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Optical Oscillator Strengths from 'Electron-impact Photoionisation' in the RCΞ Potential

R. Padma and P. C. Deshmukh

Department of Physics, Indian Institute of Technology, Madras 600 036, India.

Abstract

Electron-impact collisions excite optically allowed as well as optically forbidden transitions. In this paper we report details of optical oscillator strengths calculated using the RCΞ potential. The oscillator strengths have been calculated using the small-momentum-transfer limit ($K \to 0$) of the electron-impact generalised oscillator strength. Results for the Cooper-minimum trajectories for some high-Z (82–90) atoms and for Kr 3p ionisation are reported. These have been found to be in fair agreement with results of previous calculations in which more involved techniques were used. The present results offer further support to the utility of the RCΞ potential in atomic physics by providing first estimates of some important atomic properties, using a relativistic atomic potential which is computationally not very demanding.

1. Introduction

As is well known, very few electron–atom collisions have been studied using *relativistic* atomic potentials. In an attempt to employ a relativistic atomic potential in collision studies, we have recently carried out some investigations of generalised oscillator strengths for electron-impact atomic excitations (Padma and Deshmukh 1992) and also ionisations (Padma and Deshmukh 1993). A relativistic local-density central-potential method known as the RCΞ method (Vijayakumar *et al.* 1989; Vijayakumar and Gopinathan 1991) has been used in these studies. Our primary interest in this work is to assess the suitability of the RCΞ potential for collision studies by estimating the generalised oscillator strengths for various cases. In order to test the reliability of this approach, in the present paper we examine the optical limit of the generalised oscillator strength (GOS), where more data exist for comparison. We report here continuum optical oscillator strengths (OOS) derived from low-momentum-transfer ($K \to 0$) electron-impact ionisation calculations of the corresponding generalised oscillator strengths (GOS).

When the wavelength of the projectile is sufficiently large compared to the atomic size, the GOS for the resulting transition is proportional to the cross section for absorption of a photon with energy equal to the energy transferred in the collision process (Fano and Rau 1986). For small values of momentum transfer, the continuum *generalised* oscillator strength $\mathrm{d}f_{\mathrm{n}}(K)/\mathrm{d}(\epsilon/R)$ has the limiting behaviour (Manson 1971)

$$\frac{\mathrm{d}f_{\mathrm{n}}(K)}{\mathrm{d}(\epsilon/R)} \xrightarrow{K \to 0} \frac{\mathrm{d}f_{\mathrm{n}}}{\mathrm{d}(\epsilon/R)}, \tag{1}$$

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where $df_n/d(\epsilon/R)$ is the continuum *optical* oscillator strength (with R the Rydberg unit), which is proportional to the photoionisation cross section (Manson and Cooper 1968; Manson 1971). The above relationship provides us with a means to determine the photoionisation oscillator strengths from the low-momentum-transfer limit of the charged-particle-impact generalised oscillator strength, and is sometimes referred to as 'electron-impact photoionisation' (Samson 1981).

In high energy electron–atom collisions, the nature of energy transfer to the target is akin to what occurs in photoionisation by white light. This is due to the fact that rapid passage of an electron is manifest as a pulsed (δ-function) uniform electric field whose Fourier transform is a spectrum of white light consisting of a large number of frequencies (Samson 1981). As the momentum transfer K tends to zero, it then follows that the generalised oscillator strength approaches the optical oscillator strength (Fano and Rau 1986). We have made use of the Bethe–Born theory in generalised oscillator strength calculations (Inokuti 1971; Manson 1972*a*,*b*) employing the RCΞ potential (Vijayakumar *et al.* 1989), according to the relation

$$\mathrm{OOS} = \lim_{K \to 0} \mathrm{GOS}. \tag{2}$$

The initial state radial wavefunctions were obtained by solving the one-electron equations of the RCΞ method (Vijayakumar *et al.* 1989) by an iterative self-consistent field procedure. The corresponding RCΞ atomic potential was then substituted into the nonrelativistic Schrödinger equation (Manson 1972*b*) and subsequently, for each value of the ionised electron energy, the resulting equation was integrated once to obtain the corresponding continuum wavefunctions which appear as the final states in the evaluation of the transition matrix element. The continuum wavefunctions are thus determined in the RCΞ central field. However, the spin–orbit splitting of the continuum wavefunctions is ignored in the present work. This is, nevertheless, not a serious limitation since the spin–orbit splitting of the continuum wavefunctions is not very large. The methodology for calculating the GOS using the RCΞ potential has already been discussed elsewhere in detail (Padma and Deshmukh 1992, 1993).

We have chosen for the present study a few cases of interest for which data from other calculations were available for comparison. Also, for OOS we selected cases in which the quality of the RCΞ wavefunctions could be tested. In particular, we considered applications in which the nodal properties of the wavefunctions are important.

2. Results and Discussion

Benchmark calculations of the optical oscillator strengths were performed using the RCΞ approximation. It is well known that the occurrence of the 'Cooper minimum' (Cooper 1962; Manson and Cooper 1968) in the photoionisation cross section depends on the nodal properties of the radial wavefunctions. We have therefore determined the positions of the Cooper minima in the 6p photoionisation of some high-Z atoms. We have determined the photon energy at which the Cooper minimum in $6p \rightarrow \epsilon d$ optical channels occurs in the atoms with $Z = 82$–90. Dirac–Slater and relativistic random phase approximation (RRPA) calculations

have shown that the nonrelativistic Cooper minimum splits relativistically into three minima for the matrix elements $6p_{3/2} \rightarrow \epsilon d_{3/2}$, $6p_{3/2} \rightarrow \delta d_{5/2}$ and $6p_{1/2} \rightarrow \epsilon d_{3/2}$ (Manson *et al.* 1983; Deshmukh *et al.* 1986, 1992).

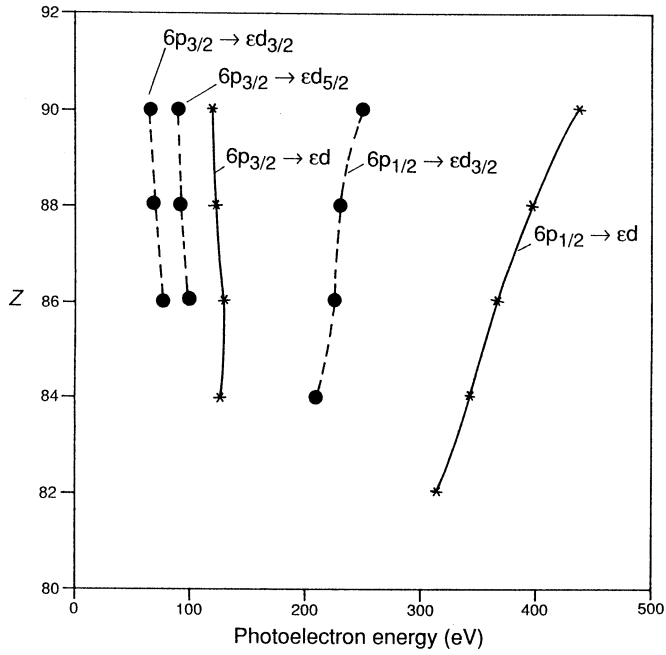

Fig. 1. Trajectory of the Cooper zeros in the $6p \rightarrow \epsilon d$ dipole matrix elements. The solid lines correspond to the present RCΞ results and the dashed lines to the Dirac–Slater results (Deshmukh *et al.* 1986).

The spin–orbit splitting of the ground state wavefunctions is included in the RCΞ method, and hence the positions of the Cooper minima in the $6p_{3/2} \rightarrow \epsilon d$ and $6p_{1/2} \rightarrow \epsilon d$ channels were determined separately. The spin–orbit splitting of the ϵd orbitals has not been considered, as mentioned above. Results of these calculations are presented in Fig. 1 along with the Dirac–Slater (DS) results (Deshmukh *et al.* 1986) for comparison. As was found in the DS approximation, we find that in the RCΞ potential the photoelectron energy at which the Cooper minimum occurs in the $6p_{1/2} \rightarrow \epsilon d$ channel shows a strong Z-dependence, whereas that at which it occurs in the $6p_{3/2} \rightarrow \epsilon d$ channel does not. The magnitude of the spin–orbit splitting of the bound state $6p_{1/2}$, $6p_{3/2}$ levels by itself is not adequate to explain the magnitude of the splitting in the positions of the Cooper minima in the photoionisation channels from these levels. In fact, the former is much smaller (by a factor of over 30) than the latter. The reason for this peculiar effect can be traced to the simultaneous consideration of two factors:

(a) the $6p_{1/2}$ radial wavefunction is more compact than the $6p_{3/2}$ radial wavefunction, and

(b) the continuum orbital ϵd has to overcome the centrifugal barrier to generate the dipole-allowed $6p_{3/2} \rightarrow \epsilon d$ and $6p_{1/2} \rightarrow \epsilon d$ matrix elements.

The condition for a Cooper minimum is thus reached earlier in the $6p_{3/2} \rightarrow \epsilon d$ channel than in the $6p_{1/2} \rightarrow \epsilon d$ channel, but the condition for the minimum in the latter does not occur merely after gaining an energy corresponding to the spin–orbit splitting. Rather, it occurs at a much higher energy since the centrifugal barrier has to be overcome, which exaggerates this effect, as has been discussed elsewhere (Deshmukh *et al.* 1992).

In the photon energy region considered in the present work, the energy dependence of the transition matrix element comes from the energy dependence of the continuum wavefunctions. With an increase in energy, the continuum wavefunction penetrates the atomic core further and becomes more compact. With a further increase in energy, it becomes more oscillatory in the region of overlap. Fig. 1 shows that the Cooper minimum occurs at a higher value of the photoelectron energy in the RCΞ results than in the DS results. The actual position of the Cooper minimum on the energy scale is sensitive to the profile of the initial and final state radial wavefunctions. Although both the RCΞ and DS potentials make use of a relativistic local-density approximation, the difference in the positions of the Cooper minima in the two approximations is predominantly due to the different treatments of the self-interaction term in the electron–electron exchange potential (Vijayakumar *et al.* 1989; Padma and Deshmukh 1992). The positions of the Cooper minima in the $6p_{3/2} \rightarrow \epsilon d_{3/2}$, $6p_{3/2} \rightarrow \epsilon d_{5/2}$ and $6p_{1/2} \rightarrow \epsilon d_{3/2}$ channels for photoionisation of atomic radon have also been reported in the RRPA (Deshmukh *et al.* 1986, 1992). For this atom, the positions of the Cooper minima determined using the RCΞ potential are in

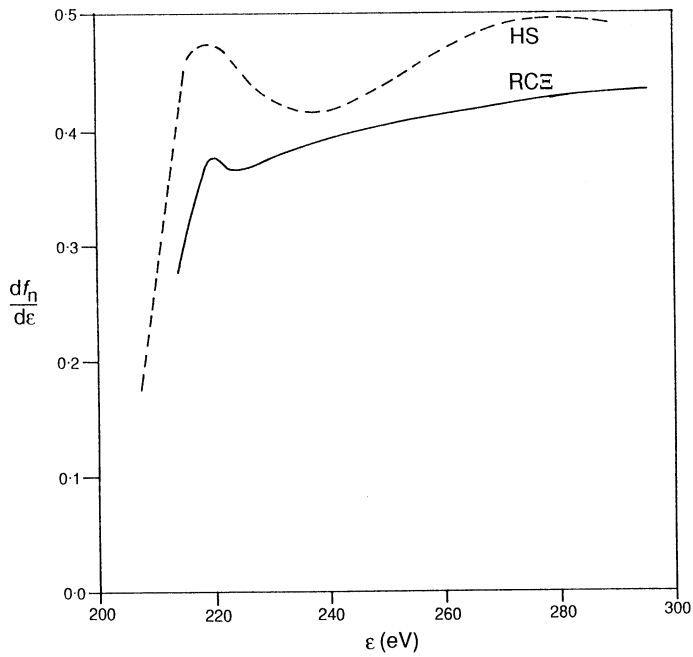

Fig. 2. Optical oscillator strengths as a function of photon energy for 3p ionisation of Kr, showing RCΞ (solid line) and Hartree–Slater (dashed line) results. The orbital energy for the 3p subshell of Kr is 214 eV in the RCΞ potential and 207·4 eV in the HS potential.

closer agreement with those determined in the RRPA than are the corresponding DS results, since the RRPA minima occur at photoelectron energies of 183·4, 189·1 and 310·4 eV in the above-mentioned three channels respectively.

We have also used the above method to calculate the optical oscillator strengths for the optically allowed Kr $3p_{1/2} \rightarrow \epsilon d$, $3p_{3/2} \rightarrow \epsilon d$ and $3p_{1/2} \rightarrow \epsilon s$, $3p_{3/2} \rightarrow \epsilon s$ ionisation channels. This was done to test the reliability of the RCΞ method's predictions in another characteristic photoionisation minimum, which is *not* a Cooper minimum. The Kr 3p dipole oscillator strengths go through a minimum which has been identified previously as a 'normalisation factor minimum' (Dillon and Inokuti 1985; Shanthi *et al.* 1988*a*,*b*). Results for the RCΞ potential are shown in Fig. 2 along with the results of calculations in the Hartree–Slater (HS) approximation (Herman and Skillman 1963), also obtained using the electron-impact photoionisation model. The *normalisation factor minimum* is seen in the HS as well as the RCΞ calculations, and the results are in fair agreement with each other. The analytical properties of the normalisation factor for continuum states have been discussed by Dillon and Inokuti (1985). This factor is the net result of the entire atomic field, and is therefore sensitive to the details of the potential employed in the calculation, thus accounting for the difference between the two curves shown in Fig. 2. The predominant influence in this case must again be the different treatments of the exchange interaction.

3. Conclusion

The fact that the RCΞ potential yields a result in fair agreement with the results of more established techniques suggests that it can be used to obtain reliable estimates of important collision and photoionisation parameters. This method has the advantage of including relativistic effects and a more appropriate treatment of the exchange interaction, while retaining the simplicity of the local-density methodology. The zero-momentum-limit generalised oscillator strengths calculated using the RCΞ potential offer reasonably good estimates of the optical oscillator strengths.

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