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ELASTIC SCATTERING OF ELECTRONS ON ATOMS WITH ONE VACANCY

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Abstract. In the framework of the random phase approximation (RPA) we investigate the process of slow elastic electron scattering on atoms with the vacancy in the closed shell. We calculated the differential cross section of the electron elastic (and quasi-elastic) scattering on the positive argon (Ar) ions.

1. INTRODUCTION

In this paper, we considered the method of calculation which is applicable to the processes of elastic scattering of electron by targets (signed by A^+) with the configuration which corresponds to one vacancy in the closed shell. This method (recently developed in Amusia et al. (1990) and Drukarev and Berezina (1975)) may be used in calculations for the processes of the inelastic scattering and some resonances, also. In the calculation we use the LS coupling. In the function of the total spin S for the system "electron + target" two cases are possible:

$$(e^- + A^+) \Leftrightarrow \text{system swith} \rightarrow \begin{cases} S = 0 \\ S = 1 \end{cases} \qquad (1)$$

The first case corresponds to the system where the intermedial and final state of atom has the closed shells; the second, corresponds to the triplet excitation of atom with the closed shells. The inter-electron interactions are responsible for the formation of the particle-hole pairs in the intermedial state of the elastic scattering $(e^- + A^+)$. By the presented method we may calculate the process of the spin-flip of the incident and atomic electron (the "quasi-elastic " collision (Amusia et al. 1990). The inter-electron interaction we calculated in the framework of the random phase approximation RPA (exactly, we use the improved version of the RPA (imRPA) Tancic 1998, Tancic and Davidovic 2006).

In the paper atomic system of units is used (energy is given in Ry).

2.THEORY

The system $(e^- + A^+)$ representS the particle-hole excitation of atom with closed shells. To described that we may using the many body theory. As the zero approximation, we use the Hartree-Fock (HF) approximation in which the particle is represented by the excitation state above the closed shells. We may calculated the wave function of the incident electron as the particle function φ_k^{N+1} (N -the number of the electrons in closed shells of the target; k - the momentum of the incident electron).The best approximation is approximation in which we calculated the wave function of incident electron in self-consistent HF atomic field with the hole in the state j. Then we have two approximation: HF1- the wave function of the incident electron φ_k^N (where averaging on the projections of the hole orbital momentum is performed); HF2- the wave function of incident electron is $\varphi_{(j)k}^{N(LS)}$ (the total orbital momentum L and spin S are fixed). The process of the particle scattering as a results of the Coulomb electron-vacancy interaction is presented in the Fig. 1. (the lines with arrow to the right (left) present the HF electronic (hole) state; the wavy line - the Coulomb interaction; the vertical arrow-the projection of the electron (hole) spin; $\nu_i \rightarrow n_i \ell_i m_i \mu_i$ - the set of quantum numbers. Fig. 1. describe the process of the elastic scattering of the polarized electrons on the polarized targets (Amusia et al. 1990).

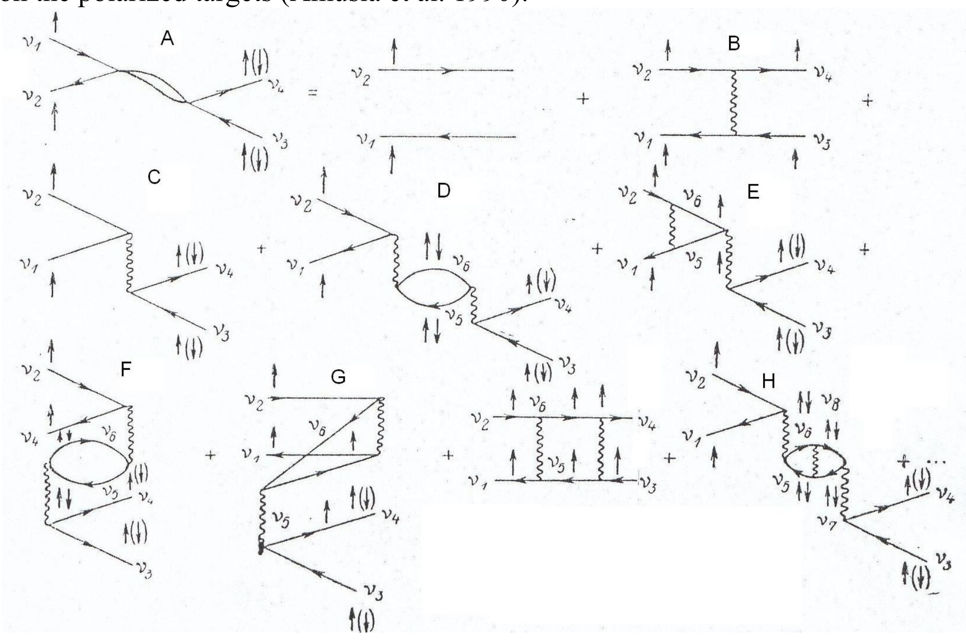

Figure 1: The particle-hole scattering in the RPA.

After some theoretical speculations, we obtain the analytical expression which corresponds some of the presented diagrams (Amusia et al. 1990, Tancic 1998, Tancic and Davidovic 2006, Amusia and Cherepkov 1975, Amusia and Chernisheva 1997):

$$\left\langle \nu_1\nu_4 \left|\Gamma(\omega)\right| \nu_2\nu_3 \right\rangle = \left\langle \nu_1\nu_4 \left|u\right| \nu_2\nu_3 \right\rangle - \left(\sum_{\substack{\nu_5 \le F \\ \nu_6 > F}} - \sum_{\substack{\nu_5 > F \\ \nu_6 \le F}} \right) \frac{\left\langle \nu_1\nu_6 \left|u\right| \nu_2\nu_5 \right\rangle \left\langle \nu_5\nu_4 \left|\Gamma(\omega)\right| \nu_6\nu_3 \right\rangle}{\omega - E_{\nu_5} + E_{\nu_6} + i\delta(1 - 2n_{\nu_5})} \tag{2}$$

The resolutions of the eq. (2) are the matrix elements of the interaction $\Gamma(\omega)$ in the particle-hole channel. If we choose the function $\varphi_{(j)k}^{N(LS)}$, the quantity $\left\langle .. \left|\Gamma(\omega)\right| .. \right\rangle$ is a function of the L and S. After integration over angular parts, we have (the details are given in Amusia et al. (1990), Amusia and Cherepkov (1975), Amusia and Chernisheva (1997)):

$$\left\langle n_1\ell_1, n_4\ell_4 \left\|\Gamma(\omega)\right\| n_2\ell_2, n_3\ell_3 \right\rangle \approx f(\left\langle ..,.. \left\|u^{LS}\right\| ..,.. \right\rangle; C\sum \left\langle ..,.. \left\|u^{LS}\right\| ..,.. \right\rangle \left\langle ..,.. \left\|\Gamma^{LS}(\omega)\right\| ..,.. \right\rangle) \tag{3}$$

where C is some constant (Amusia et al. 1990). The reduced matrix elements of u^{LS} are the radial parts of the functions $\varphi_{(j)k}^{N(LS)}$ and they are obtained by the special programs (Amusia and Cherepkov 1975, Amusia and Chernisheva 1997). The asymptotic of the radial function is given by the sum of the scattering phases on the Coulomb and HF potentials. According to the particle-hole effective interaction we obtain the phase shifts (Tancic 1998, Tancic and Davidovic 2006, Amusia and Cherepkov 1975, Amusia and Chernisheva 1997):

$$\exp[i\Delta\delta_{\ell\ell_j}^{LS}(k,n_j)]\sin\Delta\delta_{\ell\ell_j}^{LS}(k,n_j) = -(\pi/(2L+1))\left\langle n_j\ell_j, \varepsilon\ell \left\|\Gamma^{LS}(E)\right\| \varepsilon\ell, n_j\ell_j \right\rangle \tag{4}$$

where are: ε - the energy of the incident electron; $E = \omega = \varepsilon - E_j$ (E_j is the hole energy, and E ionization energy for the elastically scattered electron). Below the first discrete excitation level, the phase shifts, and the total phase shifts $\delta_{\ell\ell_j}^{LS}(k,n_j)$ are real.

3. RESULTS

In Fig. 2 we presented results of the calculations of the cross sections (c.s.) for the $e^- + Ar^+$ scattering (Amusia et al. 1990, Tancic 1998, Tancic and Davidovic 2006). Analogous to the recently presented results in Amusia et al. (1990), we take into account 5 partial waves in singlet and triplet channels ($\ell = 0, L = 1; \ell = 1, L = 0; \ell = 1, L = 2; \ell = 2, L = 1; \ell = 2, L = 3$). In Fig. 2A we have the results of the calculations of the differential cross sections in the HF1, HF2 and Coulomb approximation (Amusia et al. 1990).

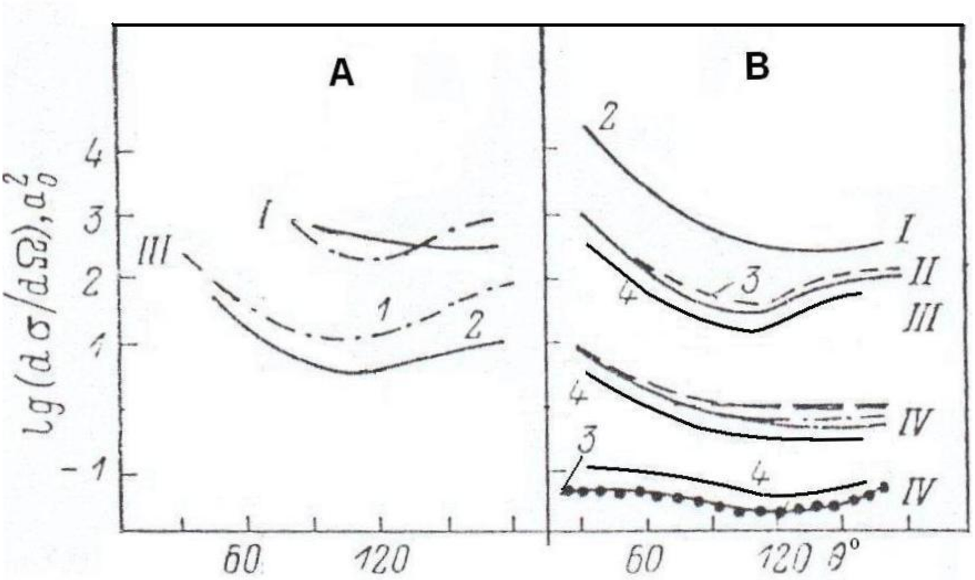

Figure 2A,B: - the differential cross sections (d.c.s.) of the $e^- + Ar^+$ scattering: $I - \varepsilon = 0.04$, $II - 0.17$, $III - 0.37$, $IV - 2.00 Ry$. The elastic scattering: 1-HF1 ($- \bullet -$), 2-HF2 (——); 3- RPA with inter-shell correlations (----) (results from Amusia et al. 1990); 4- our results, imRPA (——). Two lowest curves, Fig. 2B, correspond to quasi-elastic scattering (3- RPA with inter-shell correlations _•_•_•_ ; 4- our results, imRPA —— ; energy - IV).

Fig. 2B present the RPA (Amusia et al. 1990, Amusia and Cherepkov 1975, Amusia and Chernisheva 1997), and our improved imRPA (Tancic 1998, Tancic and Davidovic 2006) calculations. In our imRPA calculation we take into account the contributions of some third order diagrams of the Coulomb interaction (Tancic 1998, Tancic and Davidovic 2006). The main contribution to the phase shifts corrections are from transitions $3p \to \varepsilon d(^1P)$. The results of the calculations show that in the energetic interval $0.04 - 0.5 Ry$ the many-particle corrections in

RPA and imRPA are defined by inter-electron correlations in the framework of one shell and they are small. In the energetic interval $1-2Ry$ we have the main contribution of the RPA corrections: in this case the contribution comes from the transition $3p \to \varepsilon p(^1P)$ and from the inter-shell correlations (the influence from the excitations $3p \to \varepsilon d(^1P)$ and $3s \to \varepsilon p(^1P)$).

In the case of **quasi-elastic scattering** every act of the particle-hole interaction must be described by unique "exchange" component of the Coulomb matrix. As a one-particle wave functions we choose the functions $\varphi_{(j)k}^{N(L)}$. The calculations are analogous to the previous calculations for the case of the elastic scattering. We calculated 5 partial waves, which correspond to the $3p \to \varepsilon s(^1P)$, $3p \to \varepsilon p(^1S)$, $3p \to \varepsilon p(^1D)$, $3p \to \varepsilon d(^1P)$, $3p \to \varepsilon d(^1F)$ transitions. As results, we obtain that the biggest contributions from the electronic correlations comes from dipole transition $3p \to \varepsilon d(^1P)$. The results are presented in Fig. 2B (lowest two curves). The main contributions to the cross section come from the scattering in the field of the small angles ($0-30^o$ - the influence of the Coulomb interaction) and the large angles ($150-180^o$ - the main contribution is from the electronic correlations) (Amusia et al. 1990). The differential c.s. is finite at $\theta = 0$.We described the method of the calculations of the elastic and quasi-elastic scattering of electrons on the atoms (ions) with the vacancy in one of the closed shells. Our result are closed to the recently obtained results in Amusia et al. (1990).

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