Relativistic calculation of $3s$-$3p$ transition wavelengths in neonlike ions

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Wavelengths for the $2s^22p^53s$-$2s^22p^53p$ transitions in the neonlike isoelectronic sequence have been calculated by means of the relativistic code of Grant *et al.* [Comput. Phys. Commun. **21**, 207 (1980)]. Mixing with the $2s2p^63l$ configurations is found to be important. A separate optimization for the $2p^53p\ ^1S_0$ state is needed. Comparisons with observations in Ti XIII, Fe XVII, Se XXV, and Y XXX show excellent agreement.

The attempts during recent years to achieve amplification of radiation at short wavelengths have stimulated much theoretical activity on neonlike atomic systems, as one of the proposed lasing schemes involves $2p^52s$-$2p^53p$ transitions. The work that resulted in the successful observations of amplified emission from selenium and yttrium plasmas[1,2] according to this scheme included comprehensive calculations of plasma properties and atomic data.

Among the basic atomic data needed in such work are the positions of all levels involved in the populating processes and, in particular, an accurate value for the distance between the levels forming the lasing system. Experimental data for energy levels of the neonlike isoelectronic sequence have previously been available only up to Ar IX, except the $J=1$ levels of $3s$, $3d$, and some other odd configurations that had been established through ground term combinations up to Xe XLV. Recently, however, the $2p^53s$, $3p$, and $3d$ configurations of Ti XIII and Fe XVII have been analyzed,[3,4] and data are thus available for testing *ab initio* calculations for ions close to those expected to form lasing systems. Hartree-Fock calculations in Ref. 4 showed that relativistic effects start to become important already before Ti XIII, and make predictions of energy levels and transition wavelengths by means of nonrelativistic calculations beyond Fe XVII very uncertain.

Relativistic multiconfiguration Dirac-Fock (MCDF) calculations have now been performed by using the MCDF code of Grant *et al.*[5] and the transverse photon energy and QED package of McKenzie, Grant, and Norrington.[6] A detailed description of these calculations will be published elsewhere,[7] and this report will only contain a discussion of some problems that are related to the expected and observed laser transitions.

In this connection it should be noted that great confusion appears to exist in the literature concerning level designations for the neonlike ions. This is caused by the fact that the coupling conditions along the sequence—as is generally the case—change with increasing Z. While the LS representation may be a good approximation in the beginning of the sequence, the conditions at high Z approach the jj approximation. Thus the levels for low Z can be unambiguously given LS names, as is, e.g., the case for the $2p^53s$ configuration, where the three low levels form a ^3P while the upper level is a ^1P. An investigation of the LS eigenvector components shows, however, that the $J=1$ levels get increasingly mixed in the LS scheme as Z increases, and in fact the largest component of the upper level changes from ^1P to ^3P. This situation gives rise to the confusion mentioned above, as some authors use the maximum LS eigenvector component as level designation instead of keeping the ordering of the $J=1$ levels from the region of the sequence where the LS scheme is a meaningful approximation. Thus, the upper $J=1$ level should be called ^1P until the designation is changed to the jj scheme. In fact, there is good reason to make this change early in the sequence—already for Sc XII the average purity of the $3s$ configuration is 94% in jj coupling and only 58% in LS coupling. The isoelectronic development of the $3s$ level structure is shown in Fig. 2 of Ref. 4.

For the $2p^53p$ configuration the situation is still more confused due to the gradual departure from LS coupling. The mixing has been discussed in detail by Bureeva and Safronova,[8] who also point out that, as for $3s$, the only unambiguous LS designations are those obtained by application of the rule that levels with the same J do not cross; i.e., the ordering of the levels for a certain J value should be retained from the beginning of the sequence, as shown in Fig. 1. This diagram, which was obtained through Hartree-Fock calculations, also shows the correlation between the LS and the jj designations.

As examples of the results from the relativistic calculations, some $3s$-$3p$ transition wavelengths in Ti XIII and Fe XVII are shown in Table I. These lines were selected to illustrate some characteristic problems in the calculations. With one exception to be discussed below, the calculations were made by optimizing for the weighted average energy of all levels in a configuration and then calculating the fine-structure levels and the transition wavelengths. As seen in Table I, this single-configuration treatment gives good agreement with the observed wavelengths for, e.g., the two lines from $J=2$ levels in $3p$. The rest of the lines in the table show serious discrepancies.

It is known from investigations of the beginning of the neonlike sequence[9] that the $^3S_1$ level of $2s^22p^53p$ is perturbed by $^3S_1$ of $2s2p^63s$. For this reason a multiconfiguration calculation was performed, involving these two configurations and, for consistency, $2s2p^63d$. In analogy to this, $2s2p^63p$ was included in the calculation of $2s^22p^53s$. The resulting wavelengths are shown in the second row for each line in Table I. Obviously, the wavelength for the last line, where the upper level is $3p\ ^3S_1$, is drastically improved, while the other lines are less affected.

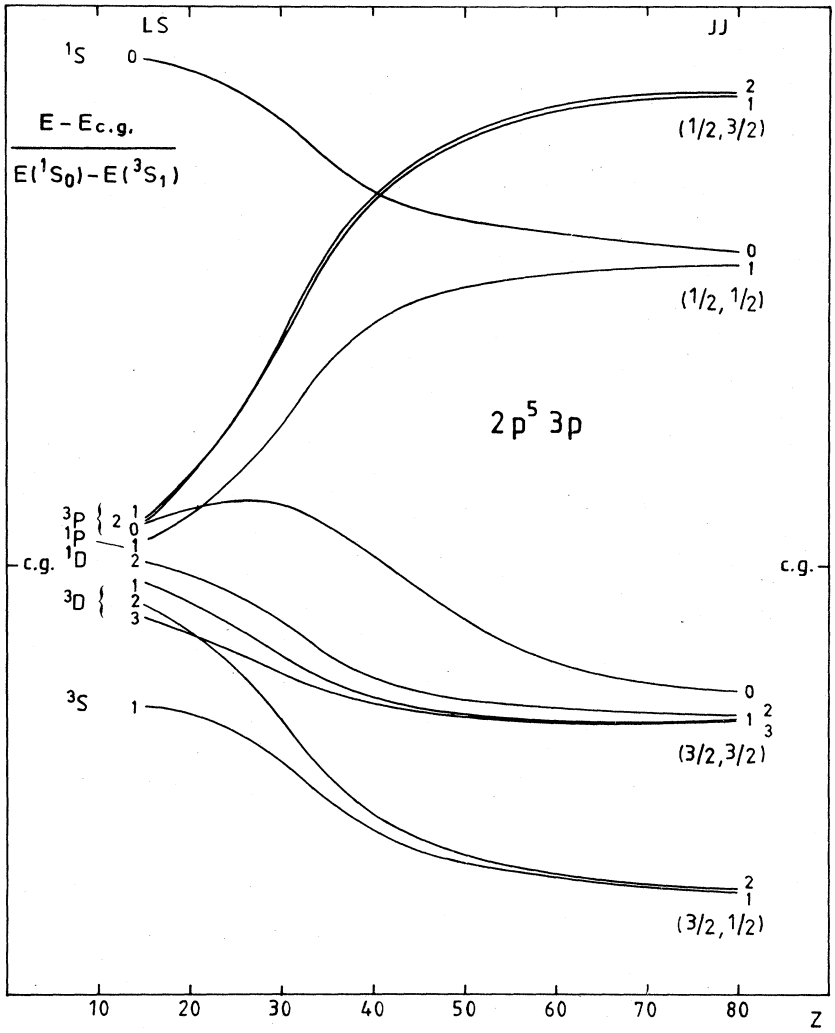

FIG. 1. Predicted structure of the $2s^22p^53p$ configuration in the neonlike sequence. The unambiguous level designations in the *LS* and *jj* representations are shown. The levels are plotted relative to the center of gravity of the configuration and the energy scale is normalized to a constant value of the $^3S_1$-$^1S_0$ interval.

TABLE I. Observed and calculated wavelengths for some $3s$-$3p$ lines in neonlike Ti XIII and Fe XVII.

Level designation			Wavelength (Å)			
			Ti XIII		Fe XVII	
$3s$ *jj*	$3p$ *LS*	*jj*	Observed[a]	Calculated	Observed[b,c]	Calculated
$(\frac{3}{2},\frac{1}{2})_1$	$^1S_0$	$(\frac{1}{2},\frac{1}{2})_0$		271.7[d]	204.65	197.2[d]
				269.6[e]		196.4[e]
				286.0[f]		204.8[f]
$(\frac{1}{2},\frac{1}{2})_1$	$^1S_0$	$(\frac{1}{2},\frac{1}{2})_0$		308.9[d]	254.87	243.9[d]
				306.3[e]		242.1[e]
				327.6[f]		254.9[f]
$(\frac{3}{2},\frac{1}{2})_1$	$^1D_2$	$(\frac{3}{2},\frac{3}{2})_2$	459.338	461.4[d]	340.40	341.7[d]
				459.3[e]		340.5[e]
$(\frac{1}{2},\frac{1}{2})_1$	$^3P_2$	$(\frac{1}{2},\frac{3}{2})_2$	472.088	473.6[d]	347.85	348.8[d]
				472.8[e]		348.0[e]
$(\frac{3}{2},\frac{1}{2})_2$	$^3S_1$	$(\frac{3}{2},\frac{1}{2})_1$	552.115	534.2[d]	409.69	389.9[d]
				550.7[e]		408.8[e]

[a]Reference 4.
[b]Reference 3.
[c]Reference 12.
[d]Single configuration.
[e]Multiconfiguration including the $2s2p^63l$ configurations.
[f]Separate optimization of the $J=0$ levels of $3p$.

TABLE II. Laser wavelengths of $3s$-$3p$ lines in Se XXV and Y XXX.

Level designation		Wavelength (Å)			
		Se XXV		Y XXX	
$3s$	$3p$	Observed[a]	Calculated	Observed[a]	Calculated
$(\frac{1}{2},\frac{1}{2})_1$	$(\frac{1}{2},\frac{1}{2})_0$	(183)[b]	181.7		154.3
$(\frac{1}{2},\frac{1}{2})_1$	$(\frac{1}{2},\frac{3}{2})_2$	209.6	209.7	157.1	157.2
$(\frac{3}{2},\frac{1}{2})_1$	$(\frac{3}{2},\frac{3}{2})_2$	206.3	206.4	155.0	155.0

[a]Reference 2.

[b]Prediction in Ref. 2.

It is also known from the beginning of the sequence that a Hartree-Fock calculation of the $3p\ ^1S_0$ state offers special problems, partly due to a different radial dependence compared with the other states arising from the $2p^5 3p$ configuration.[10] For this reason the $J=0$ states of $3p$ were optimized in a separate MCDF calculation. The resulting wavelengths for the two lines involving $3p\ ^1S_0$ are shown in Table I, and the agreement with the observations is seen to be excellent. It should be noted that all calculations are completely *ab initio,* with no fit to observations.

Calculations with the same method have now been performed for the two ions where amplification of $3s$-$3p$ emission has been reported,[1,2] viz., Se XXV and Y XXX. The resulting wavelengths are shown in Table II for the two transitions where amplification was observed and the transition that was expected to give the strongest amplification. The agreement with the reported wavelengths is found to be very good.

To conclude, we find that multiconfiguration Dirac-Fock calculations provide $3s$-$3p$ transition wavelengths that agree very well with the observed wavelengths in Ti XIII, Fe XVII, Se XXV, and Y XXX, and thus can be used for accurate predictions in highly charged ions. Generally, the $2s2p^6 3s$, $3p$, and $3d$ configurations seem to be omitted in the calculations of level structure, collision strengths, and decay rates of neonlike ions (see, e.g., Ref. 11), but we want to stress that the interaction with $2s2p^6 3s$ affects the structure of the $2s^2 2p^5 3p$ configuration. In the beginning of the sequence mainly the $^3S_1$ state is perturbed, but as the spin-orbit mixing within $3p$ increases all the $J=1$ states are likely to be affected. We also want to emphasize that the noncrossing rule for levels with the same J must be applied in order to avoid ambiguities if LS names are to be used. jj symbols should of course be used, as was done in Refs. 3 and 4, as soon as the level purity is higher in jj than in LS coupling.

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