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Combining Multiconfiguration and Perturbation Methods: Perturbative Estimates of Core–Core Electron Correlation Contributions to Excitation Energies in Mg-Like Iron

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Abstract: Large configuration interaction (CI) calculations can be performed if part of the interaction is treated perturbatively. To evaluate the combined CI and perturbative method, we compute excitation energies for the $3l3l'$, $3l4l'$ and $3s5l$ states in Mg-like iron. Starting from a CI calculation including valence and core–valence correlation effects, it is found that the perturbative inclusion of core–core electron correlation halves the mean relative differences between calculated and observed excitation energies. The effect of the core–core electron correlation is largest for the more excited states. The final relative differences between calculated and observed excitation energies is 0.023%, which is small enough for the calculated energies to be of direct use in line identifications in astrophysical and laboratory spectra.

Keywords: excitation energies; multiconfiguration Dirac–Hartree–Fock; configuration interaction

1. Introduction

Transitions from highly charged ions are observed in the spectra of astrophysical sources as well as in Tokamak and laser-produced plasmas, and they are routinely used for diagnostic purposes [1]. Often, transitions between configurations in the same complex are used, but transitions from higher lying configurations are also important (see, e.g., [2] for a discussion of the higher lying states in the case of Mg-like iron). Transition energies are available from experiments for many ions and collected in various data bases [3], but large amounts of data are still lacking. Although experimental work is aided by a new generation of light sources such as EBITs [4], spectral identifications are still a difficult and time-consuming task. A way forward is provided by theoretical transition energies that support line identification and render consistency checks for experimental level designations.

Much work has been done to improve both multiconfiguration methods and perturbative methods, each with their strengths and weaknesses, in order to provide theoretical transition energies of spectroscopic accuracy, i.e., transition energies with uncertainties of the same order as the ones obtained from experiments and observations using Chandra, Hinode or other space based missions in the X-ray and EUV spectral ranges [5–8]. Further advancements for complex systems with several electrons outside a closed atomic core calls for a combination of multiconfiguration and perturbative methods [9] and also for methods based on new principles [10,11].

In this paper, we describe how the multiconfiguration Dirac–Hartree–Fock (MCDHF) and relativistic configuration interaction (CI) methods can be modified to include perturbative corrections that account for core–core electron correlation. Taking Mg-like iron as an example, we show how the corrections improve excitation energies for the more highly excited states.

2. Relativistic Multiconfiguration Methods

2.1. Multiconfiguration Dirac–Hartree–Fock and Configuration Interaction

In the MCDHF method [12,13], as implemented in the GRASP2K program package [14], the wave function $\Psi(\gamma PJM_J)$ for a state labeled γPJM_J, where J and M_J are the angular quantum numbers and P is the parity, is expanded in antisymmetrized and coupled configuration state functions (CSFs)

$$\Psi(\gamma PJM_J) = \sum_{j=1}^{M} c_j \Phi(\gamma_j PJM_J). \tag{1}$$

The labels $\{\gamma_j\}$ denote other appropriate information of the configuration state functions, such as orbital occupancy and coupling scheme. The CSFs are built from products of one-electron orbitals, having the general form

$$\psi_{n\kappa,m}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} P_{n\kappa}(r)\chi_{\kappa,m}(\theta,\varphi) \\ \imath Q_{n\kappa}(r)\chi_{-\kappa,m}(\theta,\varphi) \end{pmatrix}, \tag{2}$$

where $\chi_{\pm\kappa,m}(\theta,\varphi)$ are 2-component spin-orbit functions. The radial functions $\{P_{n\kappa}(r), Q_{n\kappa}(r)\}$ are numerically represented on a grid.

Wave functions for a number of targeted states are determined simultaneously in the extended optimal level (EOL) scheme. Given initial estimates of the radial functions, the energies E and expansion coefficients $\mathbf{c} = (c_1, \ldots, c_M)^t$ for the targeted states are obtained as solutions to the configuration interaction (CI) problem

$$\mathbf{Hc} = E\mathbf{c}, \tag{3}$$

where $\mathbf{H}$ is the CI matrix of dimension $M \times M$ with elements

$$H_{ij} = \langle \Phi(\gamma_i PJM_J)|H|\Phi(\gamma_j PJM_J)\rangle. \tag{4}$$

In relativistic calculations, the Hamiltonian H is often taken as the Dirac–Coulomb Hamiltonian. Once the expansion coefficients have been determined, the radial functions are improved by solving a set of differential equations results from applying the variational principle on a weighted energy functional of the targeted states together with additional terms needed to preserve orthonormality of the orbitals. The CI problem and the solution of the differential equations are iterated until the radial orbitals and the energy are converged to a specified tolerance.

The MCDHF calculations are often followed by CI calculations where terms representing the transverse photon interaction are added to the Dirac-Coulomb Hamiltonian and the vacuum polarization effects are taken into account by including the Uehling potential. Electron self-energies are calculated with the screened hydrogenic formula [12,15]. Due to the relative simplicity of the CI method, often much larger expansions are included in the final CI calculations compared to the MCDHF calculations.

2.2. Large Expansions and Perturbative Corrections

The number of CSFs in the wave function expansions depend on the shell structure of the ionic system as well as the model for electron correlation (to be discussed in Section 3). For accurate calculations, a large number of CSFs are required, leading to very large matrices. To handle these large matrices, the CSFs can a priori be divided into two groups. The first group, P, with m elements ($m \ll M$) contains CSFs that account for the major parts of the wave functions. The second group, Q, with $M - m$ elements contains CSFs that represent minor corrections. Allowing interaction between CSFs in group P, interaction between CSFs in group P and Q and diagonal interactions between CSFs in Q gives a matrix

$$\begin{pmatrix} H^{(PP)} & H^{(PQ)} \\ H^{(QP)} & H^{(QQ)} \end{pmatrix}, \tag{5}$$

where $H_{ij}^{(QQ)} = \delta_{ij} E_i^Q$. The restriction of $H^{(QQ)}$ to diagonal elements results in a huge reduction in the total number of matrix elements and corresponding computational time. The assumptions of the approximation and the connections to the method of deflation in numerical analysis are discussed in [13]. This form of the CI matrix, which has been available in the non-relativistic and relativistic multiconfiguration codes for a long time [16,17], yields energies that are similar to the ones obtained by applying second-order perturbation theory (PT) corrections to the energies of the smaller $m \times m$ matrix. The method is therefore referred to here as CI combined with second-order Brillouin–Wigner perturbation theory [18]. Note, however, that the CI method with restrictions on the interactions gives, in contrast to ordinary perturbative methods, wave functions that can be directly used to evaluate expectation values such as transition rates.

3. Calculations

Calculations were performed for states belonging to the $3s^2$, $3p^2$, $3s3d$, $3d^2$, $3s4s$, $3s4d$, $3p4p$, $3p4f$, $3d4s$, $3d4d$, $3s5s$, $3s5d$, $3s5g$ even configurations and the $3s3p$, $3p3d$, $3s4p$, $3p4s$, $3s4f$, $3p4d$, $3d4p$, $3d4f$, $3s5p$, $3s5f$ odd configurations of Mg-like iron. For $3d4f$, only states below the $3p5s$ configuration were included. The above configurations define the multireference (MR) for the even and odd parities, respectively. Following the procedure in [19], an initial MCDHF calculation for all even and odd reference states was done in the EOL scheme. The initial calculation was followed by separate calculations in the EOL scheme for the even and odd parity states. The MCDHF calculations for the even states were based on CSF expansions obtained by allowing single (S) and double (D) substitutions of orbitals in the even MR configurations to an increasing active set of orbitals. In a similar way, the calculations for the odd states were based on CSF expansions obtained by allowing single (S) and double (D) substitutions of orbitals in the odd MR configurations to an increasing active set of orbitals. To prevent the CSF expansions from growing unmanageably large and in order to obtain orbitals that are spatially localized in the valence and core–valence region, at most, single substitutions were allowed from the $2s^22p^6$ core. The $1s^2$ shell was always closed. The active sets of orbitals for the even and odd parity states were extended by layers to include orbitals with quantum numbers up to $n = 8$ and $l = 6$, at which point the excitation energies are well converged.

To investigate the effects of electron correlation, three sets of CI calculations were done. In the first set of CI calculations, one calculation was done for the even states and one calculation for the odd states, the SD substitutions were only allowed from the valence shells of the MR, and the CSFs account for valence–valence correlation. In the second set of calculations, SD substitutions were such that there was at most one substitution from the $2s^22p^6$ core, and the CSFs account for valence–valence and core–valence correlation. In the final set of calculations, all SD substitutions were allowed, and the CSFs account for valence–valence, core–valence and core–core correlation. When all substitutions are allowed, the number of CSFs grows very large. For this reason, we apply CI with second-order perturbation corrections. The CSFs describing valence–valence and core–valence effects (SD substitutions with at most one substitution from the $2s^22p^6$ core) were included in group P, whereas the CSFs accounting for core–core correlation (D substitutions from $2s^2 2p^6$) were included in group Q and treated in second-order perturbation theory. The number of CSFs for the different CI calculations are given in Table 1.

Table 1. Number of CSFs for the even and odd parity expansions for the different sets of CI calculations. VV are the expansions accounting for valence–valence correlation, VV+CV are the expansions accounting for valence–valence and core–valence correlation and VV+CV+CC are the expansions accounting for valence-valence, core–valence and core–core correlation.

	VV	VV+CV	VV+CV+CC
even	2738	644,342	5,624,158
odd	2728	630,502	6,214,393

4. Results

The excitation energies from the different CI calculations, along with observed energies from the NIST database [3], are displayed in Table 2. From the table, we see that states belonging to $3l3l'$, with the exception of $3s3p\ ^3P_{0,1,2}$, are too high for the valence–valence correlation calculation. The states belonging to $3l4l'$ and $3s5l$, on the other hand, are too low. When including also the core–valence correlation, the states belonging to $3l3l'$ go down in energy and approach the observed excitation energies. The states belonging to $3l4l'$ and $3s5l$ go up and are now too high. Including also the core–core correlation results in a rather small energy change for the states belonging to $3l3l'$. The main effect of the core–core correlation is to lower the energies of the states belonging to $3l4l'$ and $3s5l$, bringing them in very good agreement with observations. The labeling of levels is normally done by looking at the quantum designation of the leading component in the CSF expansion [20]. There are two levels (67 and 69) with $3p4d\ ^3D_3$ as the leading component in the corresponding CSF expansion. To distinguish these levels, we added subscripts A and B to the labels of the dominant component. In a similar way, subscripts A and B were added to distinguish levels 78 and 80, both with $3p4f\ ^3F_3$ as the leading component.

Table 2 indicates that there are a few states that are either misidentified or assigned with a label that is inconsistent with the labels of the current calculation. The observed energy for $3p4f\ ^3D_2$ (level 84) is 2417 cm^{-1} too low compared to the calculated value and the observed energy for $3s5s\ ^3S_1$ (level 92) is 33,948 cm^{-1} too high. There seem to be no other computed energy levels that match the observed energies. The observed energy for $3s5p\ ^1P_1^o$ (level 100) is 3733 cm^{-1} too low. The observed energy matches the computed energy of $3s5p\ ^3P_1^o$ (level 97), and, thus, it seems like an inconsistency in the labeling. Finally, $3s5f\ ^1F_3^o$ (level 117) is 101,545 cm^{-1} too high and there is no other computed energy level that matches. Removing the energy outliers above, the mean relative energy differences are, respectively, 0.217%, 0.051%, 0.023% for the valence, the valence and core–valence and the valence, core–valence and core–core calculations. The energy differences are mainly due to higher-order electron correlation effects that have not been accounted for in the calculations. At the same time, one should bear in mind that the observed excitation energies are also associated with uncertainties as reflected in the limited number of valid digits displayed in the NIST tables.

In Table 3, the excitation energies obtained by including core–core correlation in the CI calculations are compared with energies from calculations by Landi [2] using the FAC code and with energies by Aggarwal et al. [21] using CIV3 in the Breit–Pauli approximation. The uncertainties of the excitation energies for the latter calculations are substantially larger. The calculations by Landi support the conclusion that some of the levels in the NIST database are misidentified. One may note that Landi gives levels 78 and 80 the labels $3p4f\ ^3F_3$ and $3p4f\ ^1F_3$, respectively, whereas Aggarwal et al. reverse the labels. This illustrates that labeling is dependent on the calculation and that the labeling process is far from straightforward [20].

Table 2. Comparison of calculated and observed excitation energies in Mg-like iron (Fe XV). E_{VV} are energies from CI calculations that account for valence–valence correlation. E_{VV+CV} are energies from CI calculations that account for valence–valence and core–valence electron correlation. $E_{VV+CV+CC}$ are energies that account for valence–valence and core–valence electron correlation and where core–core electron correlation effects have been included perturbatively. E_{NIST} are observed energies from the NIST database ([3]). ΔE are energy differences with respect to E_{NIST}. All energies are in cm^{-1}.

No.	Level	E_{VV}	ΔE	E_{VV+CV}	ΔE	$E_{VV+CV+CC}$	ΔE	E_{NIST}
1	$3s^2\ ^1S_0$	0	0	0	0	0	0	0
2	$3s3p\ ^3P^o_0$	233,087	−755	233,828	−14	233,928	86	233,842
3	$3s3p\ ^3P^o_1$	238,936	−724	239,668	8	239,741	81	239,660
4	$3s3p\ ^3P^o_2$	253,017	−803	253,829	9	253,773	−47	253,820
5	$3s3p\ ^1P^o_1$	354,941	3030	352,169	258	352,091	180	351,911
6	$3p^2\ ^3P_0$	556,594	2070	554,643	119	554,895	371	554,524
7	$3p^2\ ^1D_2$	559,900	300	559,834	234	559,661	61	559,600
8	$3p^2\ ^3P_1$	566,524	1922	564,663	61	564,674	72	56,4602
9	$3p^2\ ^3P_2$	583,327	1524	581,933	130	581,870	67	581,803
10	$3p^2\ ^1S_0$	662,999	3372	660,269	642	660,229	602	659,627
11	$3s3d\ ^3D_1$	680,522	1750	678,954	182	678,329	−443	678,772
12	$3s3d\ ^3D_2$	681,520	1735	679,986	201	679,381	−404	679,785
13	$3s3d\ ^3D_3$	683,080	1664	681,603	187	680,952	−464	681,416
14	$3s3d\ ^1D_2$	766,690	4597	762,729	636	762,176	83	762,093
15	$3p3d\ ^3F^o_2$	929,158	917	928,565	324	928,086	−155	928,241
16	$3p3d\ ^3F^o_3$	938,885	759	938,469	343	938,068	−58	938,126
17	$3p3d\ ^1D^o_2$	950,226	1713	948,768	255	948,383	−130	948,513
18	$3p3d\ ^3F^o_4$	950,300	642	949,990	332	949,451	−207	949,658
19	$3p3d\ ^3D^o_1$	986,221	3353	983,077	209	982,740	−128	982,868
20	$3p3d\ ^3P^o_2$	986,499	2985	983,765	251	983,350	−164	983,514
21	$3p3d\ ^3D^o_3$	998,324	3472	995,088	236	994,712	−140	994,852
22	$3p3d\ ^3P^o_0$	998,597	2708	996,218	329	995,835	−54	995,889
23	$3p3d\ ^3P^o_1$	999,166	2923	996,547	304	996,127	−116	996,243
24	$3p3d\ ^3D^o_2$	999,755	3132	996,892	269	996,449	−174	996,623
25	$3p3d\ ^1F^o_3$	1,066,906	4391	1,063,163	648	1,062,704	189	1,062,515
26	$3p3d\ ^1P^o_1$	1,078,913	4026	1,075,795	908	1,075,306	419	1,074,887
27	$3d^2\ ^3F_2$	1,373,374	3043	1,370,858	527	1,369,758	−573	1,370,331
28	$3d^2\ ^3F_3$	1,374,983	2948	1,372,527	492	1,371,407	−628	1,372,035
29	$3d^2\ ^3F_4$	1,376,965	2909	1,374,580	524	1,373,475	−581	1,374,056
30	$3d^2\ ^1D_2$	1,405,702	3110	1,403,474	882	1,402,237	−355	1,402,592
31	$3d^2\ ^3P_0$	1,409,066		1,406,328		1,405,381		
32	$3d^2\ ^3P_1$	1,409,639		1,406,926		1,405,672		
33	$3d^2\ ^1G_4$	1,409,702	2644	1,407,974	916	1,406,831	−227	1,407,058
34	$3d^2\ ^3P_2$	1,411,053	3280	1,408,467	694	1,407,210	−563	1,407,773
35	$3d^2\ ^1S_0$	1,489,913	2859	1,488,993	1939	1,487,460	406	1,487,054
36	$3s4s\ ^3S_1$	1,761,471	−2229	1,764,876	1176	17,63,699	−1	1,763,700
37	$3s4s\ ^1S_0$	1,785,265	−1735	1,788,455	1455	1,787,322	322	1,787,000
38	$3s4p\ ^3P^o_0$	1,880,014		1,883,187		1,882,236		
39	$3s4p\ ^3P^o_1$	1,880,440		1,883,595		1,882,588		
40	$3s4p\ ^3P^o_2$	1,887,508		1,890,703		1,889,632		
41	$3s4p\ ^1P^o_1$	1,887,872	−2098	1,891,051	1081	1,890,042	72	1,889,970
42	$3s4d\ ^3D_1$	2,029,659	−1651	2,032,907	1597	2,031,683	373	2,031,310
43	$3s4d\ ^3D_2$	2,030,413	−1607	2,033,653	1633	2,032,413	393	2,032,020

Table 2. *Cont.*

No.	Level	E_{VV}	ΔE	E_{VV+CV}	ΔE	$E_{VV+CV+CC}$	ΔE	E_{NIST}
44	$3s4d\ ^3D_3$	2,031,636	−1544	2,034,880	1700	2,033,623	443	2,033,180
45	$3s4d\ ^1D_2$	2,032,991	−2289	2,036,318	1038	2,035,053	−227	2,035,280
46	$3p4s\ ^3P^o_0$	2,051,314		2,053,909		2,053,031		
47	$3p4s\ ^3P^o_1$	2,054,922		2,057,446		2,056,493		
48	$3p4s\ ^3P^o_2$	2,071,700		2,074,376		2,073,372		
49	$3p4s\ ^1P^o_1$	2,085,097		2,087,237		2,086,235		
50	$3s4f\ ^3F^o_2$	2,105,597	−2923	2,109,821	1301	2,108,281	−239	2,108,520
51	$3s4f\ ^3F^o_3$	2,105,804	−2816	2,110,029	1409	2,108,503	−117	2,108,620
52	$3s4f\ ^3F^o_4$	2,106,098	−2782	2,110,327	1447	2,108,798	−82	2,108,880
53	$3s4f\ ^1F^o_3$	2,120,519	−2631	2,124,654	1504	2,123,180	30	2,123,150
54	$3p4p\ ^1P_1$	2,152,851		2,155,266		2,154,244		
55	$3p4p\ ^3D_1$	2,167,018		2,169,386		2,168,341		
56	$3p4p\ ^3D_2$	2,168,756		2,171,070		2,170,006		
57	$3p4p\ ^3P_0$	2,173,624		2,175,566		2,174,583		
58	$3p4p\ ^3P_1$	2,181,779		2,183,914		2,182,831		
59	$3p4p\ ^3D_3$	2,184,022		2,186,457		2,185,350		
60	$3p4p\ ^3P_2$	2,189,341		2,191,385		2,190,270		
61	$3p4p\ ^3S_1$	2,192,119		2,194,460		2,193,367		
62	$3p4p\ ^1D_2$	2,206,894		2,208,893		2,207,746		
63	$3p4p\ ^1S_0$	2,235,724		2,237,406		2,236,314		
64	$3p4d\ ^3D^o_1$	2,311,660		2,314,071		2,313,090		
65	$3p4d\ ^1D^o_2$	2,311,989		2,314,331		2,313,312		
66	$3p4d\ ^3D^o_2$	2,312,449		2,314,882		2,313,865		
67	$3p4d\ ^3D^o_{3A}$	2,313,908		2,316,401		2,315,387		
68	$3p4d\ ^3F^o_2$	2,329,261		2,331,722		2,330,678		
69	$3p4d\ ^3D^o_{3B}$	2,330,539		2,333,084		2,332,039		
70	$3p4d\ ^3F^o_4$	2,337,384		2,339,922		2,338,857		
71	$3p4d\ ^1F^o_3$	2,337,651		2,340,302		2,339,278		
72	$3p4d\ ^3P^o_2$	2,341,803		2,344,120		2,343,033		
73	$3p4d\ ^3P^o_1$	2,342,778		2,345,091		2,344,049		
74	$3p4d\ ^3P^o_0$	2,346,915		2,349,198		2,348,199		
75	$3p4d\ ^1P^o_1$	2,350,169		2,352,543		2,351,513		
76	$3p4f\ ^3G_3$	2,377,507	−2653	2,381,283	1123	2,379,714	−446	2,380,160
77	$3p4f\ ^3G_4$	2,384,217	−2483	2,387,976	1276	2,386,434	−266	2,386,700
78	$3p4f\ ^3F_{3A}$	2,384,435		2,388,118		2,386,537		
79	$3p4f\ ^3F_2$	2,388,049	−2051	2,391,670	1570	2,390,091	−9	2,390,100
80	$3p4f\ ^3F_{3B}$	2,397,860		2,401,630		2,400,029		
81	$3p4f\ ^3G_5$	2,399,542	−2558	2,403,453	1353	2,401,876	−224	2,402,100
82	$3p4f\ ^3F_4$	2,400,524	−1576	2,404,286	2186	2,402,697	597	2,402,100
83	$3p4f\ ^3D_3$	2,411,680	−1320	2,415,368	2368	2,413,758	758	2,413,000
84	$3p4f\ ^3D_2$	2,414,633	333	2,418,319	4019	2,416,717	2417	2,414,300
85	$3p4f\ ^3D_1$	2,417,852	−2248	2,421,557	1457	2,419,975	−125	2,420,100
86	$3p4f\ ^1G_4$	2,426,828	−1872	2,430,497	1797	2,429,063	363	2,428,700
87	$3p4f\ ^1D_2$	2,433,430	−2570	2,437,039	1039	2,435,534	−466	2,436,000
88	$3d4s\ ^3D_1$	2,458,614		2,460,640		2,458,997		
89	$3d4s\ ^3D_2$	2,459,450		2,461,503		2,459,846		
90	$3d4s\ ^3D_3$	2,461,283		2,463,415		2,461,742		
91	$3d4s\ ^1D_2$	2,468,780		2,470,737		2,469,163		
92	$3s5s\ ^3S_1$	2,507,700	−37,100	2,512,036	−32,764	2,510,852	−33,948	2,544,800

Table 2. *Cont.*

No.	Level	E_{VV}	ΔE	E_{VV+CV}	ΔE	$E_{VV+CV+CC}$	ΔE	E_{NIST}
93	$3s5s\ ^1S_0$	2,516,613		2,520,681		2,519,752		
94	$3d4p\ ^1D^o_2$	2,561,358		2,563,408		2,561,899		
95	$3d4p\ ^3D^o_1$	2,564,069		2,567,301		2,565,949		
96	$3s5p\ ^3P^o_0$	2,564,472		2,568,582		2,567,624		
97	$3s5p\ ^3P^o_1$	2,565,848		2,568,791		2,567,639		
98	$3d4p\ ^3D^o_2$	2,567,134		2,569,092		2,567,703		
99	$3d4p\ ^3D^o_3$	2,568,154		2,571,175		2,569,693		
100	$3s5p\ ^1P^o_1$	2,568,200	1200	2,571,834	4834	2,570,733	3733	2,567,000
101	$3s5p\ ^3P^o_2$	2,569,213		2,572,157		2,570,743		
102	$3d4p\ ^3F^o_2$	2,570,296		2,572,316		2,571,126		
103	$3d4p\ ^3F^o_3$	2,573,116		2,575,101		2,573,592		
104	$3d4p\ ^3F^o_4$	2,576,139		2,578,374		2,576,829		
105	$3d4p\ ^3P^o_1$	2,583,286		2,585,242		2,583,862		
106	$3d4p\ ^3P^o_2$	2,583,400		2,585,407		2,583,960		
107	$3d4p\ ^3P^o_0$	2,583,734		2,585,658		2,584,322		
108	$3d4p\ ^1F^o_3$	2,592,868		2,594,519		2,593,236		
109	$3d4p\ ^1P^o_1$	2,603,279		2,605,145		2,604,533		
110	$3s5d\ ^3D_1$	2,637,190	−2910	2,641,400	1300	2,640,247	147	2,640,100
111	$3s5d\ ^3D_2$	2,637,419	−2481	2,641,630	1730	2,640,442	542	2,639,900
112	$3s5d\ ^3D_3$	2,637,852	−2448	2,642,072	1772	2,640,870	570	2,640,300
113	$3s5d\ ^1D_2$	2,639,773		2,643,981		2,642,888		
114	$3s5f\ ^3F^o_2$	2,672,676	−3724	2,677,360	960	2,675,889	−511	2,676,400
115	$3s5f\ ^3F^o_3$	2,672,770	−3630	2,677,455	1055	2,675,988	−412	2,676,400
116	$3s5f\ ^3F^o_4$	2,672,907	−3693	2,677,594	994	2,676,123	−477	2,676,600
117	$3s5f\ ^1F^o_3$	2,678,041	−104,659	2,682,597	−100,103	2,681,155	−101,545	2,782,700
118	$3s5g\ ^3G_3$	2,682,487		2,687,368		2,685,680		
119	$3s5g\ ^3G_4$	2,682,654		2,687,556		2,685,877		
120	$3s5g\ ^3G_5$	2,682,855		2,687,777		2,686,099		
121	$3s5g\ ^1G_4$	2,685,580		2,690,506		2,688,841		
122	$3d4d\ ^1F_3$	2,699,116		2,701,602		2,699,874		
123	$3d4d\ ^3D_1$	2,703,542		2,705,972		2,704,354		
124	$3d4d\ ^3D_2$	2,704,742		2,707,218		2,705,580		
125	$3d4d\ ^3D_3$	2,706,116		2,708,636		2,706,964		
126	$3d4d\ ^3G_3$	2,707,934		2,710,522		2,708,828		
127	$3d4d\ ^1P_1$	2,709,315		2,711,813		2,710,163		
128	$3d4d\ ^3G_4$	2,709,360		2,711,928		2,710,264		
129	$3d4d\ ^3G_5$	2,711,220		2,713,878		2,712,174		
130	$3d4d\ ^3S_1$	2,720,698		2,723,175		2,721,783		
131	$3d4d\ ^3F_2$	2,726,309		2,728,092		2,726,350		
132	$3d4d\ ^3F_3$	2,727,568		2,729,398		2,727,634		
133	$3d4d\ ^3F_4$	2,729,029		2,730,908		2,729,156		
134	$3d4d\ ^1D_2$	2,741,839		2,743,862		2,742,627		
135	$3d4d\ ^3P_0$	2,744,213		2,746,022		2,744,706		
136	$3d4d\ ^3P_1$	2,744,807		2,746,626		2,745,163		
137	$3d4d\ ^3P_2$	2,745,935		2,747,809		2,746,300		
138	$3d4d\ ^1G_4$	2,748,985		2,751,121		2,749,474		
139	$3d4f\ ^3H^o_4$	2,765,833		2,770,098		2,768,443		
140	$3d4f\ ^1G^o_4$	2,767,533		2,771,821		2,770,030		
141	$3d4f\ ^3H^o_5$	2,767,692		2,771,943		2,770,434		
142	$3d4d\ ^1S_0$	2,775,538		2,779,275		2,777,362		

Table 2. *Cont.*

No.	Level	E_{VV}	ΔE	E_{VV+CV}	ΔE	$E_{VV+CV+CC}$	ΔE	E_{NIST}
143	$3d4f\ ^3F^o_2$	2,776,151		2,779,298		2,778,011		
144	$3d4f\ ^3F^o_3$	2,776,264		2,779,933		2,778,867		
145	$3d4f\ ^3F^o_4$	2,776,981		2,780,796		2,780,729		
146	$3d4f\ ^1D^o_2$	2,786,768		2,790,305		2,788,248		

Table 3. Comparison of calculated and observed excitation energies in Mg-like iron (Fe XV). $E_{VV+CV+CC}$ are energies that account for valence–valence and core–valence electron correlation and where core–core electron correlation effects have been included perturbatively. E_{FAC} are energies by Landi [2] using the FAC code. E_{CIV3} are energies by Aggarwal et al. [21] using the CIV3 code. E_{NIST} are observed energies from the NIST database ([3]). ΔE are energy differences with respect to E_{NIST}. All energies are in cm^{-1}.

No.	Level	$E_{VV+CV+VV}$	ΔE	E_{FAC}	ΔE	E_{CIV3}	ΔE	E_{NIST}
1	$3s^2\ ^1S_0$	0	0	0	0	0	0	0
2	$3s3p\ ^3P^o_0$	233,928	86	233,068	−774	235,013	1171	233,842
3	$3s3p\ ^3P^o_1$	239,741	81	238,900	−760	240,511	851	239,660
4	$3s3p\ ^3P^o_2$	253,773	−47	252,917	−903	253,548	−272	253,820
5	$3s3p\ ^1P^o_1$	352,091	180	356,126	4215	356,262	4351	351,911
6	$3p^2\ ^3P_0$	554,895	371	556,994	2470	560,275	5751	554,524
7	$3p^2\ ^1D_2$	559,661	61	560,266	666	563,216	3616	559,600
8	$3p^2\ ^3P_1$	564,674	72	566,832	2230	569,295	4693	564,602
9	$3p^2\ ^3P_2$	581,870	67	583,564	1761	584,856	3053	581,803
10	$3p^2\ ^1S_0$	660,229	602	665,768	6141	665,260	5633	659,627
11	$3s3d\ ^3D_1$	678,329	−443	680,146	1374	687,680	8908	678,772
12	$3s3d\ ^3D_2$	679,381	−404	681,129	1344	688,733	8948	6797,85
13	$3s3d\ ^3D_3$	680,952	−464	682,667	1251	690,401	8985	681,416
14	$3s3d\ ^1D_2$	762,176	83	769,369	7276	774,295	12,202	762,093
15	$3p3d\ ^3F^o_2$	928,086	−155	928,786	545	938,265	10,024	928,241
16	$3p3d\ ^3F^o_3$	938,068	−58	938,555	429	947,307	9181	938,126
17	$3p3d\ ^1D^o_2$	948,383	−130	949,447	934	958,402	9889	948,513
18	$3p3d\ ^3F^o_4$	949,451	−207	949,927	269	957,820	8162	949,658
19	$3p3d\ ^3D^o_1$	982,740	−128	986,082	3214	995,526	12,658	982,868
20	$3p3d\ ^3P^o_2$	983,350	−164	986,407	2893	995,767	12,253	983,514
21	$3p3d\ ^3D^o_3$	994,712	−140	997,944	3092	1,007,026	12,174	994,852
22	$3p3d\ ^3P^o_0$	995,835	−54	998,762	2873	1,006,708	10,819	995,889
23	$3p3d\ ^3P^o_1$	996,127	−116	999,173	2930	1,007,366	11,123	996,243
24	$3p3d\ ^3D^o_2$	996,449	−174	999,578	2955	1,008,124	11,501	996,623
25	$3p3d\ ^1F^o_3$	1,062,704	189	1,070,794	8279	1,077,456	14,941	1,062,515
26	$3p3d\ ^1P^o_1$	1,075,306	419	1,083,826	8939	1,089,691	14,804	1,074,887
27	$3d^2\ ^3F_2$	1,369,758	−573	1,372,400	2069	1,388,111	17,780	1,370,331
28	$3d^2\ ^3F_3$	1,371,407	−628	1,373,988	1953	1,389,834	17,799	1,372,035
29	$3d^2\ ^3F_4$	1,373,475	−581	1,375,938	1882	1,391,941	17,885	1,374,056
30	$3d^2\ ^1D_2$	1,402,237	−355	1,407,428	4836	1,421,702	19,110	1,402,592
31	$3d^2\ ^3P_0$	1,405,381		1,409,507		1,424,577		
32	$3d^2\ ^3P_1$	1,405,672		1,410,109		1,425,246		
33	$3d^2\ ^1G_4$	1,406,831	−227	1,412,127	5069	1,425,872	18,814	1,407,058
34	$3d^2\ ^3P_2$	1,407,210	−563	1,411,643	3870	1,426,815	19,042	1,407,773
35	$3d^2\ ^1S_0$	1,487,460	406	1,498,668	11,614	1,508,954	21,900	1,487,054
36	$3s4s\ ^3S_1$	1,763,699	−1	1,760,910	−2790	1,764,005	305	1,763,700

Table 3. *Cont.*

No.	Level	$E_{VV+CV+VV}$	ΔE	E_{FAC}	ΔE	E_{CIV3}	ΔE	E_{NIST}
37	$3s4s\ ^1S_0$	1,787,322	322	1,786,052	−948	1,787,950	950	1,787,000
38	$3s4p\ ^3P^o_0$	1,882,236		1,880,319		1,883,685		
39	$3s4p\ ^3P^o_1$	1,882,588		1,880,746		1,884,091		
40	$3s4p\ ^3P^o_2$	1,889,632		1,887,756		1,890,313		
41	$3s4p\ ^1P^o_1$	1,890,042	72	1,888,124	−1846	1,890,631	661	1,889,970
42	$3s4d\ ^3D_1$	2,031,683	373	2,029,563	−1747	2,034,124	2814	2,031,310
43	$3s4d\ ^3D_2$	2,032,413	393	2,030,328	−1692	2,034,848	2828	2,0320,20
44	$3s4d\ ^3D_3$	2,033,623	443	2,031,544	−1636	2,036,055	2875	2,033,180
45	$3s4d\ ^1D_2$	2,035,053	−227	2,033,212	−2068	2,037,569	2289	2,035,280
46	$3p4s\ ^3P^o_0$	2,053,031		2,051,778		2,055,797		
47	$3p4s\ ^3P^o_1$	2,056,493		2,055,514		2,059,308		
48	$3p4s\ ^3P^o_2$	2,073,372		2,072,083		2,074,452		
49	$3p4s\ ^1P^o_1$	2,086,235		2,086,607		2,088,795		
50	$3s4f\ ^3F^o_2$	2,108,281	−239	2,107,228	−1292	2,110,073	1553	2,108,520
51	$3s4f\ ^3F^o_3$	2,108,503	−117	2,107,423	−1197	2,110,281	1661	2,108,620
52	$3s4f\ ^3F^o_4$	2,108,798	−82	2,107,701	−1179	2,110,567	1687	2,108,880
53	$3s4f\ ^1F^o_3$	2,123,180	30	2,124,054	904	2,125,886	2736	2,123,150
54	$3p4p\ ^1P_1$	2,154,244		2,167,343		2,158,599		
55	$3p4p\ ^3D_1$	2,168,341		2,153,046		2,171,635		
56	$3p4p\ ^3D_2$	2,170,006		2,169,173		2,173,578		
57	$3p4p\ ^3P_0$	2,174,583		2,175,103		2,178,812		
58	$3p4p\ ^3P_1$	2,182,831		2,182,790		2,185,901		
59	$3p4p\ ^3D_3$	2,185,350		2,184,242		2,187,229		
60	$3p4p\ ^3P_2$	2,190,270		2,190,674		2,193,265		
61	$3p4p\ ^3S_1$	2,193,367		2,192,597		2,195,756		
62	$3p4p\ ^1D_2$	2,207,746		2,209,221		2,211,163		
63	$3p4p\ ^1S_0$	2,236,314		2,239,314		2,241,187		
64	$3p4d\ ^3D^o_1$	2,313,090		2,311,999		2,318,014		
65	$3p4d\ ^1D^o_2$	2,313,312		2,312,326		2,318,179		
66	$3p4d\ ^3D^o_2$	2,313,865		2,312,835		2,318,826		
67	$3p4d\ ^3D^o_{3A}$	2,315,387		23,144,663		2,320,538		
68	$3p4d\ ^3F^o_2$	2,330,678		2,329,647		2,334,178		
69	$3p4d\ ^3D^o_{3B}$	2,332,039		2,331,0213		2,335,726		
70	$3p4d\ ^3F^o_4$	2,338,857		2,338,064		2,342,277		
71	$3p4d\ ^1F^o_3$	2,339,278		2,338,703		2,343,517		
72	$3p4d\ ^3P^o_2$	2,343,033		2,342,598		2,347,544		
73	$3p4d\ ^3P^o_1$	2,344,049		2,343,850		2,348,795		
74	$3p4d\ ^3P^o_0$	2,348,199		2,347,823		2,352,406		
75	$3p4d\ ^1P^o_1$	2,351,513		2,351,661		2,356,773		
76	$3p4f\ ^3G_3$	2,379,714	−446	2,379,430	−730	2,384,306	4146	2,380,160
77	$3p4f\ ^3G_4$	2,386,434	−266	2,386,688	−12	2,391,198	4498	2,386,700
78	$3p4f\ ^3F_{3A}$	2,386,537		2,386,430		2,390,473		
79	$3p4f\ ^3F_2$	2,390,091	−9	2,390,112	12	2,393,842	3742	2,390,100
80	$3p4f\ ^3F_{3B}$	2,400,029		2,399,796		2,402,786		
81	$3p4f\ ^3G_5$	2,401,876	−224	2,401,746	−354	2,405,617	3517	2,402,100
82	$3p4f\ ^3F_4$	2,402,697	597	2,402,507	407	2,405,496	3396	2,402,100
83	$3p4f\ ^3D_3$	2,413,758	758	2,414,120	1120	2,417,151	4151	2,413,000
84	$3p4f\ ^3D_2$	2,416,717	2417	2,417,276	2976	2,420,124	5824	2,414,300
85	$3p4f\ ^3D_1$	2,419,975	−125	2,420,512	412	2,423,219	3119	2,420,100
86	$3p4f\ ^1G_4$	2,429,063	363	2,432,908	4208	2,435,828	7128	2,428,700

Table 3. *Cont.*

No.	Level	$E_{VV+CV+VV}$	ΔE	E_{FAC}	ΔE	E_{CIV3}	ΔE	E_{NIST}
87	$3p4f\ ^1D_2$	2,435,534	−466	2,438,982	2982	2,440,239	4239	2,436,000
88	$3d4s\ ^3D_1$	2,458,997		2,458,814		2,468,047		
89	$3d4s\ ^3D_2$	2,459,846		2,459,675		2,468,969		
90	$3d4s\ ^3D_3$	2,461,742		2,461,461		2,470,911		
91	$3d4s\ ^1D_2$	2,469,163		2,470,364		2,479,437		
92	$3s5s\ ^3S_1$	2,510,852	−33,948	2,507,572	−37,228			2,544,800
93	$3s5s\ ^1S_0$	2,519,752		2,517,043				
94	$3d4p\ ^1D^o_2$	2,561,899		2,561,169		2,571,814		
95	$3d4p\ ^3D^o_1$	2,565,949		2,566,041		2,576,851		
96	$3s5p\ ^3P^o_0$	2,567,624		2,564,597				
97	$3s5p\ ^3P^o_1$	2,567,639		2,564,254				
98	$3d4p\ ^3D^o_2$	2,567,703		2,567,341		2,577,905		
99	$3d4p\ ^3D^o_3$	2,569,693		2,569,518		2,583,117		
100	$3s5p\ ^1P^o_1$	2,570,733	3733	2,568,358	1358			2,567,000
101	$3s5p\ ^3P^o_2$	2,570,743		2,568,240				
102	$3d4p\ ^3F^o_2$	2,571,126		2,570,526		2,580,319		
103	$3d4p\ ^3F^o_3$	2,573,592		2,573,370		2,579,847		
104	$3d4p\ ^3F^o_4$	2,576,829		2,576,531		2,586,036		
105	$3d4p\ ^3P^o_1$	2,583,862		2,584,287		2,593,158		
106	$3d4p\ ^3P^o_2$	2,583,960		2,584,326		2,593,586		
107	$3d4p\ ^3P^o_0$	2,584,322		2,584,699		2,593,641		
108	$3d4p\ ^1F^o_3$	2,593,236		2,596,425		2,604,571		
109	$3d4p\ ^1P^o_1$	2,604,533		2,607,817		2,610,870		
110	$3s5d\ ^3D_1$	2,640,247	147	2,637,143	−2957			2,640,100
111	$3s5d\ ^3D_2$	2,640,442	542	2,637,376	−2524			2,639,900
112	$3s5d\ ^3D_3$	2,640,870	570	2,637,804	−2496			2,640,300
113	$3s5d\ ^1D_2$	2,642,888		2,640,084	0			
114	$3s5f\ ^3F^o_2$	2,675,889	−511	2,673,354	−3046			2,676,400
115	$3s5f\ ^3F^o_3$	2,675,988	−412	2,673,444	−2956			2,676,400
116	$3s5f\ ^3F^o_4$	2,676,123	−477	2,673,575	−3025			2,676,600
117	$3s5f\ ^1F^o_3$	2,681,155	−101,545	2,679,558	−103,142			2,782,700
118	$3s5g\ ^3G_3$	2,685,680		2,683,089				
119	$3s5g\ ^3G_4$	2,685,877		2,683,272				
120	$3s5g\ ^3G_5$	2,686,099		2,683,494				
121	$3s5g\ ^1G_4$	2,688,841		2,686,809				
122	$3d4d\ ^1F_3$	2,699,874		2,697,717		2,710,391		
123	$3d4d\ ^3D_1$	2,704,354		2,702,464		2,714,967		
124	$3d4d\ ^3D_2$	2,705,580		2,703,625		2,716,229		
125	$3d4d\ ^3D_3$	2,706,964		2,705,001		2,717,578		
126	$3d4d\ ^3G_3$	2,708,828		2,707,726		2,717,919		
127	$3d4d\ ^1P_1$	2,710,163		2,708,170		2,721,079		
128	$3d4d\ ^3G_4$	2,710,264		2,709,064		2,719,345		
129	$3d4d\ ^3G_5$	2,712,174		2,710,955		2,721,463		
130	$3d4d\ ^3S_1$	2,721,783		2,720,286		2,732,634		
131	$3d4d\ ^3F_2$	2,726,350		2,726,401		2,738,407		
132	$3d4d\ ^3F_3$	2,727,634		2,727,604		2,739,745		
133	$3d4d\ ^3F_4$	2,729,156		2,729,075		2,741,293		
134	$3d4d\ ^1D_2$	2,742,627		2,743,889		2,755,547		
135	$3d4d\ ^3P_0$	2,744,706		2,745,181		2,757,907		
136	$3d4d\ ^3P_1$	2,745,163		2,745,727		2,758,477		

Table 3. *Cont.*

No.	Level	$E_{VV+CV+VV}$	ΔE	E_{FAC}	ΔE	E_{CIV3}	ΔE	E_{NIST}
137	$3d4d\ ^3P_2$	2,746,300		2,747,024		2,759,619		
138	$3d4d\ ^1G_4$	2,749,474		2,752,675		2,761,254		
139	$3d4f\ ^3H^o_4$	2,768,443		2,766,350		2,778,483		
140	$3d4f\ ^1G^o_4$	2,770,030		2,768,154		2,780,096		
141	$3d4f\ ^3H^o_5$	2,770,434		2,768,448		2,780,831		
142	$3d4d\ ^1S_0$	2,777,362		2,781,322		2,792,233		
143	$3d4f\ ^3F^o_2$	2,778,011		2,775,995		2,787,305		
144	$3d4f\ ^3F^o_3$	2,778,867		2,776,790		2,787,964		
145	$3d4f\ ^3F^o_4$	2,780,729		2,777,446		2,788,842		
146	$3d4f\ ^1D^o_2$	2,788,248		2,787,354		2,798,312		

5. Conclusions

CI with restrictions on the interactions (CI combined with second-order Brillouin–Wigner perturbation theory) makes it possible to handle large CSF expansions. The calculations including core–core correlation take around 20 h with 10 nodes on a cluster and bring the computed and observed excitation energies into very good agreement. To improve the computed excitation energies, the orbital set would need to be further extended leading to even larger matrices. The combined CI and perturbation method can be applied to include core–valence correlation in systems with many valence electrons and calculations. Calculations including valence–valence correlation and where core–valence correlation is treated perturbatively are in progress for P-, S-, and Cl-like systems.

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