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LETTER TO THE EDITOR

The influence of core excitations on energies and oscillator strengths of iron group elements

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Abstract. We show that for configurations of the type $3p^M 3d^N$ the influence of core excitations, in particular the excitation $3p^2 \rightarrow 3d^2$, is important both for energies and oscillator strengths. The latter is particularly true for transitions of the type $3p^6 3d^N \rightarrow 3p^5 3d^{N+1}$ due to the fact that the core excitation in the ground configuration leads to a configuration which has an allowed dipole transition to the excited state. Differences and similarities between $3p^5 3d^N$ and the more extensively studied $3p^6 3d^N$ configurations are pointed out and illustrated with several examples concerning highly charged ions. The conclusion is that, while core excitations are important for the description of transitions out of the open 3d shell, they are absolutely essential for transitions out of the closed 3p shell. *gf* values are given for astrophysically important transitions in Ni X.

The properties of the iron group elements are important in many areas of physics and not least astrophysics. In moderately to highly charged ions of these elements, the hydrogenic ordering of the $n = 3$ orbitals has been reached so that the ground configurations are of the form $3s^2 3p^6 3d^N$ and one of the lowest excited configurations is $3s^2 3p^5 3d^{N+1}$. While much work has been done on the ground configuration much less is known about the core-excited configurations. The structure of the $3d^N$ configurations can be described using a set of orthogonal electrostatic and magnetic operators which has been used, for example, in parametric fitting of these configurations in two- to five-times ionized spectra of the iron group elements (Hansen *et al* 1988) with very good results. A variant on this method is to use, for example, the suite of computer programs due to Cowan with scaling factors for the *ab initio* integrals derived from comparison with experiment (Cowan 1981). For the more complicated $3d^N$ configurations, this is the method that has been used to calculate most of the known oscillator strengths for these elements which are of fundamental importance, for example, in astrophysics (Fuhr *et al* 1988, Fawcett 1989, Kurucz 1990). The effective operator approach or its simpler equivalents are concerned with obtaining the correct energy level positions but, in its purest form, without introducing additional configurations. This means that when using the resulting eigenvectors to describe other properties it is, in principle, necessary to introduce an effective operator for the required property that takes the effect of the simulated configurations into account (Feneuille *et al* 1970). A simpler method is to include the 'important' configurations explicitly so that the fitting only takes the 'less important', usually the more distant and thus weaker, interactions into account and

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this is the method which is most often used in practice. The effect of these configurations on other properties is usually not included but the results are nevertheless expected to be improved; for oscillator strengths, for example, because the transition energies are closer to those observed and because the mixing due to fine structure effects is expected to be improved. The validity of this argument has been discussed by Brage and Hibbert (1989) in a slightly different context. What is 'important' to include explicitly depends on the property under consideration and will be different in a calculation aimed at determining hyperfine structure, say, compared to a calculation directed at obtaining oscillator strengths. The 'art' involved in carrying out such calculations is to know which configurations must be included and this varies with the details of the case.

The iron group elements are complicated by the fact that the $n = 3$ shell is not closed so that core excitations such as $3s \rightarrow 3d$ or $3p^2 \rightarrow 3d^2$ are possible within this shell. Due to the good overlap between electrons with the same n value these interactions are very large and significantly influence the energy level structure of, for example, the $3d^N$ configurations. This effect can, however, easily be described by the effective operator technique and, in fact, some effective operators, for example T (Trees 1963), were originally introduced to take these effects into account. (For a discussion of the significance of the conventional effective parameters for the $3d^N$ configurations see Hansen and Raassen (1981).) A prominent reason behind the introduction of effective operators was the fact that the explicit introduction of these interactions leads to very large Hamiltonian matrices which even with today's computer capabilities are difficult to handle. In this letter we point out that for the calculation of oscillator strengths, the explicit introduction of core excitations is important when considering transitions out of the open $3d^N$ subshell but it is *crucial* when considering transitions out of the full $3p^6$ subshell. This point does not appear to have been appreciated in the past although the realization that core excitations are important goes back at least to Layzer (1959).

The transitions from $3p^6 3d$ to $3p^5 3d^2$ provide the simplest example of this effect. In Fe VIII and Ni X these lines are prominent in the solar spectrum and Fawcett (1989) has published calculated oscillator strengths for these transitions in the ions V V to Cu XI. A considerable amount of valence correlation is included in these calculations combined with the use of parametric fitting for some of the parameters associated with the $3p^5 3d^2$ configuration. Fawcett also considered the introduction of the core excitations $3p^2 \rightarrow 3d^2$ in the final state but did not succeed in obtaining a good fit when this configuration was included. However, he concluded that the introduction of this interaction (in the final state) could be mimicked by reducing the calculated oscillator strengths by about 10%. We agree with this observation but the purpose of this letter is to point out that the same interaction in the initial state is much more important for the oscillator strengths and leads to a substantial reduction of the f values even for the strongest transitions which are insensitive to valence correlation. Saraph *et al* (1992) have recently emphasized the importance of core excitations for the calculation of oscillator strengths for the iron group elements although few details were reported.

We consider first by way of a few examples the effect of the core excitations on the energies and subsequently on the oscillator strengths of the $3s^2 3p^M 3d^N$ configurations with $M = 5$ and 6. For the calculations we make use of the suite of programs due to Cowan (1981) which was also used in the calculations by Fawcett (1989), for example. We use the approximately relativistic HFR approximation (Cowan and Griffin 1976) and the reported transition probabilities are obtained using the length formulation of the dipole operator. The use of Ni ions for the examples is motivated by their importance in solar physics as well as by the fact that in Ni X, for example, the $3p^6 4l$ terms are located well above $3p^5 3d^2$ and do not perturb the latter. For this reason Fawcett (1989) considered his results for Ni X to be

Figure 1. Calculated and observed energy level structure of the $3s^2 3p^6 3d^2$ configuration in Ni IX. Two *ab initio* approximations are used, the one labelled 'valence correlation' has a frozen $3s^2 3p^6$ core while the other labelled 'full correlation' includes excitations from the 3s and 3p shells into the 3d shell. The results are referred to the ground level $3d^2 \ ^3F_2$.

more reliable than the results for the other ions included in his study. In Fe VIII, considered by Saraph *et al* (1992), the $3p^6 4p$ term lies in the middle of the $3p^5 3d^2$ configuration which makes the effect of the core excitations more difficult to disentangle.

Figure 1 shows the structure of the $3p^6 3d^2$ configuration in Ni IX in two approximations. The first includes valence correlation only (but no scaling) and the other includes in addition the core excitations $3s \rightarrow 3d$ and $3p^2 \rightarrow 3d^2$. (Called 'full correlation'; the effect of the $3s^2 \rightarrow 3d^2$ excitation is much smaller.) The two calculations are compared to the observations by van het Hof *et al* (1990). The figure shows that the main error in the valence correlation calculation is found for the 1S_0 level, which is nearly $10\,000\text{ cm}^{-1}$ too high, the figure also shows that this error is sharply reduced when excitations from the 3s and 3p shells are included. In fact all levels, except 1G_4 , are predicted more accurately when core excitations are included. With regard to parametric fitting, figure 1 shows that the neglect of core excitations is easy to take into account since the β parameter is available to fit the 1S_0 level (Hansen and Raassen 1981). Furthermore, this level is often unknown since it has few transitions to other levels in the spectrum.

Similarly when the $3p^5 3d$ configuration is considered, it is found that only the 1P term is seriously affected by $3s \rightarrow 3d$ and $3p^2 \rightarrow 3d^2$ excitations. Also in this case the parametric fitting is straightforward since this time the $G^1(3p, 3d)$ 'parameter' is available to fit the position of the 1P term (Hansen 1972).

Figure 2 shows equivalent results for the $3s^2 3p^5 3d^2$ configuration in Ni X. The results are again given relative to the ground level $3s^2 3p^6 3d^2 D_{3/2}$ but this time the ground level belongs to another configuration and the error in the energies includes the error in the difference between the calculated mean energies of the two configurations (including both valence and core excitations for both). The figure shows that by reducing the average energy of the $3p^5 3d^2$ configuration in the 'full correlation' calculation, reasonably good agreement is obtained for all observed levels while in the case of valence correlation only, the lowest levels in figure 2 are already lower than the observed levels so that moving the configuration as a whole does not improve the agreement materially. It is surprising that Fawcett (1989) states that including the two core excitations leads to rearrangement of many levels within the $3p^5 3d^2$ configuration which subsequently frustrated his efforts to fit the observed levels with the core excitations explicitly included. On the contrary, the results in figure 2 would suggest that parametric fitting should be easier with these included since the *ab initio* prediction is closer to the observed levels. However, for the ions where the $3p^5 3d^2$ configuration overlaps other configurations the situation is more complicated and additional core excitations must be included to get these configurations in the correct position, presumably Fawcett's remark is related to this situation.

Figure 2. Calculated and observed structure of the $3s^2 3p^5 3d^2$ configuration in Ni X. The notation is the same as in figure 1. The results are referred to the ground level $3s^2 3p^6 3d^2 D_{3/2}$, thus the results show the error in the difference between the mean energies of the two configurations as well as the error in the prediction of the term structure. Only results for the observed levels are shown.

Figure 3. Calculated and observed structure of the $3s^2 3p^5 3d^3$ configuration in Fe VII. The notation is as introduced in figure 1. The results are referred to the ground level $3s^2 3p^6 3d^2 \ ^3F_2$ and it can be seen that by lowering the $3p^5 3d^3$ configuration as a whole by approximately $20\,000\text{ cm}^{-1}$ very good agreement is obtained for all observed levels.

Finally figure 3 shows the results for the $3s^2 3p^5 3d^3$ configuration in Fe VII where more levels are known than in Ni IX. Also in this case a considerable improvement is obtained compared to the 'valence correlation' which here includes the configurations $3p^6(3d4p + 3d5p + 3d4f + 3d5f)$ and $3p^5 3d^2 4s$ in addition to the $3s^2 3p^5 3d^3$ configuration. In fact the figure shows that a displacement of all levels by about $20\,000\text{ cm}^{-1}$ leads to very good agreement with the observations for the observed levels. We note that Saraph *et al* (1992) state that the equivalent error in their calculation is about $44\,000\text{ cm}^{-1}$ which indicates that the HFR approximation is more accurate than the statistical model potential approach used by them. For the $3p^5 3d^3$ configuration, introduction of core excitations leads to rearrangements among the high levels, as the figure shows, and these rearrangements are in agreement with the observed structure so that also in this case fitting should be easier and more reliable when the core interaction is introduced explicitly. We conclude that for the calculation of energy levels, the introduction of core excitations is important in *ab initio* calculations and we believe that when attempting parametric fitting to the $3p^M 3d^N$ configurations with $M \neq 6$, it will be easier to obtain a reliable fit if these interactions are included explicitly. We will now show that this procedure is even more important when attempting to use the fits to calculate oscillator strengths.

Table 1. Observed wavelengths and calculated oscillator strengths (gf) for the strongest $3p^63d \rightarrow 3p^53d^2$ and the $3p^63d \rightarrow 3p^64f$ transitions in Ni x. Three approximations are used in the calculation of oscillator strengths: the single-configuration, the valence correlation and the 'full' (valence plus excitations from the $n \approx 3$ shell) correlation approximation (the configurations added in the final state are different for the two arrays, see text).

Transition	$\lambda_{\text{obs}}(\text{\AA})^a$	gf			
		Single conf.	Valence correlation		Full correlation
		<i>ab initio</i> ^b	Fitting ^c	<i>ab initio</i> ^b	<i>ab initio</i> ^b
$3p^63d-3p^53d^2$					
$^2D_{3/2}-(^3F)^2F_{5/2}$	159.977	4.21	3.84	3.79	2.88
$^2D_{5/2}-(^3F)^2D_{5/2}$	144.988	7.85	8.11	8.12	6.24
$^2D_{3/2}-(^3F)^2D_{3/2}$	144.216	5.00	5.07	5.18	3.99
$^2D_{5/2}-(^3P)^2P_{3/2}$	145.733	4.08	4.45	4.61	4.04
$^2D_{3/2}-(^3P)^2P_{1/2}$	146.081	2.25	2.46	2.55	2.23
$^2D_{5/2}-(^3F)^2F_{7/2}$	158.377	5.92	5.34	5.33	4.03
$3p^63d-3p^64f$					
$^2D_{5/2}-^2F_{7/2}$	91.721	3.00	4.16	4.19	3.94
$^2D_{5/2}-^2F_{5/2}$	91.728	0.15	0.21	0.21	0.20
$^2D_{3/2}-^2F_{5/2}$	91.461	2.11	2.92	2.94	2.76

^a Calculated using the observed energy levels (Sugar and Corliss 1985).

^b Calculated using the observed transition energies (column 2).

^c Fawcett (1989).

Table 1 shows results for the $3p^63d \rightarrow 3p^53d^2$ and the $3p^63d \rightarrow 3p^64f$ transitions in Ni x. The first set of transitions are particularly important for solar line intensity analysis and is discussed first. Several approximations are compared to the results due to Fawcett (1989). In the 'valence correlation' calculation, the configurations $3s^23p^6(3d + 4d + 5d + 4s + 5s)$ and $3s^23p^53d4p$ were included in the initial state and $3s^23p^5(3d^2 + 3d4s + 3d4d)$ and $3s^23p^6(4p + 5p + 4f + 5f + 6f + 7f)$ in the final state. In the 'full correlation' calculations the configurations $3s3p^63d^2$ and $3s^23p^43d^3$ were added in the initial state and, for the transitions to $3p^53d^2$, the configurations $3s3p^53d^3$ and $3s^23p^33d^4$ in the final state. Only the strongest transitions are included in table 1. To make the comparison as meaningful as possible we have used the observed transition energies in all calculations. These are given in column 2 for easy identification of the transitions. The choice of the experimental energies in the calculations also makes the comparison to Fawcett more significant, since Fawcett used fitting and therefore in general had good agreement with the observed energies. The third column shows that for the transitions to $3p^53d^2$ an *ab initio* single-configuration approximation already gives results in reasonably good agreement with Fawcett's. This is confirmed by the fact that introduction of the valence correlation used in Fawcett's approach but without fitting gives results in very good agreement with Fawcett's values. What we are seeing is that for these very strong lines valence correlation is not very important. For the many weaker lines, valence correlation can be more important and will lead to larger (percentage) changes in the calculated values.

Also introducing the core excitations, table 1 (column 6) shows on average a 20% decrease in the gf values for the $3p^63d \rightarrow 3p^53d^2$ transitions. Fawcett reported that the introduction of core excitations in the *final* state for the elements he considered leads to a reduction of about 10% while we obtain a value of 5% for Ni x. However, it is easy to see that the introduction of the core interactions in the *initial* state is far more important

and it is responsible for the main reduction in the gf values. This is because the $3s^23p^43d^3$ and the $3s3p^63d^2$ configurations, which must be introduced in the initial state, have allowed dipole transitions to the $3s^23p^53d^2$ configuration. Furthermore, the radial dipole integral $3d \rightarrow 3p$ involved in the transition from the $3s^23p^43d^3$ configuration has the same magnitude as the dipole matrix elements which connects the main configurations. On the other hand the equivalent configuration in the final state does not have an allowed transition to the initial state and this is the reason that it is more important to include the correlation in the initial than in the final state. The same discussion applies to configurations with additional $3d$ electrons. It can also be seen that the $3s^2 \rightarrow 3d^2$ excitation does not lead to a state with a dipole transition to $3s^23p^53d^2$, which is one reason that this excitation is less important for calculations of transition probabilities out of the $3p$ shell.

The results for the $3p^63d \rightarrow 3p^64f$ array in table 1 show a different behaviour. For this array the difference between the single-configuration and the valence correlation calculation (including the same configurations as before) is larger than the difference between the valence and the full correlation approximation. In this case the introduction of core excitations corresponds to adding the $3s3p^63d4f$ and $3s^23p^43d^24f$ configurations in the final state but these configurations do not combine with the ground state and the earlier mentioned core excitations in the initial state do not combine with the $3p^64f$ term which explains why the influence on the f values is small. The same applies to other transitions involving $3d$ excitations.

The results in table 1 also show that the effect of the fitting is rather small which indicates that *ab initio* calculations of these systems (using observed energies) can give results of the same quality as obtained by explicit parametric fitting. This is particularly interesting for the systems with an open $3p$ shell since a proper parametric fitting to these configurations involves effective parameters connected with the $3p \leftrightarrow 3d$ interaction (Dothe *et al* 1985), which has not been introduced in the fitting so far, in addition to the more well known parameters associated with the $3d \leftrightarrow 3d$ interaction.

In conclusion, we have shown that for calculations of $3p \rightarrow 3d$ transitions out of the closed $3p$ shell in configurations of the type $3p^63d^N$, it is essential to include core excitations. This is primarily because the $3p^2 \rightarrow 3d^2$ excitation in the initial state leads to an allowed transition to the final state with a dipole matrix element which is equal in magnitude to that for the primary transition. Also the $3s \rightarrow 3d$ excitation leads to a configuration with an allowed dipole transition to the final state. This excitation has a smaller effect on the gf values for the dipole transitions but we note that in calculations of electric quadrupole transitions, it is the introduction of this excitation that is important since it corresponds to an allowed quadrupole transition from the $3s^23p^63d^N$ configuration.

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