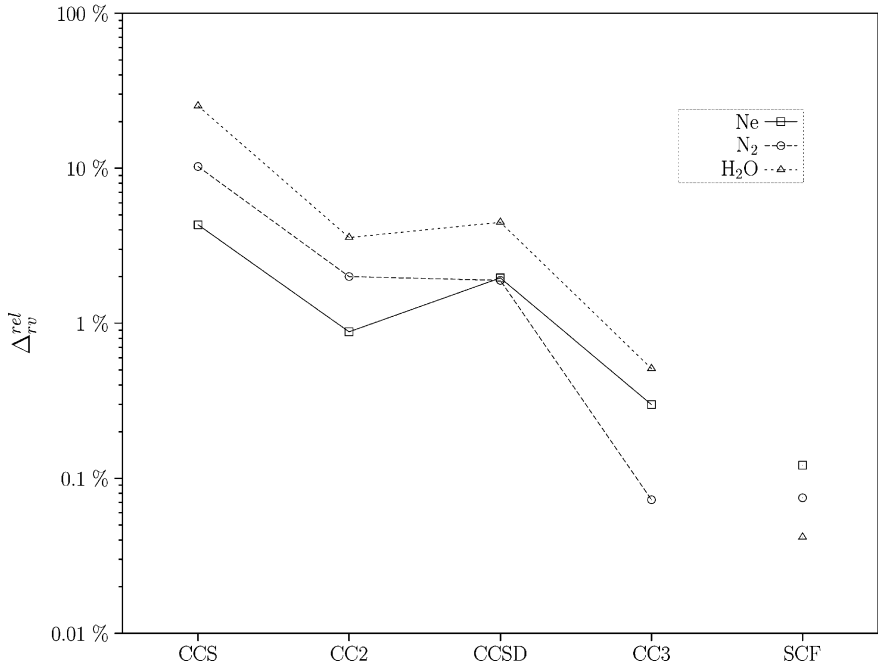


Fig. 2. The difference between the oscillator strength in the length and the velocity gauge, Δ_{rv}^{rel}, in per cent (see Eq. (7)), using d-aug-cc-pV5Z basis for Ne and N_2, and aug-cc-pV5Z for H_2O.

that the errors in the excitation energies in general decreased by about a factor 3 at each level. For CC3 the remaining errors are as small as 0.18, 0.007 and 0.02 eV for the transition in N_2, Ne and H_2O, respectively. The relative large error in the CC3 excitation energy for N_2 is due to the fact that the single excitation weight in the $^1\Pi_u$ state is 0.674 [21] in the FCI model. In Fig. 3 we have plotted the excitation energies for the various wave

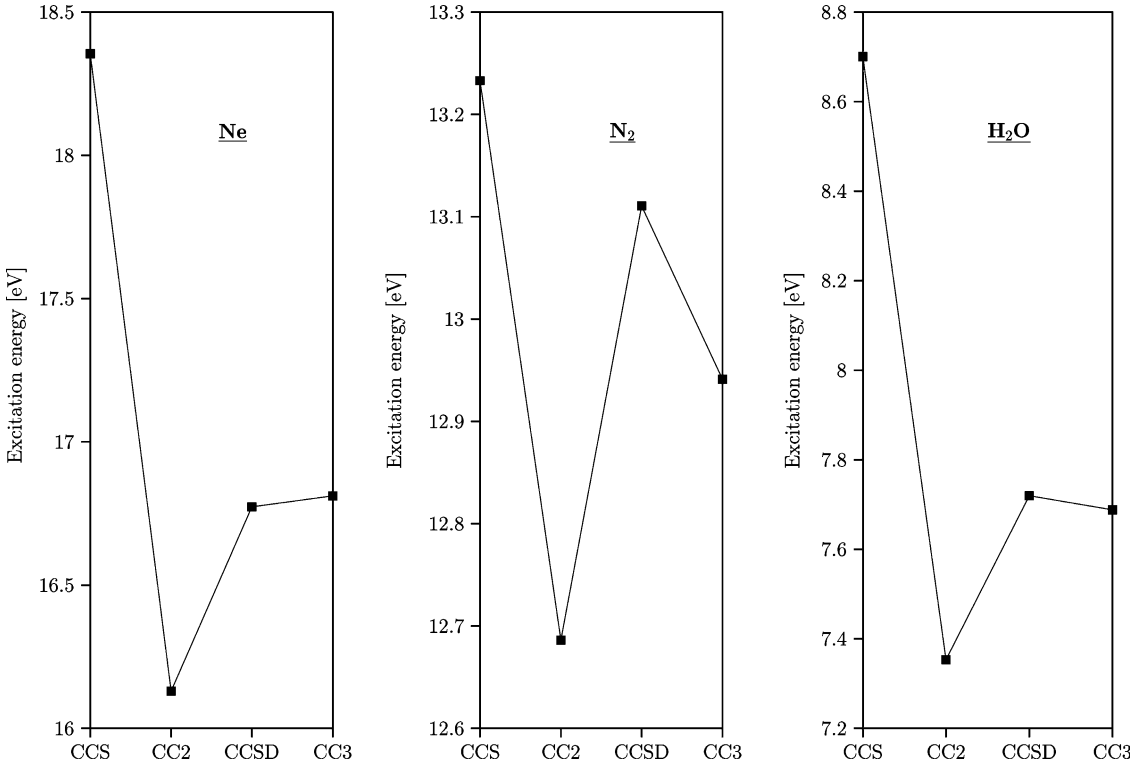


Fig. 3. The excitation energies (eV) in the various wave function approximations with d-aug-cc-pV6Z for Ne, d-aug-cc-pV5Z for N_2, and aug-cc-pV5Z for H_2O.

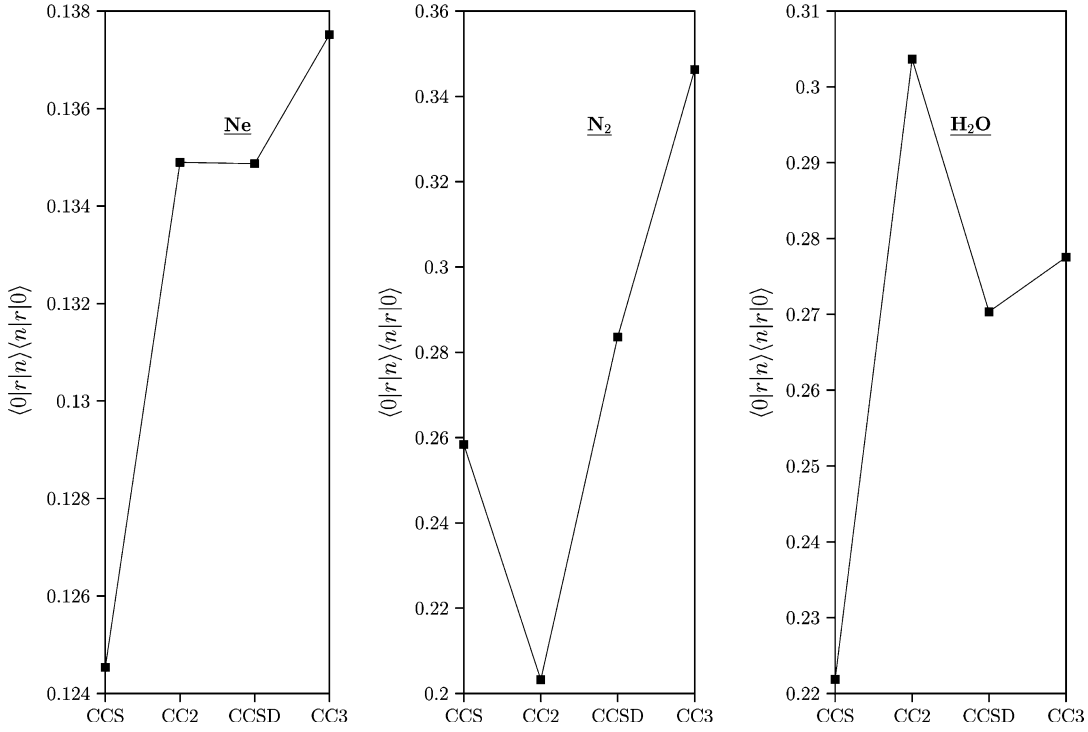


Fig. 4. The transition strengths in length gauge in the various wave function approximations with d-aug-cc-pV6Z for Ne, d-aug-cc-pV5Z for N_2, and aug-cc-pV5Z for H_2O.

function approximations calculated in the basis sets with the largest cardinal numbers. The trends in the excitation energies are very similar to the trends observed in the smaller basis sets where FCI results are available. As the difference between the FCI and CC3 excitation energies may be expected to be rather independent of the

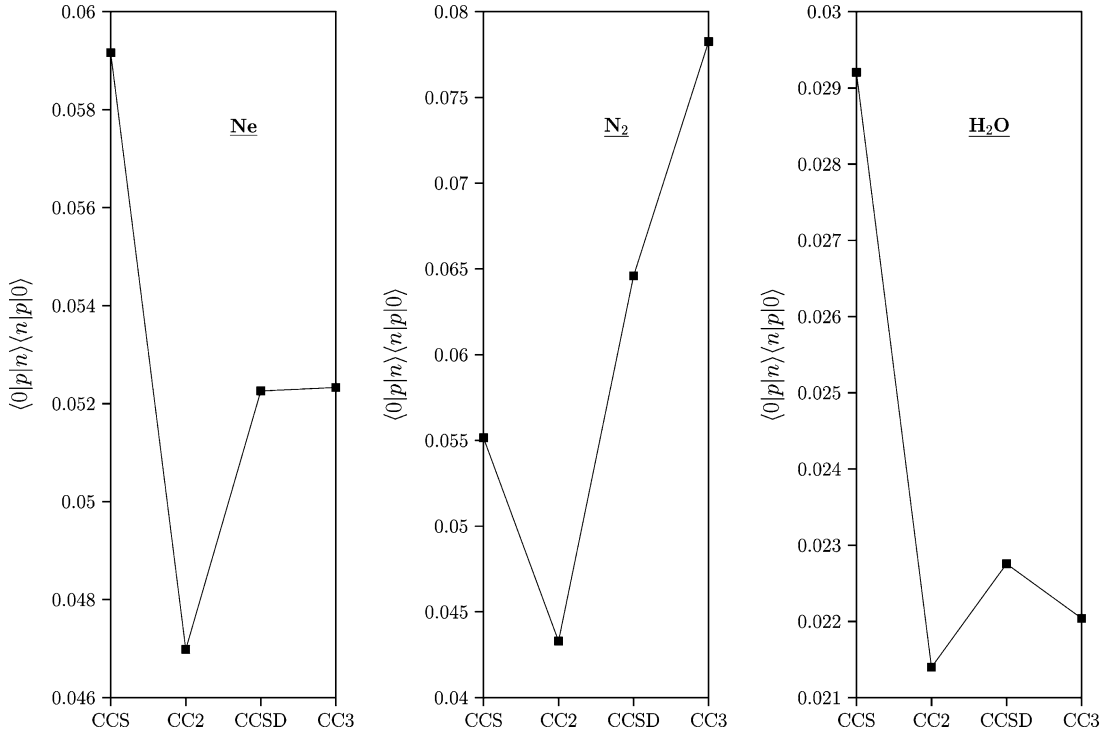


Fig. 5. The transition strengths in velocity gauge in the various wave function approximations with d-aug-cc-pV6Z for Ne, d-aug-cc-pV5Z for N_2, and aug-cc-pV5Z for H_2O.

basis set, the CC3 excitation energies in Fig. 3 are expected to be close to the FCI results also for this large basis. In Fig. 4 we have plotted the transition strength in the length gauge $S^{\mathrm{r}}_{0n} = \langle 0|\mathbf{r}|n\rangle\langle n|\mathbf{r}|0\rangle$ obtained using the various wavefunction approximations for the considered transitions in N_2, Ne and H_2O. Fig. 5 gives the corresponding results for the velocity gauge $S^{\mathrm{v}}_{0n} = \langle 0|\mathbf{p}|n\rangle\langle n|\mathbf{p}|0\rangle$. No FCI investigations have been performed for the transition strengths for the considered transitions. However, we expect improvements at each level in the CC hierarchy similar to the ones for the excitation energies. The improved equivalence between the oscillator strengths in different gauges substantiates this assumption. The CC3 intensities may thus be expected to be of very high quality. As both the excitation energies (see Fig. 3) and the transition strengths (see Figs. 4 and 5) are significantly more accurate in CCSD than in CC2, the CC2 oscillator strengths have lower quality than the CCSD ones. In particular for N_2 the CC2 oscillator strength does not have the quality of the CCSD one.

4. Concluding remarks

The equivalence of oscillator strengths in different gauges has been investigated for the hierarchy of single reference coupled cluster models CCS, CC2, CCSD, and CC3. Significant reductions of the deviations between the oscillator strengths in different gauges are found when connected double excitations are included, i.e., going from CCS to CC2, and when connected triple excitations are included, i.e., when going from CCSD to CC3, while the equivalence is very similar for CC2 and CCSD. The oscillator strengths improve at each level in the CC hierarchy, also from CC2 to CCSD, where the equivalence between the oscillator strengths in the different gauges was very similar.

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