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LETTER TO THE EDITOR

Inelastic and superelastic scattering of electrons by sodium: the role of the imaginary part of the optical potential in the DWBA analysis of the 3S–3P transition

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Abstract. The cross sections and correlation parameters of the $3^2S \leftrightarrows 3^2P$ transitions induced by intermediate-energy electrons are calculated in the distorted-wave approximation with a phenomenological optical potential. The inclusion of the imaginary part of the potential improves the agreement with experiment.

The distorted-wave Born approximation (DWBA) has proven to be a suitable approach to the theoretical interpretation of the electron impact excitation of the resonance transitions in noble gases at intermediate energies (Balashov *et al* 1981). An essential aspect of the DWBA is the choice of the complex optical potential $V_{opt}(\boldsymbol{r})$. Two approaches to the optical model of electron-atom collisions exist: the purely 'microscopic' approach in which one constructs V_{opt} from first principles (see, for example, Staszewska *et al* 1983) and the semiphenomenological approach in which V_{opt} contains adjustable parameters which are adjusted using the corresponding experimental data. Balashov *et al* (1981) used the latter approach, and the parameters of V_{opt} needed to calculate the 3p–4s excitation in Ar were determined from data on the differential elastic scattering cross section.

The purpose of this letter is to extend this approach to include atoms with unfilled shells. We begin with the sodium atom. In one respect the picture here is more diverse than for Ar or Ne atoms—for intermediate energies the $3^2S \rightleftarrows 3^2P$ transition in Na is studied experimentally not only in inelastic scattering (including the measurement of electron–photon correlations by Teubner *et al* (1985, 1986), Riley *et al* (1985, 1986), Brunger *et al* (1989)) but also in superelastic scattering (Hermann *et al* 1977, 1980, Scholten *et al* 1988). An attempt to use the DWBA in the analysis of superelastic electron scattering was made by us previously (Balashov *et al* 1983, Zaitseva 1984). In recent years new experimental data have appeared on the interaction of intermediate-energy electrons with sodium, including data on the differential and total elastic cross sections (Allen *et al* 1987). One would think that this would make it easier to determine the optical potential in the e + Na system. However, it has turned out in the course of several studies that the description of the elastic scattering of electrons by sodium is a more difficult task than in the case of noble gases (Grum-Grzhimailo and Zaitseva 1987, Mitroy *et al* 1987).

A way out of this difficulty was outlined recently (Grum-Grzhimailo 1989). It was suggested that the shape of the imaginary part of V_{opt} changes drastically within the

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electron energy range 20–50 eV, i.e. at energies where the excitation channels of the ionic core become open. Figure 1 shows the differential cross sections for elastic electron scattering at several energies. The full curves represent the results of calculations in the optical model with the semiphenomenological potential:

$$V^{\pm}_{\rm opt}(E, r) = V_{\rm st}(r) + V^{\pm}_{\rm ex}(E, r) + V_{\rm pol}(E, r) + {\rm i}V_{\rm abs}(E, r). \tag{1}$$

The real part of the potential (1) was constructed in the same manner as by Vanderpoorten (1976) and Teubner *et al* (1978). The absorptive part $V_{\rm abs}$ was used with the 'soft' truncation at small r (Grum-Grzhimailo 1989):

$$V_{\rm abs}(E, r) = \tilde{V}_{\rm abs}(r)[1 - \exp(-r/t)]. \tag{2}$$

The choice of the parameter t ensured the transition from surface absorption regime ($t = 5$ au) at 20 eV to the volume regime ($t = 0$) at 54.4 eV and higher.

Note that at 20 eV (the lowest energy under consideration) many of the characteristics of elastic and inelastic scattering (excluding the total absorption cross section $\partial_{\rm abs}$) are reproduced well by the potential (1) without $V_{\rm abs}$ at all (see, for example, figures

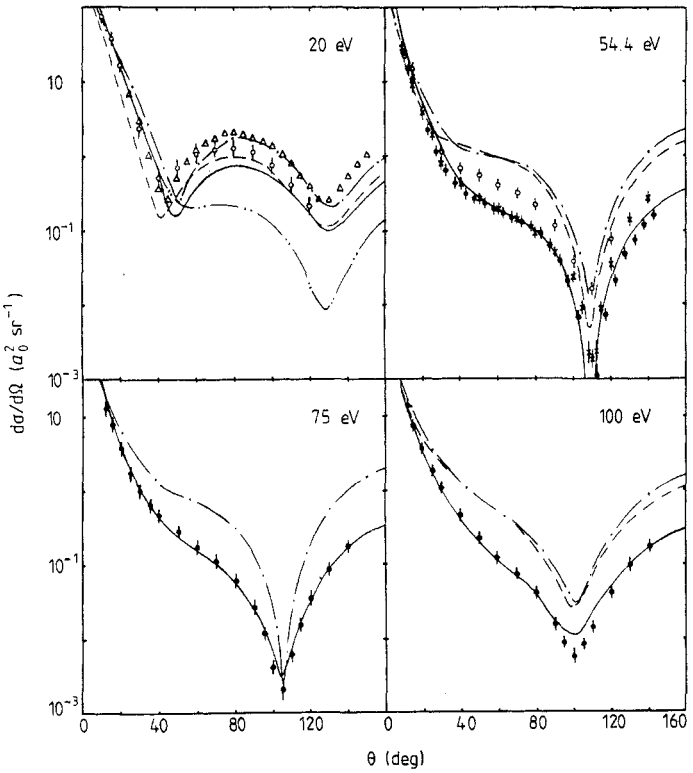

Figure 1. Differential cross sections for the elastic scattering of electrons from sodium. Theory: ——, calculation with the potential (1)-(3); — · —, calculation with $V_{\rm abs} = 0$; - - -, close-coupling calculation of Mitroy *et al* (1987); — · · —, calculation with $t = 0$ for 20 eV (expression (2)). Experiment: ○, Srivastava and Vuskovč (1980); Δ, Gehenn and Reichert (1972); ●, Buckman and Teubner (1979); ⧗, Allen *et al* (1987). The data of Gehenn and Reichert are normalised to the absolute measurements of Srivastava and Vuskovič at $\theta = 20°$.

1 and 4)†. For $\bar{V}_{abs}$ we use the exponential potential employed in the calculations of the elastic scattering of electrons by neon (Green *et al* 1981, Thirumalai and Truhlar 1982, Staszewska *et al* 1984):

$$\bar{V}_{abs}(r) = W_o[\exp(-r/d) - \exp(-r/s)]/r. \tag{3}$$

The parameters d and s, obtained by fitting, were assumed to be constant within the whole energy range under consideration (20–100 eV) and were found to have the following values: $d = 4.0$ au, $s = 0.076$ au. $W_o = -0.5$ for 20, 54.4 and 75 eV and $W_o = -0.45$ for 100 eV. The total elastic and absorption cross sections calculated with the potential (1)–(3) are given in table 1.

Table 1. Total elastic (σ_{el}) and absorption (σ_{abs}) cross sections in πa_0^2.

		E (eV)			
		20	54.4	75	100
σ_{el}	Our calculation	12.7	5.6	4.7	3.8
	Close coupling†	9.2	5.6		4.2
	Experiment‡	15.9 ± 6.1	6.1 ± 1.8		
σ_{abs}	Our calculation	31.1	25.8	22.5	18.1
	Experiment	44.8 ± 13.4‡	28.2 ± 8.5‡	22.3§	18.3§

† Mitroy *et al* (1987).
‡ Srivastava and Vuskovič (1980).
§ The lower bound from the data for 3P excitation of Enemark and Gallagher (1972) and for ionisation of sodium of McFarland and Kinney (1965).

The optical potential (1)–(3) was used to calculate the direct and exchange parts of the amplitudes $T^S_{M_L}(k_i, k_f)$ of the $3^2 \rightleftarrows 3^2P$ transition and, consequently, the density matrix of the orbital momentum L of the final 3^2P state in the process

$$e + Na(3^2S) \rightarrow e' + Na^*(3^2P) \rho(M_L, M'_L) \sim \sum_{S=0,1} T^{S*}_{M'_L} T^S_{M_L} (2S+1).$$

Hartree–Fock–Slater wavefunctions were used throughout (Herman and Skillman 1963); it was verified on part of the results, that the substitution of Hartree–Fock wavefunctions leads to minor changes. Any correlation parameter for the transitions $3^2S \rightleftarrows 3^2P$ in inelastic and superelastic scattering can be expressed in terms of the $\rho(M_L, M'_L)$. For example, the Stokes parameters of photons in the $(e, e'\gamma)$ process are calculated (as applied to photons emitted perpendicular to the scattering plane; taking the z axis along the incident electron beam) by the formulae

$$P_1 = 0.141(1 - 4\rho(1,1)) \qquad P_2 = 0.40\ \mathrm{Re}\rho(1,0) \qquad P_3 = -1.577\ \mathrm{Im}\rho(1,0) \tag{4}$$

where the numerical coefficients account for the depolarisation of radiation due to the fine- and hyperfine-structure effects (Teubner *et al* 1985). The reduced polarisation $|\bar{P}| = (\bar{P}_1^2 + \bar{P}_2^2 + \bar{P}_3^2)^{1/2}$, which is a measure of the coherence of the excitation, was found to differ only slightly from unity within the energy range under consideration throughout the range of scattering angles ($|\bar{P}|_{min} \simeq 0.97$ at $E = 22.1$ eV, $\theta \simeq 30°$). Thus, the density matrix $\rho\ (M_L, M'_L)$ describes an almost pure state. This means that the role of spin

† This observation is also confirmed by the recent paper of Mathur and Purohit (1989) where the correlation parameters at small scattering angles for the $3^2S \rightleftarrows 3^2P$ transition were reproduced quite well taking into consideration only the real part of the distorting potential.

effects, including those which are connected to an exchange scattering, is negligible (see, for example, Anderson *et al* 1988).

Figure 2 illustrates the calculations of the differential cross section for the 3^2S-3^2P excitation. On the whole the calculations give a satisfactory reproduction of the angular distribution of scattered electrons and the absolute magnitude of the cross sections. Note that, as in the case of elastic scattering (Teubner *et al* 1978, Grum-Grzhimailo and Zaitseva 1987, Grum-Grzhimailo 1989), taking into account the imaginary part of the optical potential considerably improves the agreement between theory and experiment.

Unlike the differential cross sections, the parameters of the electron-photon correlation for the 3^2S-3^2P excitation have been measured, until now, only for small scattering angles in the energy range under consideration. In figure 3 the Stokes parameters (4) obtained in the $(e, e'\gamma)$ experiments of Teubner *et al* (1985, 1986) and Riley *et al* (1985, 1986) are compared with our calculations. (We neglect the finite angular resolution, which should have an effect on P_1 and P_2 at $\theta \leqslant 5°$ at $E = 54.4$ and 100 eV, as was established by Mitroy *et al* (1987).) At $E = 22.1$ eV this picture could be supplemented with the data from the experiments on the superelastic $Na^*(3^2P) + e \rightarrow Na(3^2S) + e'$ scattering at the equivalent energy $E = 20$ eV (Hermann *et al* 1977, 1980). Unfortunately, the correlation parameters obtained by these two methods failed to agree until quite recently. It seems that this discrepancy begins to disappear after the recent experiment of Scholten *et al* (1988) on superelastic scattering.

In figure 4 the results of Scholten *et al* (1988) and the earlier data of Hermann *et al* (1977) and Riley *et al* (1985) are compared with the results of several theoretical approaches. It is seen that at $\theta \leqslant 20°$ our DWBA method is on a par with the close-coupling calculations of Mitroy *et al* (1987) and at larger angles it provides even better agreement with experiment. We share the opinion of Scholten *et al* (1988) that the

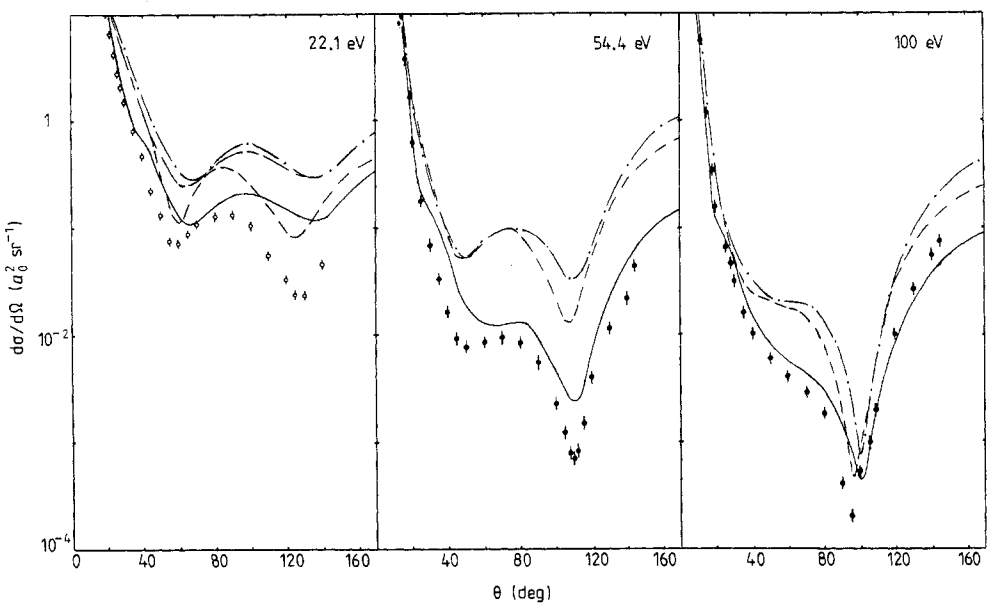

Figure 2. Differential cross sections for 3^2P excitation. Curves are as in figure 1. Experiment: ●, Buckman and Teubner (1979); ○, Teubner *et al* (1986).

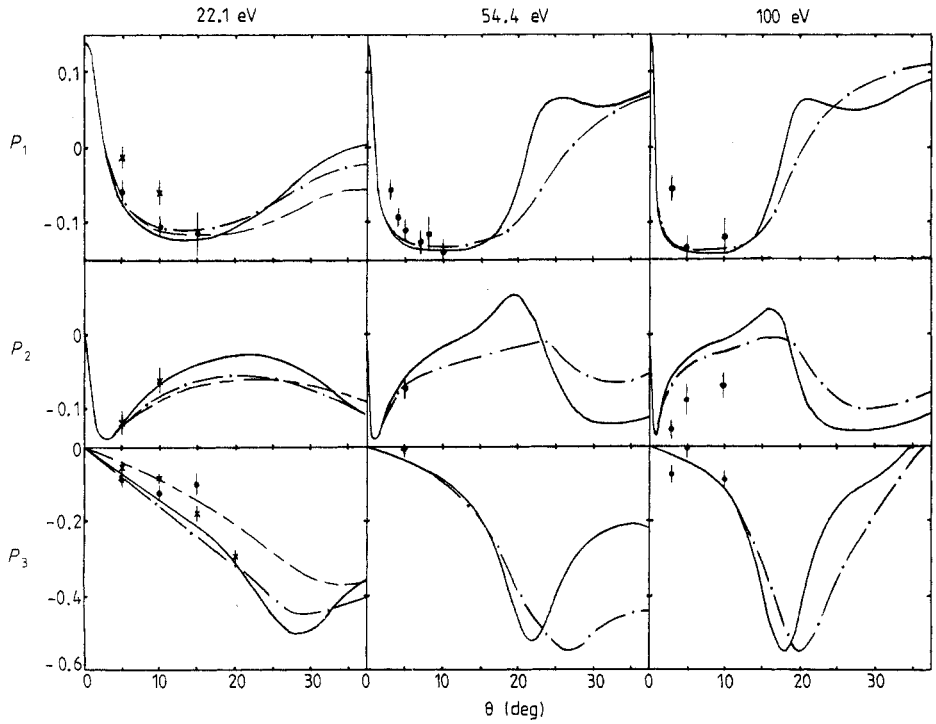

Figure 3. Stokes parameters P_1, P_2, P_3 in the $3^2S \rightleftarrows 3^2P$ transition. The curves are as in figure 1 with the following addition: — · · —, calculation with $V_{opt} = V_{st} + V_{ex}$. ⧫, inelastic scattering experiments of the Flinders University group (Teubner *et al* 1985, 1986, Riley *et al* 1985, 1986); ⧓, superelastic scattering experiments of Hermann *et al* (1977, 1980).

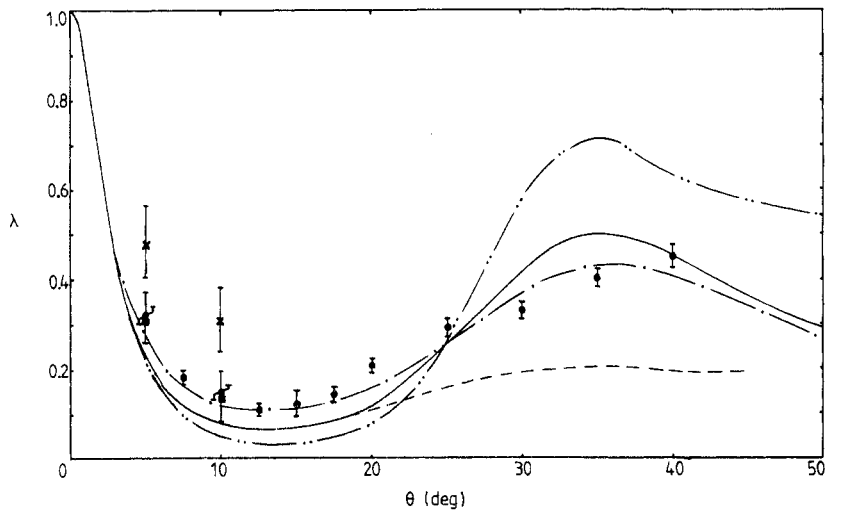

Figure 4. The parameter λ for the $3^2S \rightleftarrows 3^2P$ transition in inelastic ($E = 22.1$ eV) and superelastic ($E = 20$ eV) scattering. The curves are as in figure 1. Experiment: ⧓, Hermann *et al* (1977); ■, Riley *et al* (1985); ⧫, Scholten *et al* (1988).

few state close-coupling calculations do not seem to account fully for the distortion effects.

We believe that the present attempt to extend the DWBA with the complex optical potential to the atoms of alkali metals gives hope and we await with interest new data on the correlation parameters at large scattering angles (McClelland *et al* 1987, Brunger *et al* 1989).

The example we have studied demonstates that, in cases where the experimental investigation of the inelastic (superelastic) scattering of electrons by atoms is reinforced by a detailed study of the elastic scattering, it is possible to carry out a sound DWBA analysis. In conclusion we should emphasise, reiterating the reasoning of earlier investigations (Grum-Grzhimailo 1989), that it is expedient to carry out systematic measurements (with small steps in energy) of the superelastic (inelastic) scattering of electrons from sodium at energies of 20–55 eV.

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