

# Relativistic Many-Body Calculations of Multipole (E1, M1, E2, M2, E3, M3) Transition Wavelengths and Rates between Excited and Ground States in Nickel-Like Ions

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## Abstract

Wavelengths, transition rates, and line strengths are calculated for the 76 possible multipole (E1, M1, E2, M2, E3, M3) transitions between the  $3l-15l'$  excited states and ground state in Ni-like ions with the nuclear charges ranging from  $Z = 30$  to 100. Relativistic many-body perturbation theory (RMBPT), including the Breit interaction, is used to evaluate energy and transition rates for multipole transitions in hole-particle systems. This method agrees with multi-configuration Dirac-Fock (MCDF) calculations in lowest-order, includes all second-order correlation corrections and includes corrections from negative energy states. The calculations start from a  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$  Dirac-Fock potential. These atomic data are important in fusion-related research involving heavy ions.

## Keywords:

multipole transition, excitation energy, Breit, RMBPT, Ni-like, hole-particle system

## 1. Introduction

Atomic data for multipole transitions in heavy ions are extremely important for plasma and fusion research. In particular, radiative properties of W and Au are actively studied in fusion-related research such as in Tokamak and in hot dense Z-pinch and laser plasmas. Ni-like ions are the main contributors into M-shell spectra of W and Au. While  $3l-4l'$  transitions in Ni-like ions are mostly likely optically thick and the relevant atomic data have been published elsewhere (see, for example, [1-4]),  $3l-5l'$  transitions (in about 10 times less in intensities than  $3l-4l'$ ) are very good candidates for M-shell diagnostics in the X-ray spectral region. Ni-like spectra of W produced at LLNL electron beam ion trap device EBIT-I have been recently studied in details [5]. They were recorded with the calorimeter which provides a broad spectral range from 3 to 8 Å and at the beam energy  $E_b = 3.9$  keV which provides the dominance of Ni-like ions.  $3l-4l'$  transitions were observed together with  $3l-5l'$  transitions, which were more intense than in laboratory plasmas.

Relativistic many-body perturbation theory (RMBPT) was used recently to study atomic characteristics of particle-hole excitations of closed-shell ions [1,2,6,7]. Reduced matrix elements, oscillator strengths, and transition rates into the ground state for all allowed and forbidden electric- and magnetic-dipole

and electric- and magnetic-quadrupole transitions (E1, M1, E2, M2) in Ne-like ions were presented in Refs. [6,7]. The second-order RMBPT calculations in Ni-like ions was used in Refs. [1,2] to determine excitation energies and E1, M1, E2, M2 transition rates for  $3l-4l'$  transitions.

In the present paper, relativistic many-body perturbation theory (RMBPT) is used to determine energies of  $3s^2 3p^6 3d^9 5l(J)$ ,  $3s^2 3p^5 3d^{10} 5l(J)$ , and  $3s 3p^6 3d^{10} 5l(J)$  states of Ni-like ions with nuclear charges  $Z = 30-100$ . The calculations are carried out to second order in perturbation theory. We consider all possible  $3l$  holes and  $5l$  particles leading to the 67 odd-parity  $3d^{-1} 5p(J)$ ,  $3d^{-1} 5f(J)$ ,  $3p^{-1} 5s(J)$ ,  $3p^{-1} 5d(J)$ ,  $3p^{-1} 5g(J)$ ,  $3s^{-1} 5p(J)$ , and  $3s^{-1} 5f(J)$  excited states and to the 74 even-parity  $3d^{-1} 5s(J)$ ,  $3d^{-1} 5d(J)$ ,  $3d^{-1} 5g(J)$ ,  $3p^{-1} 5p(J)$ ,  $3p^{-1} 5f(J)$ ,  $3s^{-1} 5s(J)$ ,  $3s^{-1} 5d(J)$  and  $3s^{-1} 5g(J)$  excited states in Ni-like ions with  $Z = 30$  to 100.

Relativistic MBPT is used to determine line strengths, oscillator strengths, and transition rates for all allowed and forbidden electric-multipole and magnetic-multipole (E1, E2, E3, M1, M2, M3) from  $3s^2 3p^6 3d^9 5l(J)$ ,  $3s^2 3p^5 3d^{10} 5l(J)$ , and  $3s 3p^6 3d^{10} 5l(J)$  excited states into the ground state in Ni-like ions. Retarded E1, E2, and E3 matrix elements are evaluated in both length and velocity forms.

## 2. Method

Details of the RMBPT method were presented in Ref. [1,6] for calculation of energies of hole-particle states and in Refs. [1,2,7] for calculation of radiative electric-dipole, electric-quadrupole, magnetic-dipole, and magnetic-quadrupole rates in Ne- and Ni-like systems. The calculations are carried out using sets of basis Dirac-Fock (DF) orbitals. The orbitals used in the present calculation are obtained as linear combinations of B-splines. These B-spline basis orbitals are determined using the method described in Ref. [8]. We use 50 B-splines of order 10 for each single-particle angular momentum state and we include all orbitals with the orbital angular momentum  $l \leq 9$  in our basis set.

When starting calculations from relativistic DF wavefunctions, it is natural to use  $jj$  designations for uncoupled transition and energy matrix elements; however, neither  $jj$  nor  $LS$  coupling describes the *physical* states properly, except for the single-configuration state  $3d_{5/2}5g_{9/2}(7) \equiv 3d5g^3I_7$ .

## 3. Energy of levels

Energies, relative to the ground state, of odd-parity states with  $J = 1$  and 2, divided by  $(Z - 21)^2$ , are shown in Fig. 1. It should be noted that  $Z$  was decreased by 21 to provide better presentation of the energy diagrams. We plot the limited number of energy levels to illustrate  $Z$  dependence choosing one representative from each configuration. As a result, we show 6 levels instead of 68 in Fig. 1. The  $LS$  designations are chosen by small values of multiplet splitting for low- $Z$  ions. To confirm those  $LS$  designations we obtain the fine structure splitting for the  $3f5f^3L$  triplets.

Energy differences between levels of odd- and even-parity triplet terms, divided by  $(Z - 21)^2$ , are shown in Fig. 2. The energy intervals for the  $3d5f(^3P_1 - ^3P_0)$  and  $3d5f(^3P_2 - ^3P_1)$  states are very small and almost do not change with  $Z$  as can be seen from Fig. 1. Similar  $Z$  dependence is found for the energy intervals for the  $3d5p(^3P_2 - ^3P_1)$ ,  $3d5p(^3D_3 - ^3D_2)$ ,  $3d5p(^3F_3 - ^3F_2)$ ,  $3d5f(^3G_4 - ^3G_3)$ ,  $3d5f(^3G_5 - ^3G_4)$ ,  $3d5f(^3H_5 - ^3H_4)$ , and  $3p5s(^3P_1 - ^3P_0)$  states.

Our calculations show that the fine structures of almost all levels do not follow the Landé rules even for small  $Z$ . The unusual splittings are principally due to changes from  $LS$  to  $jj$  coupling, with mixing from other triplet and singlet states. The different  $J$  states are mixed differently. Further experimental confirmation would be very helpful in verifying the correctness of these sometimes sensitive mixing parameters.

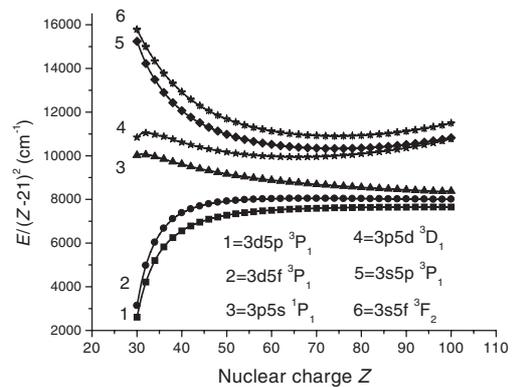


Fig. 1 Energies ( $E/(Z-21)^2$ ) in  $\text{cm}^{-1}$  for odd-parity states as functions of  $Z$ .

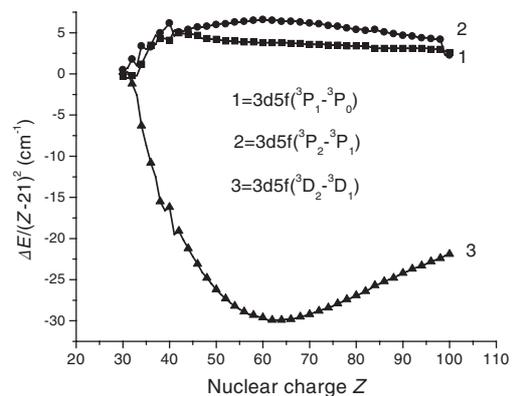


Fig. 2 Energy splitting ( $\Delta E/(Z-21)^2$ ) in  $\text{cm}^{-1}$  for terms of odd-parity states as function of  $Z$ .

## 4. Electric-dipole, electric-quadrupole, and electric-octupole matrix elements

We calculate electric-dipole (E1) matrix elements for the transitions between the 13 odd-parity  $3d_j5p_{j'}(1)$ ,  $3d_j5f_{j'}(1)$ ,  $3p_j5s_{1/2}(1)$ ,  $3p_j5d_{j'}(1)$ , and  $3s_{1/2}5p_{j'}(1)$  excited states and the ground state, electric-quadrupole (E2) matrix elements between the 17 even-parity  $3d_j5s_{1/2}(2)$ ,  $3d_j5d_{j'}(2)$ ,  $3d_j5g_{j'}(2)$ ,  $3p_j5p_{j'}(2)$ ,  $3p_j5f_{j'}(2)$ , and  $3s_{1/2}5d_{j'}(2)$  excited states and the ground state, and electric-octupole (E3) matrix elements between the 15 odd-parity  $3d_j5p_{j'}(3)$ ,  $3d_j5f_{j'}(3)$ ,  $3p_j5s_{1/2}(3)$ ,  $3p_j5d_{j'}(3)$ ,  $3p_j5g_{j'}(3)$ , and  $3s_{1/2}5f_{j'}(3)$  excited states and the ground state in Ni-like ions with nuclear charges  $Z = 30 - 100$ . Analytical expressions for multipole matrix elements in the first and the second order RMBPT are given in Refs. [1,2].

Transition rates for the four E1 lines from  $3d5f^3P_1$ ,  $^3D_1$ ,  $^1P_1$  and  $3p5s^1P_1$  levels to the ground state are plotted in Fig. 3. The sharp features in the curves shown in these figures can be explained in many cases by strong mixing of states inside the odd-parity complex with  $J = 1$ . In Fig. 3, the double cusp in the interval  $Z = 57 - 59$  is due to mixing of the  $3d_{5/2}5f_{5/2}(1)$

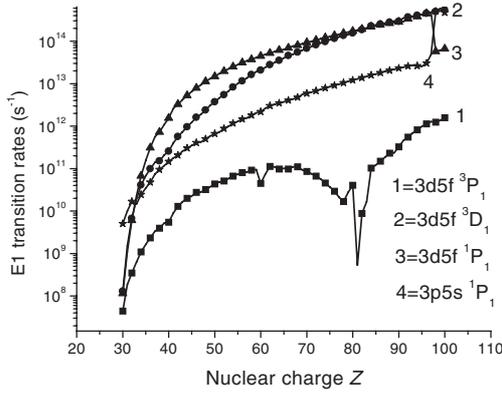


Fig. 3 E1 transition rates for transitions between the  $3/5l'$  odd-parity states with  $J=1$  and the ground state.

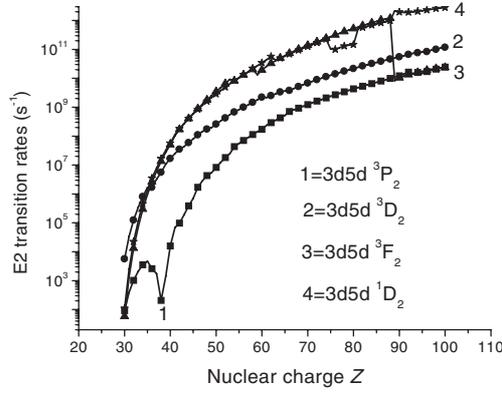


Fig. 4 E2 transition rates for transitions between the  $3/5l'$  even-parity states with  $J=2$  and the ground state.

and  $3d_{5/2}5f_{7/2}$  (1) states. The mixing of the  $3d_{5/2}5f_{7/2}$  (1) and  $3d_{3/2}5f_{5/2}$  (1) states in the  $Z = 55 - 56$  range gives a singularity in the curve with the  $3d5f\ ^3D_1$  label. The mixing of the  $3d_{3/2}5f_{5/2}$  (1) and  $3p_{3/2}5s_{1/2}$  (1) states in the  $Z = 49 - 50$  range gives a singularity in the curves with the  $3d5f\ ^1P_1$  and  $3p5s\ ^1P_1$  labels.

Transition rates for the four E2 lines from  $3d5d\ ^3P_2$ ,  $^3D_2$ ,  $^3F_2$ ,  $^1D_2$  levels to the ground state are plotted in Fig. 4.

## 5. Magnetic-dipole, magnetic-quadrupole, and magnetic-octupole matrix elements

We calculate magnetic-dipole (M1) matrix elements for the transitions between the 13 even-parity  $3d_j5s_{1/2}(1)$ ,  $3d_j5d_j(1)$ ,  $3d_j5g_j(1)$ ,  $3p_j5p_j(1)$ ,  $3p_j5f_j(1)$ ,  $3s_{1/2}5s_{1/2}(1)$ , and  $3s_{1/2}5d_j(1)$  excited states and the ground state, magnetic-quadrupole (M2) matrix elements between the 16 odd-parity  $3d_j5p_j(2)$ ,  $3d_j5f_j(2)$ ,  $3p_j5s_{1/2}(2)$ ,  $3p_j5d_j(2)$ ,  $3p_j5g_j(2)$ ,  $3s_{1/2}5p_j(2)$ , and  $3s_{1/2}5f_j(2)$  excited states and the ground state, and magnetic-octupole (M3) matrix

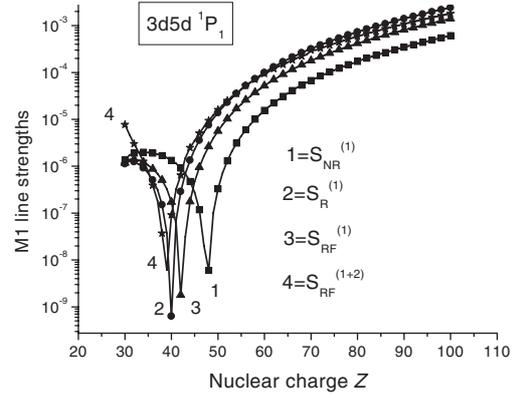


Fig. 5 The total M1 line strengths ( $S_{RF}^{(1+2)}$ ) between the  $3d5d\ ^1P_1$  and the ground states in Ni-like ions as function of  $Z$ .

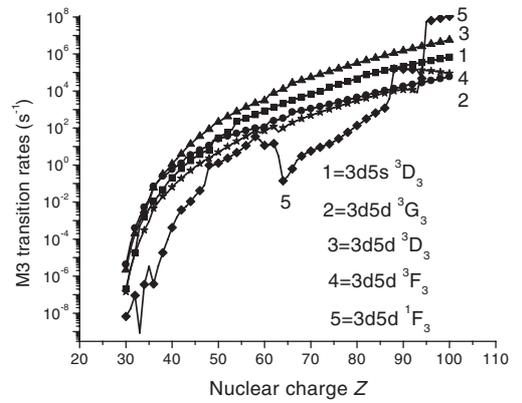


Fig. 6 M3 transition rates for transitions between the  $3/5l'$  even-parity states with  $J=3$  and the ground state.

elements for the transitions between the 16 even-parity  $3d_j5s_{1/2}(3)$ ,  $3d_j5d_j(3)$ ,  $3d_j5g_j(3)$ ,  $3p_j5p_j(3)$ ,  $3p_j5f_j(3)$ , and  $3s_{1/2}5d_j(3)$  excited states and the ground state in Ni-like ions with nuclear charges  $Z = 30 - 100$ .

In Fig. 5, we illustrate the  $Z$ -dependence of the line strengths of M1 transition from the  $3d5d\ ^1P_1$  excited state to the ground state. In this figure, we plot the values of the first-order line strengths  $S_{NR}^{(1)}$ ,  $S_R^{(1)}$ , and  $S_{RF}^{(1)}$  calculated in nonrelativistic, relativistic frequency-independent, and relativistic frequency-dependent approximations, respectively. The total  $S^{(1+2)}$ , which include second-order corrections, are also plotted. Strong mixing between  $3d_{5/2}5d_{3/2}(1)$  and  $3d_{5/2}5d_{5/2}(1)$  states occurring for small  $Z$  leads to the sharp features in the line strengths seen in the graphs. The deep minimum in Fig. 5 shifts when different approximations are used for the calculation of line strengths. This shift in the placement of the minimum leads to difficulties in comparison of data for M1 transitions obtained in nonrelativistic and relativistic approximations.

Transition rates for the five M3 lines from  $3d5s\ ^3D_3$  and  $3d5d\ ^3G_3, ^3D_3, ^3F_3, ^1F_3$  levels to the ground state are plotted in Fig. 6.

## 6. Conclusion

We have presented a systematic second-order relativistic RMBPT study of excitation energies, reduced matrix elements, line strengths, and transition rates for  $\Delta n = 1$  electric- and magnetic-dipole, electric- and magnetic-quadrupole, and electric- and magnetic-octupole transitions in Ni-like ions with nuclear charges  $Z = 30 - 100$ . Good agreement of our RMBPT data with other accurate theoretical results leads us to conclude that the RMBPT method provides accurate data for Ni-like ions. Results from the present calculations provide benchmark values for future theoretical and experimental studies of the nickel isoelectronic sequence. Ni-like lines dominate in M-shell spectra of heavy ions in X-ray region and atomic data in particular for W and Au are important in fusion research.

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