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*LETTER TO THE EDITOR*

# ELECTRON IMPACT EXCITATION OF AUTOIONIZING LEVEL IN Na

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Electron-impact integral cross sections for the excitation of the lowest lying autoionizing level generated by the inner-shell $1s^2\ 2s^2\ 2p^6\ 3s\ {}^2S^e \rightarrow 1s^2\ 2s^2\ 2p^5\ 3s^2\ {}^2P^0$ complex transition in sodium (Na) atomic system have been calculated. In the calculation, single-configuration Hartree-Fock (HF) wave functions for both initial and final states involved in the transition matrix element within the asymptotic Green function approximation (AGFA) proposed by Tiwary (1981) were employed. The calculation was done exactly in the same way as in the earlier work in the case of the lightest alkali-metal atom lithium (Tiwary (1985), Tiwary, Macek and Madison (1985)) and the heaviest alkali-metal atom caesium (Tiwary (1983)) in the bombarding energy range from the threshold to 1500 eV. For the first time, Tiwary (1983) predicted the resonance behaviour in near vicinity of the excitation threshold in Cs using AGFA. Feuerstein et al. (1998) performed the experiment and observed resonance behaviour in the neighbourhood of excitation threshold in Na. Comparison has been made with available relevant experimental observations and other theoretical predictions. Our present AGFA theoretical result is qualitatively in accord with the experimental results.

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There has been a growing interest in the inner-shell excitation of alkali and alkaline earth metal atoms from both experimentalists and theorists because inner-shell

[1]This work was partly done while the author was Alexander von Humboldt (AvH) Fellow, Berlin, Germany.

excitation leads to autoionization which plays an important role in explaining the structure observed in the total ionization cross section curves for electron impact. Consequently, theoretical predictions of the cross sections of inner-shell excitation process in atoms or ions are of special interest. The contribution of autoionization to the direct ionization process is very important in alkali-metal atoms [1 – 41]. The scattering cross sections for the excitation of the autoionizing levels have been calculated in lithium (Li) and caesium (Cs) alkali-metal atoms [1, 3, 12, 18, 23, 25]. We applied the asymptotic Green function approximation (AGFA) [12, 23], the distorted wave Born approximation (DWBA) [25], the plane wave Born approximation (PWBA) [1], the Glauber approximation (GA) [18], the R-matrix method [17] and the Coulomb Born approximation (CBA) [23].

Our primary purpose of this work is to test the usefulness of AGFA and single configuration Hartree-Fock wave function to describe initial and final states involved in the inner-shell excitation transition by electron impact in sodium (Na I) atomic system. We have performed calculations for electron impact integral cross sections for the excitation of the lowest-lying autoionizing level in Na I using single-configuration Hartree-Fock wave functions for both initial and final states within the AGFA exactly in the same way as Tiwary [12] did in the case of Cs. Hence, the method is not given here.

Tiwary et al. [31] have also calculated the optical oscillator strengths (OOS) for the $1s^2\ 2s^2\ 2p^6\ 3s\ {}^2S^e \rightarrow 1s^2\ 2s^2\ 2p^5\ 3s^2\ {}^2P^0$ transition in Na I in both length and velocity forms ($f_L$ and $f_V$, respectively) exactly in the same way as in our earlier work [20] in order to examine the accuracy of the Hartree-Fock wave functions. We found that the Hartree-Fock length and velocity values of OOS differ considerably, which reflects that the Hartree-Fock wave functions are not adequate for such complex inner-shell excitation transition which leads to autoionization. We have treated the $1s^2\ 2s^2\ 2p^6\ 3s\ {}^2S^e \rightarrow 1s^2\ 2s^2\ 2p^5\ 3s^2\ {}^2P^0$ transition exactly in the same way as in our earlier work on alkali-metal atoms. The expressions for OOS are well known, hence they are not given here.

Figure 1 displays the present AGFA integral cross sections ($\sigma$) for the inner-shell excitation transition in the sodium atomic system by electron impact with the available experimental observations and other theoretical predictions. Several features of importance emerge from the figure.

First, the AGFA exhibits the resonance behaviour near the threshold as it displayed in the case of the cesium atomic system which is in a reasonably good agreement with the experimental curve, whereas PWBA differs significantly and qualitatively in the low and intermediate energy regions and in is good accord in the high energy range as is expected for the PWBA. It may be due to the fact that PWBA is not valid in the low and intermediate energy regions but is valid in the high energy range. Second, the AGFA curve tends to lie below the experimental curve in the entire energy range under consideration. It is probably due to the lack of configuration mixing, i.e., correlation and inadequacy of the AGFA in the low energy region. Third, cross section is sensitive to methods employed, e.g.,

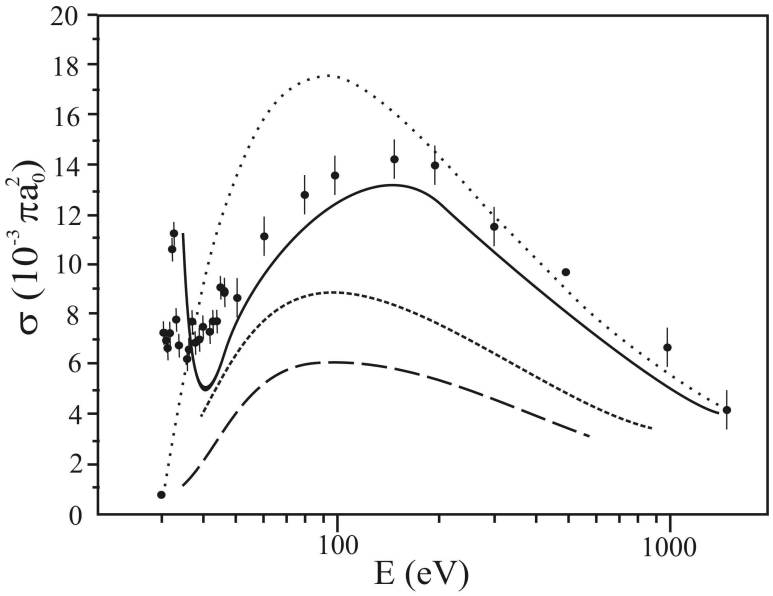


*Fig. 1. Integral cross section ($\sigma$) for* 2p–3s *excitation of* Na *as a function of electron impact energy E.*
*Legend:*

| | |
|---|---|
| ϕ | *experimental results, Feuerstein et al. (Ref. [41]),* |
| ····· | *PWBA, Feuerstein et al. (Ref. [41]),* |
| - - - - - | *PWBA, Pangantiwar and Srivastava (Ref. [30]),* |
| — — — — | *PWBA, Liepinsh and Peterkop (Ref. [9])* |
| ——— | *AGFA, present results.* |

PWBA, GA and Vainshtein, Presnykov and Sobelman approximation (VPSA) methods are not capable to produce resonance whereas the R-matrix method and AGFA are capable of producing resonance behaviour in the vicinity of the threshold.

In conclusion, our present theoretical investigation demonstrates that the AGFA is capable of producing resonance behaviour near threshold in the integral cross section curve which is qualitatively in good agreement with the available experimental data, whereas PWBA does not exhibit resonance character. Our calculated results also suggest that it is indispensable to take account of (1) the electron correlation, (2) the interaction between the autoionizing level and the associated continuum and (3) the modification of AGFA near the coordinate origin in order to get reliable cross sections for the inner-shell excitation, particulary in the low and intermediate incident energy regions. If these are feasible, the idea of using the asymptotic separability of the Green function could provide a significant advantage in more complex scattering calculations, e.g., in calculation of electron-molecule collisions.

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## UZBUDA AUTOIONIZACIJSKOG STANJA U Na UDAROM ELEKTRONA

Izračunali smo integralne udarne presjeke za uzbudu najnižeg autoionizacijskog stanja koje nastaje udarom elektrona te putem kompleksnog prijelaza $1s^2\ 2s^2\ 2p^6\ 3s\ {}^2S^e$ Q $1s^2\ 2s^2\ 2p^5\ 3s^2\ {}^2P^0$ među unutarnjim ljuskama u atomima natrija. U računu smo primijenili jedno-konfiguracijske Hartree-Fockove (HF) valne funkcije za odnosna početna i konačna stanja u matričnom elementu unutar asimptotskog približenja za Greenove funkcije (AGFA), predloženog Tiwary-em (1981). Račun je proveden točno na način kao u ranijem radu za najlakši alkalijski metalni atom litij (Tiwary (1985), Tiwary, Macek and Madison (1985)) i najteži alkalijski metalni atom cezij (Tiwary (1983)), za energije elektrona od praga do 1500 eV. Tiwary (1983) je prvi predvidio rezonanciju blizu iznad uzbudnog praga u Cs primjenom AGFA-e. Feuerstein et al. (1998) izveli su mjerenja i vidjeli rezonanciju u blizini uzbudnog praga u Na. Načinili smo usporedbu poznatih eksperimentalnih podataka i drugih teorijskih predviđanja. Naši su sadašnji teorijski rezultati u skladu s eksperimentalnima.