## Comments and Addenda

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# Systematic trends for the oscillator strengths of resonance transitions in the Cu and Zn isoelectronic sequences

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New systematic trend curves for the oscillator strengths of the $4s$-$4p$ resonance transitions of Cu- and Zn-like ions have been derived from a critical analysis. This analysis takes into account recent theoretical results as well as a simulation study of cascade effects in beam-foil experiments which showed that the currently available experimental data for high ions may be too low by as much as 40–70%. The new analysis yields reliable interpolated data for many ions within the Cu and Zn isoelectronic sequences.

## I. INTRODUCTION

The principal resonance lines of the Cu and Zn isoelectronic sequences are important spectral features for the diagnostics and modeling of high-temperature magnetically confined plasmas. Many such plasmas contain heavy element impurities (Mo, W), produced by wall bombardment, which are sufficiently ionized to lie in the Cu- and Zn-like isoelectronic sequences. These ionic species are especially attractive for diagnostic purposes since their spectra are quite simple and the principal resonance lines are prominent transitions. Furthermore, the upper levels associated with these lines are so close to the ground state that in the usually encountered coronal plasma regime very strong collisional excitation takes place, producing high line intensities.

Some time ago we studied the oscillator strength data for the resonance lines of Cu-like ions and found large systematic discrepancies between beam-foil experimental data and calculations.[1] Subsequently, due mainly to this discrepancy and the increasing importance of these transitions, additional improved measurements and calculations were undertaken which narrowed the difference but still left the calculated oscillator strength data a substantial 40% and 70% above the measurements for the higher ions of the Cu and Zn sequences, respectively. Suspecting a major problem with the experimental approach, we undertook a detailed analysis and simulation study of beam-foil lifetime experiments, and found that the measured data may indeed be seriously deficient, producing $f$ values significantly too small. Based on the conclusions of that study we now present new critically analyzed systematic trend curves which should provide much more reliable interpolated data.

## II. EXISTING DATA

On the theoretical side, Fischer[3] has computed $f$ values by the multiconfiguration-Hartree-Fock (MCHF) method for a number of ions in the Cu isoelectronic sequence, using wavelengths corrected for relativistic effects according to the Pauli approximation. Correlation between the $4l$ electron and the core, which was neglected in earlier calculations but which was suspected to have significant effects, was included and reduced the values by 25% or more. Good agreement was obtained between theory and experiment at the neutral end of the trend, but there still remained a (10–40)% discrepancy for Ga III and higher ions. Independent calculations by one of us[4] using many-body diagrammatic perturbation theory confirm Fischer's results. Migdalek[5] has recently computed oscillator strengths for a number of transitions of Ga III using a semiempirical relativistic potential, but without explicit correlation. Since correlation effects reducing the $f$ value are large for low ions, it is not surprising that his results are higher than those of Fischer.

For the Zn sequence, Weiss[6] has calculated oscillator strengths for many low-lying transitions using superposition of configuration wave functions in intermediate coupling. Shorer[7] has applied the relativistic random-phase approximation to the computation of excitation energies and oscillator strengths for three transitions from the ground state. Both of these calculations include only correlation within the $n=4$ shell. Very recent calculations by Fischer and Hansen[8] include core polarization in addition to $n=4$ correlation, and utilize experimental wavelengths where available to compute oscillator strengths.

On the experimental side, several new beam-foil measurements[9-12] for Cu- and Zn-like Kr and Br ions have been reported since our earlier analysis. These generally conform with existing beam-foil data, confirming the earlier indicated large discrepancies between theoretical and experimental results.

## III. ANALYSIS

In our earlier paper on the oscillator strength situation for the Cu and Zn sequence resonance lines,[1] we suggested two likely reasons for the large discrepancy between data from beam-foil experiments and theoretical calculations. These were the neglect of correlation effects in the theoretical work and the inadequate treatment of cascading effects in beam-foil experiments. (The latter constitutes the only currently available experimental approach for the higher ions of the sequences.) Recent calculations[3,4,6,7] show that correlation effects now taken into account indeed have a significant effect, reducing Hartree-Fock values by 25% (even more at the neutral end of the sequence). Although there is now good agreement between theory and experiment for the lowest ions, there still exist large systematic discrepancies for higher ions which do not appear to be caused by correlation effects.

In order to analyze the experimental beam-foil lifetime data for the more highly ionized species, we have recently undertaken a detailed simulation of the cascade problem in heavy ion lifetime measurements.[2] As our main example, we chose the $4p\,^2P$ state of Kr VIII, for which a detailed measured beam-foil decay curve is available.[12] Our assumptions for the values of the calculated transition probabilities of cascade transitions and for the distribution of the initial populations of the excited states could be checked by comparison of our simulation with the experimental curve. A model for the population distribution was found which accurately reproduced the experimental decay curve at both short and long times, and which was consistent with other experimental studies of population distributions. The main result of the study was that once the decay curve is constructed, one is not able to extract from it by the usual cascade analysis, i.e., a two-exponential fit with both the coefficients and exponents as variables, the actual primary lifetime used in constructing it. The lifetimes which were extracted, however, were in good agreement with those derived from the experimental decay curve. Thus for Kr VIII, the average of four beam-foil lifetimes is 0.36 nsec; the simulation result is 0.35 nsec, but the primary tabulated lifetime used in the simulation is 0.26 nsec or 40% smaller. An analogous simulation study has been carried out by us for the $4p$ level of the Zn sequence. Here the simulation is complicated by the presence of doubly excited $4p^2$ states, for which it is obviously difficult to model initial populations. Nevertheless, this simulation yields results analogous to those for the Cu sequence. We propose that similar situations actually occur in beam-foil experiments on heavy ions, and that this is the principal cause of remaining discrepancies. It should be emphasized that such cascading occurs through a rather complex scheme involving many high angular momentum states. The effects are rather subtle and cause, for example, the initial important part of the decay curve to be approximately linear in a semilog presentation as one would expect from an apparently cascade-free lifetime.

## IV. RESULTS FOR THE NEW SYSTEMATIC TRENDS

Based on the above discussions, we present in Figs. 1 and 2 new systematic trends for the oscil-

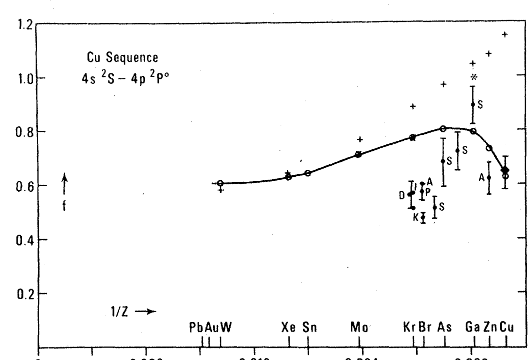


FIG. 1. Systematic trend for the resonance transition $4s\,^2S$–$4p\,^2P^0$ of the Cu isoelectronic sequence. ◆, critical compilation, Ref. 13; ●, beam-foil data: $P$, Ref. 9; $K$, Ref. 10; $I$, Ref. 11; $D$, Ref. 12; $A$, Ref. 14; $S$, Ref. 15; $A'$, Ref. 16; ○, MCHF, Ref. 3; ×, many-body diagrammatic perturbation theory, Ref. 4; *, semiempirical, Ref. 5; HF, Ref. 6.

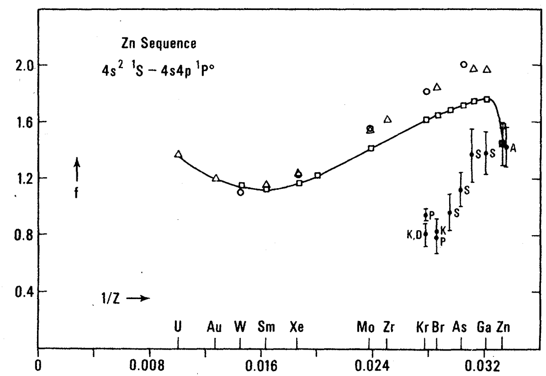


FIG. 2. Systematic trend for the resonance transtion $4s^{2}\,{}^{1}S-4s4p\,{}^{1}P^{0}$ of the Zn isoelectronic sequence. ■, absorption, Ref. 17; ●, beam foil: *P*, Ref. 9; *D*, Ref. 12; *K*, Ref 10; *A*, Ref. 14; *S*, Ref. 15; Δ, RPA, Ref. 7; o, SOC, Ref. 6; □, MCHF, Ref. 8.

lator strengths of the $4s$-$4p$ transitions of the Cu and Zn sequences. In view of the results of our beam-foil cascade analysis, we lean heavily toward the new theoretical data, except for the neutral atoms. The almost-exact agreement of the results of several different theoretical approaches in each sequence is a strong indication that correlation effects have been accurately evaluated. The systematic trend curves are estimated to be accurate to within 25% for the indicated range, and should be most accurate for the lower ions. Approximate relativistic corrections to the line strengths, which become important at about $Z \sim 50$, are included in the graphs.

## ACKNOWLEDGMENT

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