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Strong monopole electron-collisional excitation in highly stripped ions

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The collision strengths for electric monopole collisional excitation of the outermost subshell of highly stripped closed-shell ions are examined and found to scale nearly hydrogenically. The collision strength near threshold for the principal monopole excitation process (in the distorted-wave approximation) is written as $\Omega(Z) = \xi_{nl}(Z)\eta_{nl}(Z)N_{nl}I_H/\Delta E(Z)$, where $\xi_{nl}(Z)$ is near 0.3, 0.5, and 0.6 for the He-like (1s-2s), Ne-like (2p-3p), and Ni-like (3d-4d) sequences, respectively, and where $\eta_{nl}(Z)$ accounts for mixing effects and is near unity at low Z. The excitation process in nickel-like ions is more effective per electron than for neonlike ions and is favorable to the development of x-ray lasers below 44 Å. The extension of the monopole excitation scheme to Nd-like ions appears very attractive for longer wavelengths.

Electric monopole transitions play a key role in the physics of electron collisional schemes in x-ray lasers¹⁻⁶ and are of interest due to the fact that some of the strongest transitions in highly stripped ions are monopole transitions.^{7,8} Our interest in this paper was originally generated by the possibility of developing x-ray lasers in the spectral regime below 44 Å (within the so-called water window which lies between the K edges of carbon and oxygen⁹).

Monopole transitions in nickel-like ions appear particularly attractive as a possible route towards the development of a 44-Å x-ray laser and amplification has already been observed at 66 Å in nickel-like europium^{10,11} at the Lawrence Livermore National Laboratory (LLNL). Preliminary experimental work has also begun there in search of possible amplification at 50.2 Å in nickel-like ytterbium.¹²

In this work we discuss the scaling of the electric monopole transitions in nickel-like ions. We have previously reported multiconfiguration relativistic distorted-wave calculations of n = 3-4 electron collisional cross sections in gadolinium,¹³ and we discussed briefly the various monopole transitions which occur. The strongest monopole transition occurs between the $3s^23p^{6}3d^{10}S_0$ ground state and the high-lying $(3s^23p^{6}3d^3_{3/2}3d^6_{5/2}4d_{3/2})_0({}^1S_0)$ state, the latter of which serves as the upper laser state in the experiments mentioned above.

The collision strength for the strong monopole transition in the distorted-wave approximation is approximately constant near threshold and in Table I the nearthreshold distorted wave values for the collision strengths of the strong monopole transitions for selected elements between silver and rhenium are presented. The product of the excitation energy and collision strength $\Delta E(Z)\Omega(Z)$ is roughly constant as a function of Z, as may be found from inspection of the data in Table I. This result is consistent with standard "hydrogenic" \overline{Z}^{-2} scaling of collision strengths, where \overline{Z} is an effective charge.¹⁴

There are two possible laser transitions from the $(3s^23p^63d_{3/2}^34d_{3/2})_0$ monopole-excited upper state in the nickel-like sequence. At low Z, the lower energy transition will have higher small signal laser gain, since the gain is proportional to oscillator strength f (which we have tabulated in Table I for both transitions). At high Z (>Z = 68), the higher energy transition is dominant, which has important consequences for the development of a sub-44-Å laser. Simply put, it would take more than twice the incident pump laser power to drive a laser at high Z had the low-energy 4d-4f transition been favored.

Although the discussion presented here so far relates to the scaling of the monopole excitation cross section in nickel-like ions, we are also interested in examining the scaling of collisional excitation between sequences. Gain has now been observed on transitions both in the neonlike sequence^{15,16} and in the nickel-like sequence where the upper laser level is a monopole-excited ${}^{1}S_{0}$ state. (We note that in the neonlike lasers, the laser transitions with the highest gain are pumped both by indirect excitation and through dielectronic recombination as discussed previously.¹⁷⁻¹⁹) The monopole transition is calculated to be very strong for both sequences, and it may

37 1357

be asked how these excitation processes compare against one another. For example, is the collision strength for the nickel-like electric monopole transition basically the same as it is for the neonlike case, except perhaps scaled by the number of electrons within the relevant subshell?

In order to shed light on this issue, we have plotted (see Fig. 1) the scaled total monopole collision strength (based on near-threshold distorted-wave-models) defined as follows:

$$\xi(Z) = \frac{\Delta E(Z)\Omega(Z)}{NI_{\rm H}} , \qquad (1)$$

where N is the number of subshell electrons and $I_{\rm H}$ is 13.606 eV, as a function of threshold excitation energy for the He-like $1s^2-1s2s$ ${}^{1}S_{0}$ transition,²⁰ for the sum of the two Ne-like $2s^22p^{6}-2s^22p^{5}3p$, J=0 transitions,²¹ and for sum of the two Ni-like $3s^23p^{6}3d^{10}-3s^23p^{6}3d^{9}4d$ J=0 transitions. We note that near-threshold resonances are known to be important for monopole excitation in the He-like sequence,²² and since the discussion in this paper is based primarily on the distorted-wave model in the absence of resonance contributions for the neonlike and nickel-like sequences, there will be corrections to be applied once these contributions are better understood.

Inspection of Fig. 1 indicates that the scaled total collision strengths are slowly varying functions of the excitation energy for the three isoelectronic sequences and monotonically increasing with increasing principal quantum number. It may be concluded that in terms of the scaled total collision strength, the 3d-4d monopole excitation strength in the nickel-like ions is roughly 25%stronger than the corresponding value for the 2p-3ptransitions in the neonlike ions per electron.

In the neonlike sequence there are two $2s^22p^{5}3p$, J=0 levels, corresponding to ${}^{1}S_{0}$ and ${}^{3}P_{0}$ states at low Z. Due to configuration interaction effects these states are mixed. One finds that in iron the collision strength for the transition up to the ${}^{1}S_{0}$ state is 93% of the 2p-3p monopole total (see Fig. 2), whereas in yttrium the ratio is 65%. In silver (not shown) the collision strength is split evenly between the two transitions. In the nickel-

ΔEΩ NI_H 0.6 3d-4d 0.5 20 0.4 0.3 ls-2s 0.2 0.1 õ 1.5 2.0 0.5 1.0 2.5 THRESHOLD ENERGY DE IN KeV

FIG. 1. The scaled total collision strength $\xi_{nl}(Z)$ from Eq. (1) of the text is plotted as a function of threshold excitation energy for He-like, Ne-like, and Ni-like ions.

like sequence in the same range of excitation energy the collision strength is dominated by the upper J=0 level (for which a label ${}^{1}S_{0}$ is justified). For example, in gadolinium the collision strength for the transition to the $(3s^{2}3p^{6}3d_{3/2}^{3}3d_{5/2}^{6}4d_{3/2})_{0}$ state constitutes 94% of the total collision strength for monopole excitation.

From the discussion in the above paragraphs, it seems reasonable to propose a simple expression for the monopole collision strengths of the following form:

$$\Omega(nl,Z) = \xi_{nl}(Z)\eta_{nl}(Z)N_{nl}\frac{I_{\rm H}}{\Delta E(Z)} , \qquad (2)$$

where N_{nl} is the number of subshell electrons (2, 6, and 10 for the $1s^2$, $2p^6$, and $3d^{10}$ shells, respectively) and where $\xi_{nl}(Z)$ is approximately 0.3, 0.5, and 0.6 for the He-like, Ne-like, and Ni-like sequences, respectively (as shown in Fig. 1). The function $\eta_{nl}(Z)$ includes the dilution of the monopole strength due to deviations from a pure *LS* picture ultimately due to relativistic effects. At low *Z* the function $\eta_{nl}(Z)$ is close to unity (although it is always less than unity even at low *Z* due to the occurrence of exchange excitation) as shown in Fig. 2. The

TABLE I. Atomic data relevant to the electric monopole collisional excitation scheme in nickel-

like ions. The high-energy 4p-4d line is the $(3s^23p^63d_{3/2}^33d_{5/2}^64p_{1/2})_1 - (3s^23p^63d_{3/2}^33d_{5/2}^64d_{3/2})_0$ tran-
sition and the low-energy $4p-4d$ line is the $(3s^23p^63d_{3/2}^33d_{5/2}^64p_{3/2})_1 - (3s^23p^63d_{3/2}^33d_{5/2}^64d_{3/2})_0$ transi-
tion. The wavelengths were estimated through correcting a multiconfiguration relativistic Hartree-
Fock calculation with a Z-independent decrement of the upper $J=0$ state to obtain approximate
agreement with experimental data for europium. The collision strengths are for the $3d$ -4d monopole
transition from the $(3s^23p^63d^{10})_0$ ground state to the $(3s^23p^63d^3_{3/2}3d^5_{5/2}4d_{3/2})_0$ upper state. ΔE is the
transition energy for the monopole excitation process.

Scaling in Ni-like systems							
	High energy 4p-4d Low energy 4p-4d						
Ζ	λ	f	λ	f	Ω	ΔE	
47	135.0 Å	0.0084	139.9 Å	0.180	0.136	485	
54	95.7 Å	0.0360	100.1 Å	0.130	0.091	787	
63	65.9 Å	0.0620	71.0 Å	0.084	0.060	1272	
64	63.4 Å	0.0640	68.6 Å	0.080	0.057	1333	
70	50.3 Å	0.0750	56.2 Å	0.061	0.044	1726	
75	41.6 Å	0.0820	47.8 Å	0.048	0.036	2092	



FIG. 2. The ratio $\eta_{nl}(Z)$ of the collision strength for excitation of the dominant $(J=0) 2s^2 2p^5 3p$ state to total $2p \cdot 3p$ (J=0) collision strength for the neonlike sequence and the ratio of the collision strength for excitation of the dominant $(J=0) 3s^2 3p^6 3d^9 4d$ state to total $3d \cdot 4d$ (J=0) collision strength in the nickel-like sequence. In the He-like sequence there is only one (J=0) 1s 2s state, and for this case the function $\eta_{nl}(Z)$ is unity.

results given in this paper and expressed in Eq. (2) are of use in the consideration of the scaling of gain and power requirements in x-ray lasers.^{23,24}

The extension of the collisional excitation scheme to the next shell (in Nd-like) ions is perhaps an obvious next step. It is reasonable to expect that the total scaled collision strength for the 4f-5f monopole transitions in the Nd-like sequence will be even larger than that for the Ni-like sequence [we anticipate that $\eta_{nl}(Z)$ will be approximately 0.7 at high Z]. Furthermore, little dilution of the monopole excitation strength between the two $(4s^24p^{6}4d^{10}4f^{13}5f)_0$ levels is expected, both from a consideration of the scaling of $\eta_{nl}(Z)$ from sequence to sequence and from examination of mixing coefficients resulting from a relativistic multiconfiguration atomic structure calculation for U.

For U (which is the highest Z which could plausibly be incorporated into an x-ray laser experiment), the principle electric monopole collisionally excited laser transition is the $(4s^24p^{6}4d^{10}4f_{5/2}^{6}4f_{7/2}^{7}5d_{5/2})_{1}-(4s^24p^{6}4d^{10}4f_{5/2}^{5}4f_{7/2}^{8}5f_{5/2})_{0}$ transition, which is calculated to occur near 67 Å.²⁵ The excitation energy for the 4f-5f monopole transition is calculated to be 608 eV. From Eq. (2) we estimate that the collision strength near threshold for monopole excitation will be 0.22. Although the Nd-like sequences will not be of particular use in the quest for a sub-44-Å laser, it is clear from the present discussion and from a consideration of the pump laser power required to produce Nd-like ions (such ions are much easier to generate than their Ni-like or Ne-like analogs given a desired x-ray laser wavelength) that the collisional excitation scheme in Nd-like ions will be extremely important for longer-wavelength laboratory x-ray lasers.

SUMMARY AND CONCLUSIONS

We have examined the scaling of strong monopole excitation in the outermost subshell of highly ionized closed-shell ions, both as a function of Z and of sequence. We find that the collision strengths scale principally with the number of subshell electrons and are inversely proportional to the threshold excitation energy (consistent with the usual "hydrogenic" scaling law). Our expression for the collision strength [Eq. (2)] includes both a factor $\xi_{nl}(Z)$ which varies primarily with subshell as shown in Fig. 1 and a factor $\eta_{nl}(Z)$ which takes into account the dilution of the principal monopole excitation due to mixing between the two J=0 singly excited states (and is given in Fig. 2).

Total monopole collisional excitation is more effective in the nickel-like sequences than in the neonlike sequence by about 25% on a per electron basis. Additionally, the stronger of the two nickel-like monopole transitions is less diluted by the effects of mixing than the analog in the neonlike sequence at the same excitation energy. We propose that further advantages could be obtained through use of Nd-like sequence. The nickel-like sequence appears to be attractive for obtaining lasing below 44 Å, while the Nd-like sequence will be most important at longer wavelengths.

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