Electron-correlation effects on the $3C$ to $3D$ line-intensity ratio in the Ne-like ions Ar^{8+} to Kr^{26+}

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We present a theoretical and experimental investigation of the $3d \rightarrow 2p$ resonance to the intercombination line ratio in low- to mid-Z neonlike ions of astrophysical interest, i.e., of the $2p_{1/2}2p_{3/2}^4 3d_{3/2}\,{}^1P_1^o \rightarrow 2p^6\,{}^1S_0$ and $2p_{1/2}^2 2p_{3/2}^3 3d_{5/2}\,{}^3D_1^o \rightarrow 2p^6\,{}^1S_0$ transitions commonly labeled $3C$ and $3D$, respectively. In particular, we have employed the configuration-interaction method with three different numbers of basis states and the many-body perturbation theory method to calculate oscillator strengths and energies for neonlike ions from $Z = 18$ to 36. Combining our calculations with a systematic study of previous works in the literature, we show that these methods can predict accurate and converged energies for these transitions. We also find convergence for the oscillator strengths, but the ratio of oscillator strengths, which can be compared to experimental values of the relative intensity ratios of these lines, appears to converge to values higher than measured. We speculate that this is due to the role of electron-electron correlations. While the amount of electron correlations associated with the intercombination line $3D$ appears to be well described, it seems that the contributions from highly excited states are not sufficiently accounted for in the case of the resonance line $3C$. In order to augment the body of available experimental data for neonlike ions, we present a measurement of the $3C$ and $3D$ lines in neonlike Ar^{8+}. We report a wavelength of 41.480 ± 0.001 Å for line $3C$ and 42.005 ± 0.001 Å for line $3D$. The intensity ratio of the two lines was determined to be $I(3C)/I(3D) = 11.32 \pm 1.40$.

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I. INTRODUCTION

The resonance-to-intercombination line-intensity ratio in Fe^{16+}, the so-called $3C/3D$ line ratio, has been the focus of many experimental [1–8] and theoretical studies [9–28]. The large amount of work has been stimulated, on the one hand, by the potential application of these lines as diagnostics of astrophysical plasmas [4,29–31] and, on the other hand, by the unexpected deviation between the measured and the theoretical $3C/3D$ line ratios [1,6,8,27,28]. The deviation has prevented the full application of the lines as diagnostic tools and has raised concern about the accuracy of modern atomic physics theory. To explain the discrepancy between experiment and theory, many effects relevant to the collisional models have been invoked, such as resonance contribution, radiative cascades, or collisional depopulation, among others [27,28]. Moreover, a possible deficiency in the wave function of the collisional system was pointed out by Beiersdorfer *et al.* [5] as well as by Brown *et al.* [3] and Gu *et al.* [12,19]. They proposed that the deviation arises because the approximated wave functions do not properly describe the level mixing (or electron-correlation effects). Beiersdorfer *et al.* [5], for example, have pointed out that a simple shift of the atomic number Z by $\Delta A = 1.5$ would greatly improve agreement between calculations and experiment, indicating that the screening of the nuclear Coulomb potential was inaccurate.

The possible deficiency in the wave function was further studied in recent work by Bernitt *et al.* [32]. They measured the ratio of weighted oscillator strengths gf of the $3C$ and $3D$ lines in Fe^{16+} by x-ray laser spectroscopy. The experiment allowed a direct comparison of experimental and theoretical results. The measured gf^{3C}/gf^{3D} ratio was 2.61 ± 0.23 [32]. This value was compared with results from large-scale multiconfiguration Dirac-Fock (MCDF) calculations and previous second-order many-body perturbation theory (MBPT). We note that the effect of level mixing in the $3C/3D$ line ratio in neonlike ions was extensively studied [11,13], particularly in Fe^{16+} [12,15–18] and Ni^{+18} [12] before the work of Bernitt *et al.* [32]. These studies, however, are based on configuration-interaction methods with a relatively small number of mixing levels. In their MCDF calculations, Bernitt *et al.* [32] used a configuration space systematically increasing in size, reaching close to 10^5 coefficients, to describe the upper levels in the $3C$ and $3D$ lines. Moreover, the MCDF calculated gf^{3C}/gf^{3D} ratio was extrapolated to the infinitely large configuration space limit. Comparison of the MCDF and previous theoretical ratios showed the most accurate predictions to overestimate the measured ratio by over 30% [32]. This result demonstrates the difficulty to properly account for electron-correlation effects with current theoretical methods. It seems that an explicit full MCDF or higher-order MBPT calculation is required. Yet such calculations are impractical or rather difficult even nowadays.

A simple approach to study electron-correlation effects on the $3C/3D$ line-intensity ratio is to explore the ratio along the Ne isoelectronic sequence. For an isoelectronic sequence, in general, one expects the effects of electron correlation to decrease with increasing Z because of the stronger nuclear attraction. Then one may anticipate that if the incorrect prediction of the $3C/3D$ line-intensity ratio relates to electron-correlation effects, the agreement between theory and experiment will vary with Z and the deviation will vanish for large Z. Such a trend of the deviation of theoretical (e.g.,

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MCDF) and experimental data as a function of Z is commonly observed for transition energies in isoelectronic sequences [3,33–38].

In order to perform the comparative study of the $3C/3D$ ratio in the Ne ion isoelectronic sequence outlined above, we need the corresponding measured ratios. The most complete data sets available of the $3C/3D$ ratio in various neonlike ions were measured in the Livermore electron-beam ion trap (EBIT) [3] and the Princeton Large Torus (PLT) tokamak [5]. While the combined data set is limited to mid-Z neonlike ions, $Z = 24$–36, Brown *et al.* [3] show the $3C/3D$ ratio of these ions to have a Z dependence proportional to Z^{-4}. Therefore, one may in principle interpolate the ratio for ions that have not been measured yet. To apply this simple procedure to ions with Z below 24, an additional measurement is necessary. We have performed such a measurement for $Z = 18$, Ar^{8+}, as is discussed below.

Moreover, we would have to compare the measured gf^{3C}/gf^{3D} ratio with the corresponding calculated values to study the effect of electron correlation on the $3C/3D$ line-intensity ratio. However, such a measurement has only been performed for Fe^{16+} [32] so far. Instead, we will use the $3C/3D$ line-intensity ratio measured with the EBIT [3] and the PLT tokamak [5]. As discussed in Ref. [32], the $3C/3D$ line-intensity ratio measured in typical plasma conditions reflects not only radiative contributions, but also kinetic contributions and collisional effects. Nevertheless, the EBIT $3C/3D$ line-intensity ratios may be taken as an upper bound of the gf^{3C}/gf^{3D} ratio. One can justify such an assumption based on the measured value for Fe^{16+}; the value from x-ray laser spectroscopy [32] of the gf^{3C}/gf^{3D} ratio is 2.61 ± 0.23, while that from the EBIT [3] for the $3C/3D$ line-intensity ratio is 3.04 ± 0.12. One may expect a similar trend of higher $3C/3D$ line ratios (compared to ratios of gf values) for other neonlike ions when the ratio is measured under plasma conditions [5,13]. We note that kinetic effects in our comparison with EBIT data can be mostly ignored, as they may at best affect the ratios by about 5%. This approximation has been shown to be valid in some of the earliest measurements using an electron-beam ion trap [39]. The effect may be higher in a plasma where indirect processes are allowed to contribute, but in measurements on an electron-beam ion trap some processes, such as dielectronic resonances, recombination from fluorinelike ions, and cascades from high-lying levels, do not contribute by choice of the electron-beam energy.

In the current work, we present EBIT measurements of the $3C/3D$ line-intensity ratio in Ar IX. This ion was chosen because its atomic number is substantially below that of ions used in previous measurements. Furthermore, in ions with lower Z there is a crossing of the $2p_{3/2}3d_{5/2}$ upper level of the $3D$ line with the $2p_{3/2}3d_{3/2}$ level [40] and the Z^{-4} dependence of the $3C/3D$ ratio is not preserved. We combine this point with the previous EBIT and PLT tokamak results [3,5] to interpolate the $3C/3D$ ratio of $Z = 20$ and 22. With this extended data set, we study the effects of electron correlation on the $3C/3D$ ratio in neonlike ions from Ar^{8+} to Kr^{26+}. For this we compare theoretical gf^{3C}/gf^{3D} ratio with the measured $3C/3D$ line-intensity ratio. The theoretical ratio for each ion was evaluated with the relativistic configuration-interaction (CI) and CI plus second-order MBPT correction methods.

II. EXPERIMENT

The spectrum of neonlike Ar^{8+} has been measured earlier at the electron-beam ion-trap facility at Livermore [41]. This measurement utilized the x-ray and extreme ultraviolet spectrometer (XEUS) [42–44]. XEUS employed a varied-line-spacing flat-field grating with a mean spacing of 2400 lines/mm and with a Rowland circle of radius of 15.9 m, resulting in a spectral resolution of 0.1 Å ($\lambda/\Delta\lambda \sim 400$ at 40 Å). XEUS, however, proved unsuitable for an accurate measurement of the $3C/3D$ ratio because its response function dropped to near zero at the 284-eV carbon edge [45], which coincides with the location of the argon $3D$ line; the effect here is due to an antireflective carbon coating on the Photometrics CCD camera originally used with this spectrometer. Moreover, this problem rendered the wavelength determination of the Ar IX $3D$ line very inaccurate compared to that of $3C$ and of other Ar IX lines [41].

Because Ar IX provides crucial information on the low-Z behavior of the $3C/3D$ ratio, we have revisited the Ar IX spectrum in order to obtain accurate relative line intensities and wavelengths of the $3C$ and $3D$ lines. The present measurements were carried out at the Lawrence Livermore EBIT-I electron-beam ion-trap facility [46]. For this work we utilized an extreme ultraviolet spectrometer that afforded considerably higher spectral resolution than XEUS, allowing for a very high signal-to-noise measurement. This instrument utilizes a varied-line-spacing flat-field grating with a Rowland radius of 44.3 m and a mean (inverse) spacing of 2400 lines/mm [47]. The resulting spectral resolution of approximately 0.025 Å corresponds to a resolving power $\lambda/\Delta\lambda \sim 1700$ at the wavelengths studied here. Wavelength calibrations were periodically performed with the well-known [48,49] $1s2p\ ^1P_1, ^3P_1 \rightarrow 1s^2\ ^1S_0$ lines of C V, i.e., the resonance and intercombination lines, dubbed w and y, respectively, the Lyman-α and Lyman-β lines of C VI, and, in second order, those corresponding lines from O VII and O VIII. Data were collected with an uncoated, liquid-nitrogen-cooled Princeton

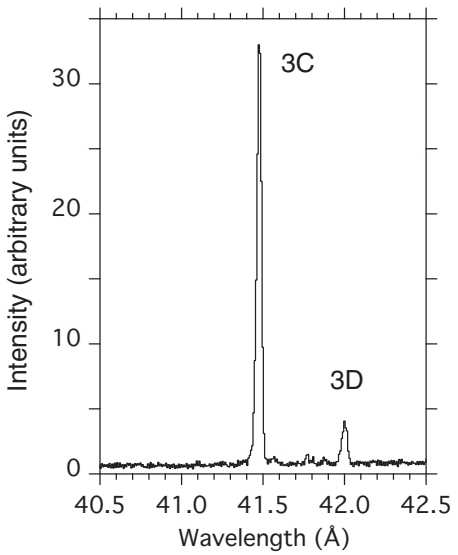

FIG. 1. Spectrum of neonlike Ar IX in the 40.5–42.5 Å region showing the $3C$ and $3D$ lines. The spectrum was acquired with the high-resolution EUV spectrometer on EBIT-I.

TABLE I. Experimental energies [3] and intensity ratio [3] of the $3C$ and $3D$ lines in neonlike ions ($Z = 18$–36).

Z	$3C$ energy (eV)	$3D$ energy (eV)	$3C/3D$ intensity ratio
18	298.894[a]	295.159[a]	11.32[a] ± 1.40
20	407.201[b]	401.672[b]	8.24[c]
22	530.851[b]	523.188[b]	5.92[c]
24	670.101	659.577	4.37 ± 0.43
25	745.815	733.808	3.42 ± 0.30
26	825.772	812.406	3.04 ± 0.12
27	909.287	893.720	2.59 ± 0.18
28	997.115	979.401	2.30 ± 0.16
29	1089.055	1068.897	1.97 ± 0.14
30	1185.143	1162.202	1.71 ± 0.10
32	1390.549[d]	1360.937[d]	1.50[e] ± 0.14
34	1611.193[e]	1573.367[e]	1.12[e] ± 0.05
35	1729.163	1685.961	0.93 ± 0.07 (1.04)[c]
36	1850.976	1802.175	0.99 ± 0.07

[a]Present result.
[b]Energies of the $3C$ and $3D$ lines from the NIST Database [103].
[c]Interpolated values from the measured $3C/3D$ line ratios.
[d]Energies of the $3C$ and $3D$ lines from Boiko *et al.* [73].
[e]Results of Beiersdorfer *et al.* [5].

Instruments CCD camera having an image size of 1300 × 1340 of 20-μm-wide pixels. Data processing consisted of filtering for cosmic rays and subtraction of background signal.

Five measurements of argon were taken at an electron beam energy of 500 eV. Figure 1 shows the $3C$ and $3D$ lines as seen in a typical measurement with the high-resolution spectrometer.

For the wavelength of line $3C$ we obtained 41.480 ± 0.001 Å and for the wavelength of line $3D$ we obtained 42.005 ± 0.001 Å. This compares to 41.485 ± 0.002 and 42.041 ± 0.030 Å, respectively, in our earlier measurement [41]. The present result for $3D$ is thus an order of magnitude more accurate than our earlier value.

For the $3C/3D$ intensity ratio, we found a weighted-mean ratio of 11.32 ± 1.40 (Table I), from individual data in the range 9.68–12.55. Here we note that the emission from neonlike ions excited by an electron beam is generally polarized [42]. Although the grazing-incidence spectrometer we used has little sensitivity to polarization, we need to account for the fact that the measured intensities depend on the angle at which the emission is measured relative to the electron-beam direction [50]. In our analysis we assumed that the polarizations of lines $3C$ and $3D$ are the same and about 40% [1]. This assumption was reaffirmed in a recent calculation by Zhang *et al.* [21].

III. CALCULATION

A large number of calculations have been performed on the electronic structure of the ions in the Ne isoelectronic sequence [23,40,51–71]. From these calculations, one can notice a disparity between the calculation of excitation energies and radiative rates. Nowadays, the advance in the methodology to treat both electron-correlation and relativistic effects allows one to determine excitation energies of the neonlike isoelectronic sequence, for instance, that agree with experimental results at the 0.1% level [23,40,61,65–68,70,71]. These great advances in the theoretical accuracy to determine excitation energies come in part due to the extensive experimental data [72–86] available to benchmark any predictions. This experiment-theory interchange helped to develop methods to optimize the calculation of excitation energies. For radiative rates, on the order hand, there are fewer experimental results and the benchmarking of theoretical methods has been performed with ions other than neonlike [87–91]; a very few cases where neonlike high-Z ions were studied [92,93] are the exception. (There also have been studies of transition rates in low-Z ions of the Ne isoelectronic sequence, with reviews that illustrate the pitfalls of experiment and calculation [94–96].) Thus, theoretical radiative rates in neonlike ions often differ considerably when calculated with various theoretical methods [40,52,58–60,64] even while excitation energies may be in good agreement. Experimental results such as those reported for the gf^{3C}/gf^{3D} ratio in Fe^{16+} [32] are therefore of great value to validate theoretical methods.

We have calculated weighted oscillator strengths and transition energies of the $3C$ ($2p_{1/2}2p_{3/2}^4 3d_{3/2}\ {}^1P_1^o \rightarrow 2p^6\ {}^1S_0$) and $3D$ ($2p_{1/2}^2 2p_{3/2}^3 3d_{5/2}\ {}^3D_1^o \rightarrow 2p^6\ {}^1S_0$) lines with the relativistic CI and the combined relativistic CI plus MBPT methods as implemented in the flexible atomic code (FAC) [97–99]. These two methods mainly differ in their treatment of electron-correlation effects. In the CI method, correlation effects are better described by increasing the number of mixing levels. To study the effects of level mixing, we used three model configuration spaces to represent the upper levels of the $3C$ and $3D$ lines. In the first model, CI-1, the upper levels were represented by the minimal 7 jj-coupled states coming from the singly excited $n = 3$ levels, $[1s^2]2\ell^7 3\ell$. In a second model, CI-2, 105 states with singly and doubly excited $n = 3$ levels were included: $2\ell^7 3\ell$ and $2\ell^6 3\ell^2$. The third model, CI-3, included 816 states to represent the upper levels where up to triply excited $n = 3$ levels were considered: $2\ell^7 3\ell^1$, $2\ell^6 3\ell^2$, and $2\ell^5 3\ell^3$. The lower level $[1s^2]2\ell^8(^1S_0)$ of the $3C$ and $3D$ lines was also represented with the same configuration spaces of the upper levels, even though configuration mixing in this case is small [100]. We have also performed calculations for Fe^{16+} where the upper levels of the $3C$ and $3D$ lines were represented with a configuration space including four electrons in the $n = 3$ excited states. However, the oscillator strengths and transition energies of the $3C$ and $3D$ lines from this calculation differ by less than 0.0001 and 0.005 eV, respectively, from the results of model CI-3.

In the CI plus MBPT method, electron-correlation effects are treated with the CI approach and the Rayleigh-Schrödinger perturbation theory ansatz [98]. The present MBPT calculations were performed with the configuration model space CI-1. Moreover, we also performed MBPT calculations with the model CI-2 for Fe^{16+}, but the results were similar to the model CI-1.

Details of the CI and CI plus MBPT methods implemented in the FAC code can be found in the FAC documentation [99] and Ref. [98], respectively. In FAC, atomic processes are treated with basis wave functions generated from a single potential. The potential is optimized for a fictitious average configuration, instead of a single physical configuration, to represent the electronic screening of the nuclear potential. In our present CI calculations, the potential is optimized only

with the $1s^2 2\ell^8$ ground-state configuration, as the energy levels of Ne-like ions are then closer to experiment than in calculations with an average configuration [99]. In the CI plus MBPT calculations, however, separate Dirac-Fock-Slater self-consistent-field calculations are performed for the $1s^2 2\ell^8$ and $1s^2 2\ell^7 3\ell$ configurations. In this case, optimizing the two configuration groups separately improves the accuracy [101].

IV. RESULTS AND DISCUSSION

A. Transition energies

In a previous study of the $3C$ and $3D$ lines in the neonlike isoelectronic sequence, Fournier and Hansen [13] found the experiment-theory agreement of the $3C/3D$ intensity ratio to correlate with the corresponding agreement of the relative excitation energies of the $3C$ and $3D$ lines. They also showed these relative excitation energies to be predicted with better accuracy for high-Z neonlike ions than for the low-Z ions [13]. This trend is a result of the larger electron-correlation effects in low-Z ions [55]. Along this line of thought, we have performed a comparison of the experimental and calculated transition energy of the $3C$ and $3D$ lines in the neonlike ions with $Z = 18$–36 (see Fig. 2). We have also included in our comparison previous results from Liang and Badnell [23] and Hibbert *et al.* [62].

The effect of electron correlation is evident for the transition energies of the $3C$ and $3D$ lines. As expected, the energies calculated with the small model CI-1 deviate significantly from the measured values. Moreover, the deviation clearly depends on the value Z of a given neonlike ion, monotonically decreasing from 1% in Ar^{8+} to 0.15% in Kr^{26+} (Table II). The accuracy is dramatically increased, by an order of magnitude in many cases, for calculations with the model CI-2. The difference between models CI-1 and CI-2 is the inclusion of doubly excited $n = 3$ levels; clearly, pair excitation effects need to be included to accurately predict the transitions energies of the $3C$ and $3D$ lines. This behavior has been seen already in a comparison between experiment and theory of much-higher-Z neonlike ions than are discussed here [76,79]. Inclusion of triply excited $n = 3$ levels, model CI-3, only leads to a small further improvement in the accuracy. Application of the second-order perturbation corrections (MBPT results) to the model CI-1 also leads to very accurate results.

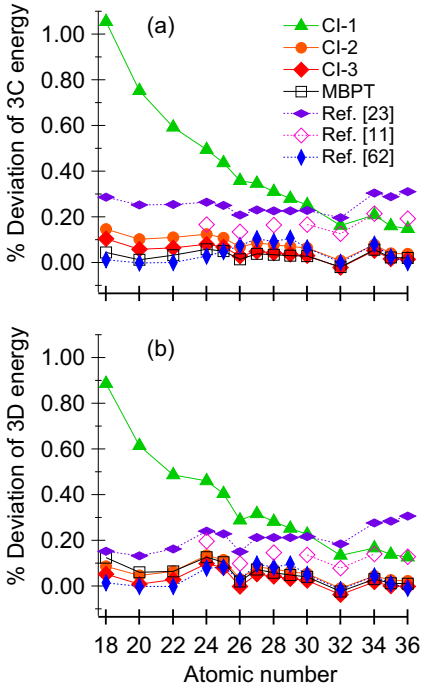

FIG. 2. (Color online) Difference (in percent) between the theoretical and experimental excitation energy of the (a) $3C$ and (b) $3D$ lines in neonlike ions as a function of the atomic number. Results are shown for the present calculations (Cl-1, CI-2, CI-3, and MBPT) and the previous calculations of Liang and Badnell [23], Dong *et al.* [11], and Hibbert *et al.* [62]. Experimental and present calculated excitation energies are collected in Tables I and II.

We can see in Fig. 2 that the Z dependence of the experiment-theory deviation is essentially removed when a larger fraction of the electron-correlation effects is correctly described. One can similarly rationalize the lack of Z dependence in the previous results of Dong *et al.* [11] and Liang and Badnell [23] as their MCDF and Breit-Pauli CI-type calculations, respectively, included pair excitation effects. However, the overall accuracy of the calculations of Liang and Badnell [23] is up to three times poorer than those of the other calculations, as seen by the increased deviation in Fig. 2. Moreover, there is an apparent discontinuity in the calculations by Liang and Badnell [23] at $Z = 34$, which further reduces the accuracy of their calculations.

There are still some unaccounted-for electron-correlation effects in our calculations, as indicated by the (small) variation of the predicted energies as a function of atomic number. In addition, we note that there are two dips in the otherwise smooth variation of the experiment-theory deviation shown in Fig. 2. One occurs at $Z = 32$, i.e., for germanium. The other occurs at $Z = 26$, i.e., for iron. There has been only one measurement for $Z = 32$; the dip might therefore be due to the uncertainty in the experimental data. The values for iron, however, have been measured multiple times and this dip appears to be more likely to result from an artifact of theory. It will be very important to confirm these dips by future, targeted measurements, as they may indicate additional, unaccounted-for correlation effects [102].

Finally, we note that for the mid-Z ions, particularly Z above 32, the predicted energies of model CI-2, model CI-3, and MBPT are essentially the same. To some extent, this indicates that electron-correlation effects have been properly described in these ions.

B. Line intensities

The effect of level mixing or electron correlation in the $3C/3D$ line-intensity ratio in neonlike ions have been previously studied [11–13,15–18,32]. Yet a systematic study of this effect, by comparing experimental results and highly accurate predictions, has not been presented for the neonlike isoelectronic sequence. Aiming to do so, we display in Fig. 3(a) the $3C/3D$ line-intensity ratio measured with the EBIT [3] and with the PLT tokamak [5] as well as the predicted gf^{3C}/gf^{3D} ratio. The figure closely resembles those previously presented in Refs. [3,11,13]. The difference, however, is our present

TABLE II. Calculated energies E (in eV) of the 3C and 3D lines in neonlike ions with different methods: CI-1, CI-2, CI-3, and MBPT. The percentage of deviation (% dev.) of the calculated excitation energies from experimental values is also given.

	E (3C)	E (3D)	% dev. (3C)	% dev. (3D)	E (3C)	E (3D)	% dev. (3C)	% dev. (3D)
Z	CI-1				CI-2			
18	302.045	297.773	1.054	0.886	299.330	295.413	0.146	0.086
20	410.269	404.136	0.753	0.614	407.622	401.855	0.103	0.046
22	534.000	525.738	0.593	0.487	531.433	523.528	0.110	0.065
24	673.414	662.609	0.494	0.460	670.932	660.460	0.124	0.134
25	749.070	736.773	0.436	0.404	746.630	734.652	0.109	0.115
26	828.733	814.756	0.359	0.289	826.334	812.660	0.068	0.031
27	912.436	896.555	0.346	0.317	910.079	894.483	0.087	0.085
28	1000.214	982.170	0.311	0.283	997.898	980.121	0.078	0.074
29	1092.105	1071.601	0.280	0.253	1089.827	1069.573	0.071	0.063
30	1188.143	1164.845	0.253	0.227	1185.904	1162.838	0.064	0.055
32	1392.821	1362.778	0.163	0.135	1390.655	1360.811	0.008	−0.009
34	1614.567	1575.978	0.209	0.166	1612.468	1574.052	0.079	0.044
35	1731.945	1688.310	0.161	0.139	1729.877	1686.405	0.041	0.026
36	1853.718	1804.468	0.148	0.127	1851.680	1802.584	0.038	0.023
	CI-3				MBPT			
18	299.205	295.313	0.104	0.052	299.027	295.525	0.044	0.124
20	407.437	401.708	0.058	0.009	407.255	401.911	0.013	0.060
22	531.194	523.337	0.065	0.028	531.020	523.530	0.032	0.065
24	670.645	660.228	0.081	0.099	670.494	660.413	0.059	0.127
25	746.322	734.400	0.068	0.081	746.187	734.581	0.050	0.105
26	826.008	812.388	0.029	−0.002	825.891	812.566	0.014	0.020
27	909.735	894.192	0.049	0.053	909.638	894.368	0.039	0.073
28	997.538	979.812	0.042	0.042	997.460	979.983	0.035	0.059
29	1089.453	1069.246	0.037	0.033	1089.398	1069.417	0.031	0.049
30	1185.516	1162.493	0.031	0.025	1185.486	1162.666	0.029	0.040
32	1390.243	1360.433	−0.022	−0.037	1390.267	1360.615	−0.020	−0.024
34	1612.036	1573.643	0.052	0.018	1612.111	1573.835	0.057	0.030
35	1729.435	1685.980	0.016	0.001	1729.539	1686.182	0.022	0.013
36	1851.229	1802.145	0.014	−0.002	1851.363	1802.359	0.021	0.010

datum for Ar^{8+}. This point follows the Z^{-4} dependence of the $3C/3D$ line-intensity ratio observed in mid-Z neonlike ions [3,5]. A similar Z dependence can be seen for the predicted gf^{3C}/gf^{3D} ratio; an exception is the previous MBPT results of Safronova *et al.* [70], where, interestingly, the dependence is less steep for Ar^{8+} and Ca^{+10}.

From Fig. 3(a) we see that the gf^{3C}/gf^{3D} ratios calculated with model CI-1 deviates significantly from the measured $3C/3D$ line-intensity ratio, particularly for ions with relatively-low-Z values. The measured ratios are better reproduced with the model CI-2. Model CI-3 leads only to slightly better values than model CI-2. The predictions of MBPT are the closest to the measurement. This general trend for the experiment-theory agreement of the calculational results of models CI-1, CI-2, and CI-3 and MBPT is similar to that discussed above for the transition energies. Therefore, one may expect a Z dependence on the experiment-theory deviation of the $3C/3D$ ratio as well.

Figure 3(b) shows the deviation between the calculated gf^{3C}/gf^{3D} and the measured $3C/3D$ line-intensity ratios as a function of Z. The deviation clearly depends on Z and on the particular theoretical method. The calculation with model CI-1 overestimates the ratio by 48% for the lower-Z value (Table III). This deviation decreases as Z increases, reaching 25% for Kr^{26+}. The poor agreement of CI-1 reflects the lack of electron-correlation effects in this model calculation. The calculations of Liang and Badnell [23] show a trend very similar to our CI-1 calculations. The similarity is somehow unexpected since their calculations included pair excitation effects and as a result, one would have expected a smaller deviation from experiment. For instance, the calculations where we have included pair excitation effects, CI-2 and CI-3, deviate by 30%–20% for most ions (Table III). In other words, CI-2 and CI-3 calculations do not show an obvious dependence on Z. Inclusion of pair electron-correlation effects clearly leads to ratios closer to the measured values even at low atomic number, in line with our results for the excitation energies.

The deviation between experiment and theory at low Z is significantly reduced when considering the MBPT calculations. Our MBPT values reproduce the measured ratio for ions with $Z = 18$–24 to within 10% (Table III). For higher Z, the deviation, however, grows and it is around 20% for $Z \geqslant 34$. The MBPT calculations of Safronova *et al.* [70] follow a trend similar to our MBPT results, as they also increase with atomic number. However, at the lowest Z they exhibit a negative deviation, i.e., the calculated ratio is smaller than measured, while our MBPT calculations predict ratios that are in perfect agreement with measurement for the neonlike ion with the

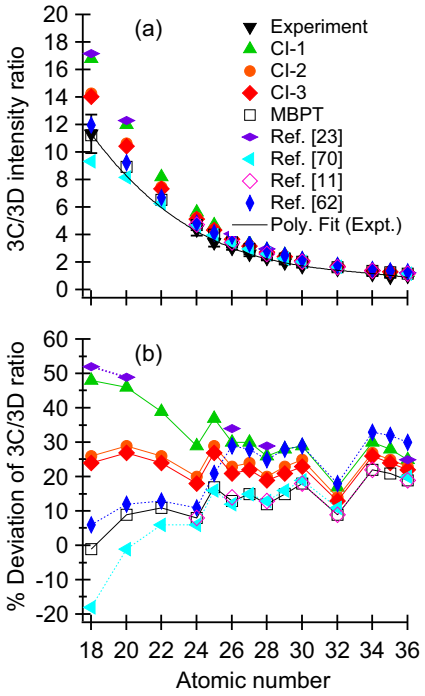

FIG. 3. (Color online) (a) Experimental $3C/3D$ line-intensity ratio and theoretical gf^{3C}/gf^{3D} ratio of neonlike ions as a function of atomic number. (b) Difference (in percent) between the theoretical and experimental $3C/3D$ ratios. Results are shown for the present calculations (Cl-1, CI-2, CI-3, and MBPT) and the previous calculations of Liang and Badnell [23], Safronova *et al.* [70], Dong *et al.* [11], and Hibbert *et al.* [62]. Experimental $3C$ and $3D$ line intensities and calculated gf^{3C} and gf^{3D} are collected in Tables I and III, respectively.

lowest Z. For neonlike iron and the ions with higher Z the two calculations are essentially in perfect agreement with each other.

Interestingly, the results obtained by Dong *et al.* [11], using MCDF calculations with a configuration model of single and double excitation up to $n = 5$, are very close to measurements and indistinguishable from MBPT. However, Ref. [11] is not specific about how the result was achieved and apparently there are no later CI-based calculations with a similar model space that have reproduced the results. Only very recently [32], a very large-scale MCDF computation with about 90 000 levels has come close to such agreement with experiment and MBPT.

Given the good agreement between the calculated and measured transition energies for the higher-Z ions, one may have expected that the experiment-theory deviation of the $3C/3D$ ratio calculated with the various methods converged and approached 0% for the ions with the highest atomic number. We indeed found that the different types of calculations converge. However, they do not converge to perfect agreement with experiment. Instead they approach a deviation of 20%–30% for Kr^{26+} ($Z = 36$). This discrepancy is only a lower bound for the expected deviation of the experimental gf^{3C}/gf^{3D} ratio, if we take guidance from the measurement of Bernitt *et al.* [32], and might be even larger if the experiments were to measure the actual gf^{3C}/gf^{3D} ratio instead of the $3C/3D$ line-intensity ratio.

C. Implications for theory

The nonzero result obtained for the highest-Z ions in Fig. 3(b) indicates one of two things: (i) The deviation does not originate from missing electron-correlation effects or (ii) second-order MBPT cannot describe the missing correlation effects in both $3C$ and $3D$ lines or in one of them. Point (i) derives from the similarity of the calculated gf^{3C}/gf^{3D} ratio of ions with the highest Z regardless of the calculational approach used, although MBPT, for example, correctly describes the electron-correlation effects for the transition energies of these ions. Point (ii) derives from the fact that our most accurate calculation is nevertheless only an approximation at the second-order level of perturbation. Moreover, point (ii) implies that for the $3C$ and $3D$ lines, transition energy calculations converge faster than calculations of the transition amplitude, with respect to the perturbation series or number of CI coefficients.

It is rather difficult to distinguish between points (i) and (ii) solely based on the data in Fig. 3(b). An analysis of electron-correlation effects affecting each individual line could help to differentiate the two points.

In the spirit of Gu *et al.* [12], we present in Fig. 4 the calculated gf^{3D} and gf^{3C} ratios relative to the values evaluated with model CI-1. From Fig. 4(a) we can see that accounting for electron-correlation effects (using either the CI-2, CI-3, or MBPT methods) leads to larger values of gf^{3D} in the low-Z ions. For the high-Z ions, the difference between all predictions is small, within 3%. Even though there are no experimental gf^{3D} values for these ions, these intertheory comparisons indicate that second-order MBPT and CI method

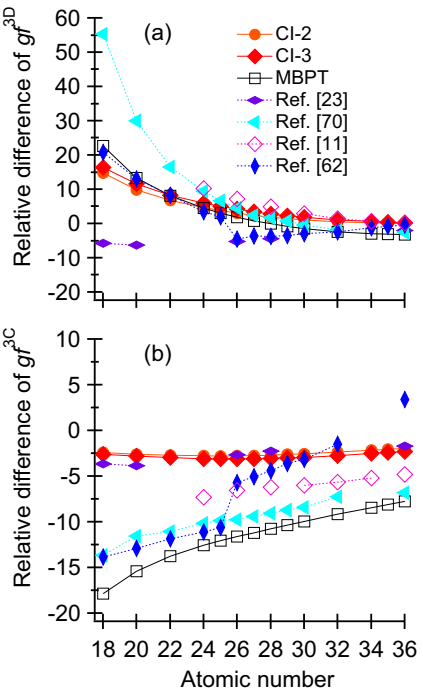

FIG. 4. (Color online) Comparison of various calculations of the (a) $3D$ and (b) $3C$ weighted oscillator strengths with the results of calculations in the CI-1 model (Cl-2, Cl-3, and MBPT from our own calculations). Other works shown are by Liang and Badnell [23], Safronova *et al.* [70], Dong *et al.* [11], and Hibbert *et al.* [62].

TABLE III. Calculated weighted oscillator strength gf (in the length form) of the 3C and 3D lines in neonlike ions evaluated with different methods: CI-1, CI-2, CI-3, and MBPT (see the text). The $3C/3D$ intensity ratio (gf^{3C}/gf^{3D}) and percentage of deviation (% dev.) from the experimental $3C/3D$ ratio are given.

	gf^{3C}	gf^{3D}	gf^{3C}/gf^{3D}	% dev.	gf^{3C}	gf^{3D}	gf^{3C}/gf^{3D}	% dev.
Z	CI-1				CI-2			
18	2.138	0.1273	16.79	48	2.086	0.1462	14.27	26
20	2.381	0.1985	12.00	46	2.320	0.2182	10.63	29
22	2.507	0.3055	8.21	39	2.439	0.3263	7.48	26
24	2.539	0.4511	5.63	29	2.468	0.4721	5.23	20
25	2.525	0.5371	4.70	37	2.455	0.5575	4.40	29
26	2.497	0.6302	3.96	30	2.428	0.6496	3.74	23
27	2.455	0.7285	3.37	30	2.388	0.7464	3.20	24
28	2.405	0.8301	2.90	26	2.340	0.8461	2.77	20
29	2.347	0.9327	2.52	28	2.286	0.9466	2.42	23
30	2.286	1.035	2.21	29	2.228	1.046	2.13	25
32	2.161	1.230	1.76	17	2.110	1.236	1.71	14
34	2.041	1.406	1.45	30	1.997	1.409	1.42	27
35	1.985	1.486	1.34	28	1.944	1.487	1.31	25
36	1.933	1.560	1.24	25	1.895	1.560	1.21	23
	CI-3				MBPT			
18	2.083	0.1483	14.05	24	1.757	0.1563	11.24	–1
20	2.315	0.2214	10.45	27	2.015	0.2250	8.95	9
22	2.433	0.3310	7.35	24	2.163	0.3302	6.55	11
24	2.461	0.4782	5.15	18	2.220	0.4714	4.71	8
25	2.447	0.5642	4.34	27	2.221	0.5536	4.01	17
26	2.419	0.6567	3.68	21	2.207	0.6419	3.44	13
27	2.379	0.7538	3.16	22	2.181	0.7345	2.97	15
28	2.331	0.8536	2.73	19	2.146	0.8295	2.59	12
29	2.277	0.9541	2.39	21	2.104	0.9251	2.27	15
30	2.219	1.053	2.11	23	2.059	1.020	2.02	18
32	2.102	1.243	1.69	13	1.963	1.201	1.63	9
34	1.989	1.415	1.41	26	1.869	1.365	1.37	22
35	1.937	1.493	1.30	24	1.824	1.440	1.27	21
36	1.888	1.565	1.21	22	1.783	1.509	1.18	19

(including at least double excitation in the $n = 3$ levels) correctly describe electron correlation in the radiative rate of the 3D line.

We note that our results for gf^{3D} values are in line with the result from Gu *et al.* [12] for Ni^{+18}; they showed that the excitation rate evaluated with a small number of CI coefficients is similar to that evaluated with a more extensive CI calculation that includes double excitations at the $n = 3$ level. On the other hand, the present results are different from the theoretical results presented by Bernitt *et al.* [32], who found the gf^{3D} value in Fe^{16+} evaluated with close to 10^5 CI coefficients to be over 7% larger than that evaluated with a minimum number of CI coefficients.

Figure 4(b) shows the Z-dependent behavior for the calculated values of gf^{3C}. The MBPT predictions for gf^{3C} are significantly different from those calculated with the CI-2 and CI-3 approaches. The CI-2 and CI-3 values are very similar to those obtained with the CI-1 approach, within 3%, for all ions. However, the MBPT values are over 15% lower for low-Z ions. This difference slightly decreases with Z, reaching 8% for Kr^{26+}. Similar to what we found for the gf^{3D} values, our results in general agree with those of Gu *et al.* [12]. However, they differ from the theoretical results of Bernitt *et al.* [32], who evaluated gf^{3C} for Fe^{16+} with a small number of CI coefficients and found the results to be similar to that obtained with an extensive CI space.

The present different Z-dependent trends in Fig. 4 indicate that electron-correlation effects have different roots for gf^{3D} and gf^{3C}. The effect on the gf^{3D} values seems to come mainly from pair correlation, as illustrated by the similarity in the gf^{3D} values derived from MBPT and from CI-2. Therefore, the gf^{3D} values predicted by the MBPT method are likely to be correct. By contrast, the effects on the gf^{3C} values likely involve highly excited states. The experiment-theory deviation of the $3C/3D$ ratio thus can be thought to arise because theory overestimates the rate of the 3C line [12].

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