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Collisional excitation of neon-like Ni XIX using the Breit–Pauli *R*-matrix method

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Abstract. Collision strength for the transition within the first five fine-structure levels in Ni XIX are calculated using the Breit–Pauli *R*-matrix method. Configuration interaction wave functions are used to represent the target states included in the *R*-matrix expansion. The relativistic effects are incorporated in the Breit–Pauli approximation by including the one-body mass correction, Darwin and spin–orbit interaction terms in scattering equations.

Keywords. Collisional excitation; configuration interaction; Breit–Pauli *R*-matrix method.

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1. Introduction

In recent years, there has been great interest in the study of isoelectronic sequence of neon as ions of this very stable sequence occur in numerous types of plasmas, including astrophysical plasmas [1], magnetically-confined plasmas [2] and *Z*-pinch plasmas [3]. Recently, Feldman *et al* [4] have identified the $2s^2 2p^6 {}^3P_0$–$2s^2 2p^5 3s$ $^3P_1$ line of Ni XIX in solar flare spectra. Zhang *et al* [5] have reported the fine-structure collision strengths in Coulomb–Born exchange method for transitions from the ground state to $n = 3$ levels of many neon-like ions including Ni XIX, but to our knowledge, no results for collision strengths have been reported so far for the transitions within different fine-structure levels.

In the present work we have used the Breit–Pauli *R*-matrix method [6,7] to calculate the collision strengths for the transition within the first five fine-structure levels corresponding to the configurations $[1s^2]2s^2 2p^6({}^1S^e)$, $2s^2 2p^5 3s({}^1P^o_1,\ {}^3P^o_{0,1,2})$ in Ni XIX, which are represented by the configuration interaction (CI) wave functions.

2. Calculation

In the present scattering calculation on neon-like Ni XIX, the five lowest fine-structure levels belonging to the configurations $2s^2 2p^6 ({}^1S^e)$ and $2s^2 2p^5 3s ({}^1P^o_1, {}^3P^o_{0,1,2})$ are represented by configuration interaction wave functions [8] of the form

$$\Phi(J) = \sum_{i=1}^{M} a_i \phi_i(\alpha_i, LSJ), \tag{1}$$

where each of the single configuration function ϕ_i is constructed from one-electron orbitals (or spin-orbitals), whose angular momenta are coupled as specified by α_i (called the seniority number) to form states of given total L, S and J. The radial part of each orbital is written as a linear combination of normalized Slater-type orbitals (STO)

$$P_{nl}(r) = \sum_{i=1}^{k} c_i r^{p_i} \exp(-\zeta_i r). \tag{2}$$

The parameters $\{c_i\}$, $\{p_i\}$ and $\{\zeta_i\}$ in (2) and the mixing coefficients a_i in (1) are determined variationally. In our calculations, we have used seven orthogonal one-electron orbitals 1s, 2s, 2p, 3s, 3p, 3d and 4d. The parameters of the radial functions were optimized as follows. The 1s, 2s and 2p orbitals are taken as the HF orbitals of the ground state $1s^2 2s^2 2p^5\ {}^2P^o$ of iso-nuclear fluorine-like ion. The 3s orbital is optimized on $2s^2 2p^5 3s\ {}^3P^o$ state and the 3p orbital is optimized on the $2s^2 2p^6$ ground state, with configurations $2s^2 2p^6$ and $2s^2 2p^5 3p$, so that 3p acts as a first-order correction for the 2p orbital of the ground state. The optimization of 3d is done on $2s^2 2p^5 3s$ state, with configurations $2s^2 2p^5 3s$ and $2s^2 2p^5 3d$. The 4d orbital is optimized on the $2s^2 2p^5 3d\ {}^3P^o$ state, with configuration $2s^2 2p^5 3d$ and $2s^2 2p^5 4d$. The optimal value of parameters for non-HF orbitals are given in table 1. In table 2, we present the excitation threshold, calculated with our fairly simple wave functions which agree reasonably well with the experimental results [9]. Table 3 gives a list of the configurations included in the scattering calculations to represent the target state. The total wave function describing the $(N + 1)$-electron system

Table 1. Parameters of the radial functions of Ni XIX.

Orbitals	Power of r	Exponent	Coefficients
3s	1	20.60692	0.2312505
	2	8.98607	−1.1264039
	3	6.92923	1.6002710
3p	2	9.83896	2.3803094
	3	10.38145	−2.7699178
3d	3	13.18651	1.0000000
4d	3	14.11282	0.6332913
	4	7.81852	−1.1473076

Table 2. Configuration used in the CI expansion of Ni XIX.

Target states	Key no.	Configuration used
$^1S^e$	1	$[1s^2]2s^2 2p^6$, $[1s^2]2s^2 2p^5 3p$, $[1s^2]2s^2 2p^5 4p$, $[1s^2]2s2p^6 3d$
$^3P^o$	2, 4, 5	$[1s^2]2s^2 2p^5 3d$, $[1s^2]2s^2 2p^5 3s$ $[1s^2]2s^2 2p^5 4d$, $[1s^2]2s2p^6 3p[1s^2]2s2p^6 4p$
$^3P^o$	3	$[1s^2]2s^2 2p^5 3d$, $[1s^2]2s^2 2p^5 3s[1s^2]2s^2 2p^5 4d$, $[1s^2]2s2p^6 3p[1s^2]2s2p^6 4p$

in an inner region is expanded on a discrete basis of R-matrix states as discussed by Burke and Robb [10]. We have imposed a zero logarithmic derivative ($b = 0$) at the boundary radius $a = 2.20$ a.u. and we have retained 12 continuum orbitals for each angular symmetry to ensure convergence in the energy range considered here. In the outer region ($r \geq a$), it is important to take into account the long-range coupling between the channels. The resulting coupled equations are solved using a perturbation method developed by Seaton [11] to yield K matrix and then the collision strengths. In our calculations, we have considered all partial waves up to $L = 9$ for both parities and spin multiplicities (singlets and triplets).

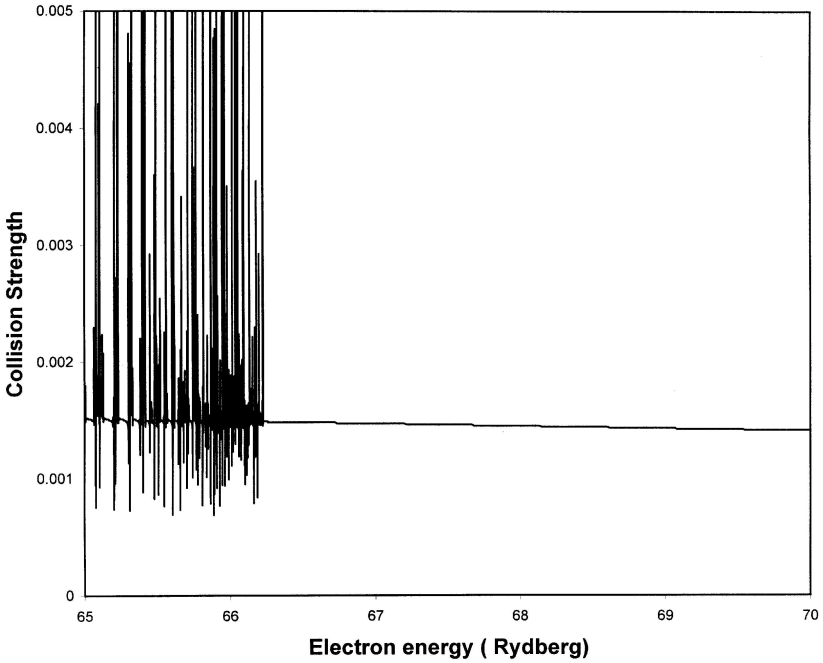

Figure 1. Total collision strength for the transition $1s^2 2s^2 2p^6\, ^1S^e$ to $1s^2 2s^2 2p^5 3s\, ^3P^o_2$ in Ni XIX as a function of the electron energy.

Table 3. Excitation threshold for Ni XIX (In Ryd).

Key	Level	State	J	Present	Expt.
1	$[1s^2]2s^22p^6$	$^1S^e$	0	00.00000	00.00000
2	$[1s^2]2s^22p^53s$	$^3P^o$	2	64.82234	64.73631
3	$[1s^2]2s^22p^53s$	$^1P^o$	1	65.00092	64.89123
4	$[1s^2]2s^22p^53s$	$^3P^o$	0	66.13064	
5	$[1s^2]2s^22p^53s$	$^3P^o$	1	66.22816	66.13419

Table 4. Collision strengths Ω in Ni XIX in the energy range 65 to 150 Ryd.

Transitions $(i \rightarrow f)$	$1 \rightarrow 2$	$1 \rightarrow 3$	$1 \rightarrow 4$	$1 \rightarrow 5$	$2 \rightarrow 3$
E (in Ryd)	Ω	Ω	Ω	Ω	Ω
65.0	1.475(−3)				
70.0	1.405(−3)	1.607(−3)	2.977(−4)	1.421(−3)	5.200(−2)
80.0	1.328(−3)	1.932(−3)	3.729(−4)	1.520(−3)	4.989(−2)
90.0	1.218(−3)	2.150(−3)	2.272(−4)	1.877(−3)	3.477(−2)
100.0	1.029(−3)	2.215(−3)	2.145(−4)	1.961(−3)	3.022(−2)
110.0	8.365(−3)	2.332(−3)	1.630(−4)	2.071(−3)	2.435(−2)
120.0	7.859(−4)	2.589(−3)	1.599(−4)	2.142(−3)	2.109(−2)
130.0	7.039(−4)	2.697(−3)	1.412(−4)	2.224(−3)	1.922(−2)
140.0	6.785(−4)	2.847(−3)	1.297(−4)	2.330(−3)	1.795(−2)
150.0	5.361(−4)	3.359(−3)	1.037(−4)	2.344(−3)	1.679(−2)
Transitions $(i \rightarrow f)$	$2 \rightarrow 4$	$2 \rightarrow 5$	$3 \rightarrow 4$	$3 \rightarrow 5$	$4 \rightarrow 5$
70.0	9.497(−3)	4.904(−2)	2.390(−2)	7.600(−2)	1.649(−2)
80.0	8.708(−3)	4.158(−2)	2.108(−2)	6.215(−2)	1.600(−2)
90.0	8.334(−3)	3.544(−2)	1.497(−2)	3.634(−2)	9.792(−3)
100.0	7.824(−3)	3.329(−2)	1.206(−2)	2.939(−2)	8.184(−3)
110.0	7.425(−3)	2.615(−3)	1.204(−2)	2.381(−2)	7.875(−3)
120.0	6.967(−3)	2.383(−2)	7.989(−3)	1.829(−2)	5.558(−3)
130.0	6.895(−3)	2.222(−2)	6.910(−3)	1.630(−2)	4.860(−3)
140.0	6.867(−3)	2.120(−2)	6.155(−3)	1.505(−2)	4.411(−3)
150.0	6.456(−3)	2.100(−2)	5.083(−3)	1.381(−2)	2.344(−3)

3. Results and discussion

Figure 1 illustrates the results for the excitation from the ground state $1s^22s^22p^6\ ^1S^e$ to the first excited state $1s^22s^22p^53s\ ^2P^o_2$ as a function of incident electron energy (in Ryd). It clearly shows that at low energies, the collision strengths are dominated by close channel (or Feshback) resonances. These resonances converge to threshold beyond the first excited state. In table 4 we present the total collision strength

Table 5. Comparison of fine-structure collision strengths obtained by Zhang *et al* (Ω_z) with our results (Ω).

Transitions ($i \to f$)	$1 \to 2$	$1 \to 2$		$1 \to 3$	$1 \to 3$
E (Ryd)	Ω	Ω_z	E (Ryd)	Ω	Ω_z
77.67	1.334(−3)	1.13(−3)	77.85	1.878(−3)	1.88(−3)
97.09	1.104(−3)	9.04(4)	97.31	2.171(−3)	2.28(−3)
122.98	7.711(−4)	6.90(−4)	123.26	2.619(−3)	2.85(−3)
161.82	4.648(−4)	4.84(−4)	161.82	3.712(−3)	3.70(−3)
Transitions ($i \to f$)	$1 \to 4$	$1 \to 4$		$1 \to 5$	$1 \to 5$
79.29	2.872(−4)	2.27(−4)	79.35	1.489(−3)	1.56(−3)
99.06	2.170(−4)	1.87(−4)	99.19	1.83(−3)	1.84(−3)
125.64	1.570(−4)	1.38(−4)	125.64	2.166(−3)	2.25(−3)
165.09	9.097(−5)	9.68(−5)	165.31	2.862(−3)	2.87(−3)

at incident electron energies from 65 to 150 Ryd for all transitions within the first five fine-structure levels corresponding to $1s^2 2s^2 2p^6\ ^1S^e$ and $1s^2 2s^2 2p^5 3s(^1P^o, ^3P^o)$ configurations of Ni XIX. As shown in table 4, among the transitions from the ground state, the transition 1 to 3, i.e. $^1S^e$ to $^1P^o$ transition has the largest collision strength as it is dipole-allowed (E1) transition and corresponds to excitation of electron from 2p state to 3s state. For the transitions from the first excited state we find that the collision strength for $^3P^o_2$ to $^3P^o_0$ (i.e., 2 to 4) is lowest as it corresponds to electric quadruple transitions. Other two transitions from first excited state (i.e. 2 to 3 and 2 to 5) have large collision strength. The magnetic dipole transition from 4 to 5, i.e. $^3P^o_0$ to $^3P^o_1$ which was observed recently in solar flare by Feldman *et al* [4] also has high collision strength. In table 5 we have compared our results with those obtained by Zhang *et al* [5] and found that there is reasonably good agreement between the two calculations.

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