PRAMANA
— journal of
physics

Vol. 67, No. 3
September 2006
pp. C553–C557

Electron impact excitation collision strengths for neon-like Ni XIX calculated using the relativistic *R*-matrix method

K M AGGARWAL and F P KEENAN
Department of Physics and Astronomy, Queen's University, Belfast BT7 1NN, Northern Ireland, UK
E-mail: K.Aggarwal@qub.ac.uk

MS received 2 November 2005; accepted 15 April 2006

Abstract. In a recent paper [*Pramana – J. Phys.* **64**, 129 (2005)] results have been presented for electron impact excitation collision strengths for transitions among the fine-structure levels of the $2s^2 2p^6$ and $2s^2 2p^5 3s$ configurations of Ni XIX. In this paper we demonstrate through an independent calculation with the relativistic *R*-matrix code that those results are unreliable and the conclusions drawn are invalid.

Keywords. Collisional excitation; Dirac atomic *R*-matrix code.

PACS No. 34.80.Kw

1. Introduction

In a recent paper, Singh and Mohan [1] have presented results for electron impact excitation collision strengths (Ω) for transitions among the fine-structure levels of the $2s^2 2p^6$ and $2s^2 2p^5 3s$ configurations of Ni XIX. For their calculations they have adopted the CIV3 [2] and *R*-matrix [3] programs for the generation of wave functions and computations of Ω, respectively. Furthermore, they have included configuration interaction (CI) as well as relativistic effects in a Breit–Pauli approximation. In the present paper, we undertake an independent calculation for Ni XIX using the relativistic *R*-matrix code, and find large discrepancies with the Singh and Mohan's results for many transitions. We discuss these discrepancies in detail, and demonstrate that the Singh and Mohan's data are unreliable.

2. Collision strengths

For our calculations we have adopted an independent approach by employing the GRASP (general-purpose relativistic atomic structure package) [4] and DARC

(Dirac atomic R-matrix code) [5] programs for the generation of wave functions and the computations of collision strengths, respectively. Our calculations are fully relativistic and CI has been included as by Singh and Mohan [1]. All partial waves with angular momentum $J \leq 9.5$ have been included, which are found to be sufficient for the convergence of Ω for all the ten transitions under consideration here, and for the energy range of interest, i.e. below 150 Ryd. Additionally, this range of partial waves is similar to that of Singh and Mohan, who adopted $L \leq 9$.

To make comparisons meaningful with the reported results of Singh and Mohan [1], we have performed three sets of calculations with increasing complexity. In the first calculation (DARC1), we have included only the lowest five levels of the $2s^2 2p^6$ and $2s^2 2p^5 3s$ configurations, but CI has been included with the additional 22 levels of the $2s^2 2p^5 3p$ and $2s^2 2p^5 3d$ configurations. This calculation is similar to that of Singh and Mohan. In the second calculation (DARC2), we have included all the 27 levels in the $2s^2 2p^6$ and $2s^2 2p^5 3\ell$ configurations, mainly to demonstrate the effect of resonances in the threshold region. In the third calculation (DARC3), we have included all the 89 levels of the $2s^2 2p^6$, $2s^2 2p^5 3\ell$, $2s 2p^6 3\ell$, $2s^2 2p^5 4\ell$, and $2s 2p^6 4\ell$ configurations of Ni XIX. This calculation is comparatively more challenging as the Hamiltonian size increases up to 10086, but has been performed in order to check the consistency of the results, and to observe the effect of the inclusion of additional CI. Inclusion of a larger number of levels in a calculation not only improves the accuracy of wave functions, but also increases the range of threshold energies and subsequently of the resonances. Since our focus is on a limited range of transitions among the lowest five levels only, and in a limited range of electron energy above thresholds but below 150 Ryd, we find that all three sets of calculations yield values of Ω which agree within $\sim$10% for all transitions and at all energies. Therefore, for conciseness, we will focus on a comparison of results only between our DARC2 and the Breit–Pauli R-matrix calculations of Singh and Mohan [1].

In figures 1a and 1b we compare our results of Ω with those of Singh and Mohan [1] for a few transitions. For some of the transitions, such as $(2s^2 2p^5 3s)\ {}^1P^o_1$–$^3P^o_0$ (3–4) and $^1P^o_1$–$^3P^o_1$ (3–5, see table 3 of Singh and Mohan for level indices), the Ω values of Singh and Mohan differ from ours by over a factor of three, particularly at lower energies. At higher energies, all transitions from the ground state to the higher excited levels differ up to 30%, and their values of Ω are invariably lower, as shown in figure 1a. Not only do the magnitudes of Ω differ in the two independent (but similar) R-matrix calculations, but the behaviour of the Singh and Mohan's results is erratic as seen for many transitions, such as 1–3, 2–3 and 3–5. At energies above thresholds ($E \geq 67$ Ryd), values of Ω are expected to vary smoothly as shown by our calculations, and there is no reason to observe sudden changes in Ω, as found by Singh and Mohan. Based on this comparison, and the consistency of results observed in our three sets of calculations, we conclude that the Ω values reported by Singh and Mohan are unreliable.

Finally, in figure 2 we demonstrate resonances in the threshold regions for the $2s^2 2p^6\ {}^1S_0$–$2s^2 2p^5 3s\ {}^3P^o_2$ (1–2) transition of Ni XIX. This is an important transition as its emission line (λ 14.08 Å) has already been observed [6] in the spectrum of the solar corona. Our results in figure 2 are in clear contrast with the corresponding data in figure 1 of Singh and Mohan [1]. They observed that for this transition resonances have converged to thresholds beyond the first excited level, whereas

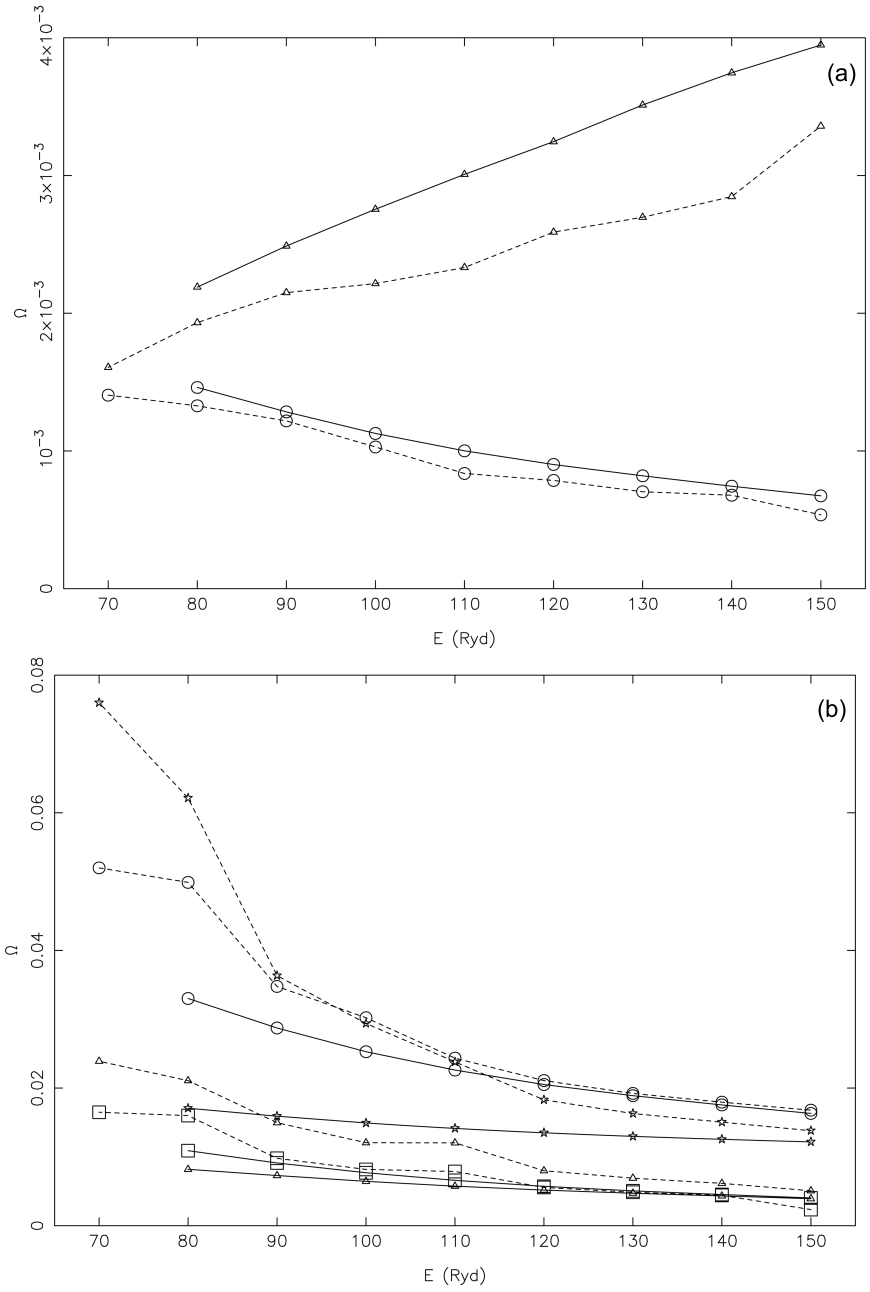

Figure 1. Collision strengths for transitions in Ni XIX. Continuous curves: present results, broken curves: Singh and Mohan [1]. (**a**) (○) $2s^22p^6\ {}^1S_0$–$2s^22p^53s\ {}^3P^o_2$ (1–2), (△) $2s^22p^6\ {}^1S_0$–$2s^22p^53s\ {}^1P^o_1$ (1–3). (**b**) (○) $2s^22p^53s\ {}^3P^o_2$–$2s^22p^53s\ {}^1P^o_1$ (2–3), (△) $2s^22p^53s\ {}^1P^o_1$–$2s^22p^53s\ {}^3P^o_0$ (3–4), (∗) $2s^22p^53s\ {}^1P^o_1$–$2s^22p^53s\ {}^3P^o_1$ (3–5), and (□) $2s^22p^53s\ {}^3P^o_0$–$2s^22p^53s\ {}^3P^o_1$ (4–5) transition.

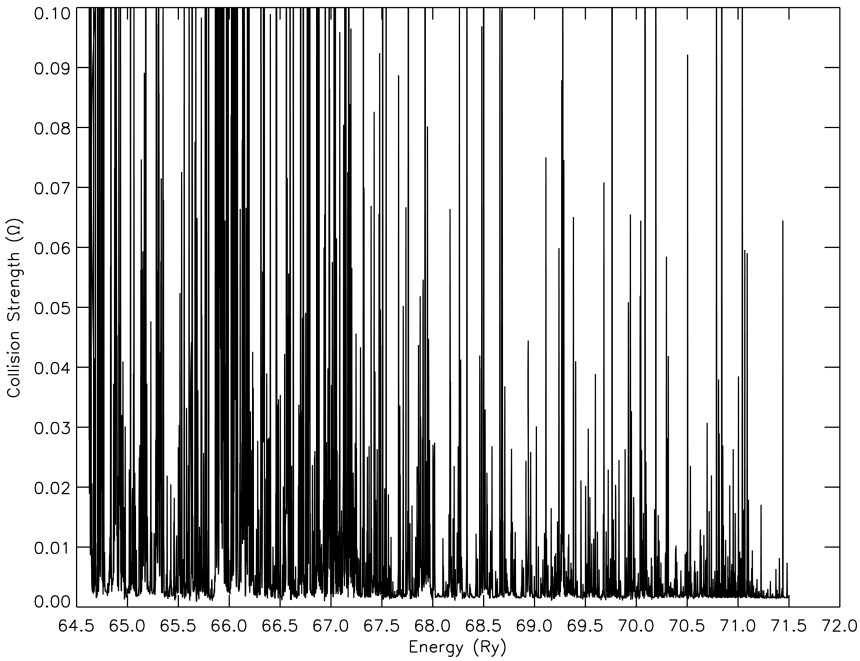

Figure 2. Collision strengths in the threshold regions for the $2s^2 2p^6\ {}^1S_0$–$2s^2 2p^5 3s\ {}^3P^o_2$ (1–2) transition of Ni XIX.

our calculations show that these are not converged even up to the $2s2p^5 3\ell$ levels. The reason they did not observe resonances beyond the $2s^2 2p^5 3s\ {}^3P^o_1$ level is that they did not include the higher excited levels in their collisional calculations. Since these closed-channel (Feshbach) resonances are spread over a wide range of energy (more than 7 Ryd as seen in figure 2), their contribution to the determination of excitation rates will be highly significant up to $T_e = 5 \times 10^6$ K, the temperature of maximum ion abundance for Ni XIX in ionization equilibrium [7]. For this very reason even a larger calculation, such as our 89 level one, is necessary in order to accurately determine values of collision strengths and subsequently excitation rates. The importance of a larger calculation can be appreciated from figure 12 of Chen *et al* [8], who have demonstrated resonances for the same 1–2 transition, but for Fe XVII which is a Ne-like system similar to Ni XIX.

3. Conclusions

In this short paper we have demonstrated the unreliability of the collisional data reported by Singh and Mohan [1] for transitions in Ni XIX. Not only do their values of Ω differ in magnitude for many transitions, but they also show unexplained erratic behaviour with energy. In order to accurately determine the collisional data, which are highly desired in the modelling and diagnostic calculations of plasmas, a significantly larger calculation than that performed by Singh and Mohan is desirable. To

fulfill this requirement our 89-level calculations are in progress, which will not only cover a wider range of transitions but also a wider range of energy/temperature. The detailed results from this larger calculation will be reported in a future publication. However, in the meantime, it is recommended that the distorted-wave atomic data for Ni XIX [9,10] continue to be employed for modelling purposes.

Acknowledgements

This work has been financed by the Engineering and Physical Sciences and Particle Physics and Astronomy Research Councils, and AWE Aldermaston of the United Kingdom. We thank Dr Patrick Norrington for making his code available to us prior to publication.

References

[1] N Singh and M Mohan, *Pramana – J. Phys.* **64**, 129 (2005)
[2] A Hibbert, *Comput. Phys. Commun.* **9**, 141 (1975)
[3] K A Berrington, W Eissner and P H Norrington, *Comput. Phys. Commun.* **92**, 290 (1995)
[4] K G Dyall, I P Grant, C T Johnson, F A Parpia and E P Plummer, *Comput. Phys. Commun.* **55**, 424 (1989)
[5] P H Norrington and I P Grant, *Comput. Phys. Commun.* (2006) (in preparation)
[6] M Loulergue and H Nussbaumer, *Astron. Astrophys.* **45**, 125 (1975)
[7] P Mazzotta, G Mazzitelli, S Colafrancesco and N Vittorio, *Astron. Astrophys. Suppl.* **133**, 403 (1998)
[8] G X Chen, A K Pradhan and W Eissner, *J. Phys.* **B36**, 453 (2003)
[9] H L Zhang, D H Sampson, R E H Clark and J B Mann, *At. Data Nucl. Data Tables* **37**, 17 (1987)
[10] H L Zhang and D H Sampson, *At. Data Nucl. Data Tables* **43**, 1 (1989)