A theoretical investigation of K-shell photoionization of neon

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Abstract. The total photoionization cross section is calculated for neon (Z = 10) near the 1s threshold using the relativistic random-phase approximation, the relativistic random-phase approximation modified to include relaxation effects, and the relativistic random-phase approximation modified to include relaxation effects and Auger decay. Comparisons are made between theoretical calculations and experimental data. The need to include Auger decay along with relaxation is demonstrated.

1. Introduction

The outer subshells of neon (Z = 10) have been the subject of numerous studies, both theoretical and experimental; less attention has, however, been given to the K-shell. The closed-shell structure makes an analysis of neon accessible to a large variety of theoretical techniques. Without careful study, one might assume that a hydrogenic approximation would suffice for calculations of deep inner-shell photoionization.

An early theoretical study of the photoionization cross section in the 1s threshold region was reported by Sukhorukov et al [1]. Sukhorukov et al modelled the photoionization cross section by modifying the Hartree–Fock (HF) equation to include orbital relaxation. In 1993 Tulkki and Mäntykenttä [2] used a multichannel multiconfigurational Dirac–Hartree–Fock (MMDHF) calculation to show how the relaxation effect depends on the Auger electron energy.

Recently Kutzner et al [3] compared the relativistic random-phase approximation (RRPA), the relativistic random-phase approximation modified to include relaxation effects (RRPAR), and the relativistic random-phase approximation modified to include relaxation and Auger decay (RRPAPA) results for the 1s subshell of Ar and concluded that good agreement was attained only after including the effects of relaxation, relativity and Auger decay.

This work is a theoretical investigation of the photoionization of the 1s subshell of neon atoms to determine the effects of core relaxation and Auger decay on cross section. We compare four theoretical models; the HF modified to include orbital relaxation as reported by Sukhorukov et al [1], the RRPA, RRPAR, and RRPAPA, with the experimental results measured by Bearden [4], Henke et al [5, 6] and Esteva et al [7]. Comparisons presented in this way yield valuable insights into the effects of various types of electron correlation.

2. Method

Detailed discussions of both the RRPA and the RRPAR can be found elsewhere [8, 9]. Here we will point out that in the RRPA, the partial photoionization cross section for a given subshell
is given by
\[
\sigma_{n\kappa} = \frac{4\pi^2\alpha_\omega}{3} (|D_{n\ell\to j-\ell}|^2 + |D_{nj\to j}|^2 + |D_{nj\to j+1}|^2).
\] (1)

In this equation, \(n\) is the principal quantum number and \(\kappa = \tau(j + \frac{1}{2})\) for \(j = \ell \pm \frac{1}{2}\), where \(j\) and \(\ell\) are the single electron total and orbital angular-momentum quantum numbers. The dipole matrix element \(D_{nj\to j'}\) is the reduced RRPA dipole matrix element for the photoionization channel \(nj\to j'\).

The RRPAR method approximates the effects of core relaxation by calculating the continuum photoelectron orbital in the potential of the relaxed ion. The ionic core with the hole in the level with \(j = \ell + \frac{1}{2}\) has a lower ionization threshold energy and also represents the most populated of the two levels. Thus, we generally place the hole in the subshell with the largest \(j\) for the purpose of obtaining the \(V^{\infty-1}\) potential. Overlap integrals of the form \(\text{Det} \langle \Phi_i^\prime | \Phi_i \rangle\) between orbitals of the unrelaxed ground state \(\Phi_i\) and the corresponding orbitals of the final relaxed state \(\Phi_j^\prime\) are included in the RRPAR dipole matrix element for each electron of the ionic core. Inclusion of these overlap integrals is important for calculations of the partial photoionization cross sections since they approximately remove oscillator strength due to double-excitation shake-up and shake-off processes from the single-excitation channel oscillator strength [10]. However, for calculations of the total photoionization cross section which include oscillator strength from doubly-excited channels, these overlap integrals need not be included. To approximately include the effects of Auger decay in the RRPARA model, we include overlap integrals between orbitals of the ground state and the continuum orbitals of the final state. According to Åberg [11], this factorization of the post-collision interaction matrix element into a one-electron energy-dependent Auger decay amplitude and the one-electron overlap matrix element is equivalent to approximating that the many-electron Hamiltonian matrix element that involves the final scattering wavefunction describes the emission of the slow photoelectron and the fast Auger electron.

The RRPA-type calculations reported here have included all nine dipole allowed channels. Photoionization thresholds in the strict RRPA model use the DHF eigenvalues. However, experimental thresholds are frequently utilized. In this work experimental ionization energies were used in calculating the total cross section for the RRPA, RRPAR and RRPARA models. Another frequently used threshold is the difference in total self-consistent field energies of the neutral atom and ion (\(\Delta E_{\text{SCF}}\)). Subshells where the experimental thresholds match \(\Delta E_{\text{SCF}}\) are also subshells where relaxation effects are found to be important [3]. The experimental ionization and \(\Delta E_{\text{SCF}}\) energies for the K-shell of neon are 31.983 [12] and 31.964 au, respectively. The DHF threshold (32.817 au) is not as close to the experimental value as the \(\Delta E_{\text{SCF}}\) threshold. DHF and \(\Delta E_{\text{SCF}}\) energies were obtained using the Oxford multiconfiguration DF computer code of Grant et al [13].

3. Results

Deep inner-shell photoionization is influenced by a number of effects. Rearrangement, Auger decay, radiative decay, polarization, and post-collision interaction can all play a role. The importance of the effects of rearrangement and Auger decay can be seen in figure 1, where the total photoionization cross sections in the RRPA, the RRPAR, and the RRPARA models are shown along with the relaxation modified HF calculation by Sukhorukov et al [1] and experimental data [4–7]. The RRPA result (which includes no rearrangement effects) is in excellent agreement with Bearden [4] and Henke et al [5] at energies below approximately 35 au, but above 35 au predicts cross sections slightly lower than experiment. RRPA
**Figure 1.** Total photoionization cross sections above the 1s threshold of neon. The full curve is the RRPA calculation; the double-dot-dashed curve is the RRPAR calculation; the long broken curve is the RRPARA calculation. The single-dotted curve is the relaxed HF calculation by Sukhorukov et al. [1]. Open squares are Bearden’s [4] experimental results and the open triangles [5] and full circles [6] are the results of Henke et al.’s experiments. Esteve’s [7] results are shown by the light full curve between 32 and 34 au. Experimental threshold energies were used for the present RRPA-type calculations. The geometric means of the length and velocity calculations are shown for each approximation. Experimental and DHF thresholds are indicated by EXP and DHF respectively. On the scale of this plot EXP is indistinguishable from the difference in total self-consistent field energies of the neutral atom and ion ($\Delta E_{SCF}$).

Calculations using the DHF ionization energies (not shown in figure 1) are above experimental results near threshold, but agree very well at higher energies. The RRPAR, which includes relaxation effects, is in poor agreement with experimental data near threshold, predicting cross sections much lower than observed experimentally. However, as the energy is increased, the predicted cross section rises to meet the experimental results and then declines following the experimental data. Applying the effects of Auger decay (RRPARA) to the RRPAR model restores the calculated cross section to close agreement with observed values near threshold. Sukhorukov et al.’s [1] relaxed HF results predict cross sections lower in value and with a steeper gradient than experiment. Sukhorukov et al.’s [1] calculations are similar in nature to the shown RRPARA calculations but they do not include interchannel coupling or relativistic effects, which could account for the differences. Esteve et al.’s [7] experimental results are consistent in magnitude with both the RRPA and RRPARA near threshold; the slope of Esteve et al.’s data does not however seem to match the theoretical results of either the RRPA or RRPARA.

In the strict RRPA with all possible dipole channels included, the results are independent of whether the length or velocity gauge is chosen. When experimental thresholds or relaxation effects are included, this no longer holds. Figure 1 shows the geometric mean of length and velocity total cross sections for the RRPA, RRPAR, and RRPARA calculations. The RRPA and RRPARA take on their maximum deviations between length and velocity at threshold of 4.89% and 9.65% respectively, and as the photon energy is increased, the difference between length and velocity for both models decreases. The RRPAR takes on its minimum deviation
between length and velocity at its peak, where its difference is about 1.48%. At higher energies the difference between length and velocity calculations stays approximately constant at around 0.005 Mb.

It is important to note the relative contributions of various channels to the total photoionization cross section. Near threshold, the 1s contribution to the total cross section in RRPA (RRPARA) is 96% (76%), and the 2p and 2s contributions are 1.4% (2.2%) and 2.6% (3.7%), respectively. In addition, the RRPARA theory provides an estimate of photoionization-with-excitation and double-photoionization channels which are computed from overlap integrals and amount to approximately 18% (independent of photon energy).

Figure 2 shows the geometric mean of the length and velocity partial cross sections for the RRPA and the RRPARA calculations. Although the total photoionization cross sections in the RRPA and RRPARA models do not differ greatly, as seen in figure 1, the predicted partial cross sections are significantly different. The differences are due largely to the inclusion of overlap integrals in the RRPARA calculations. The sums of the calculated partial cross sections for the 2p and 2s subshells in the RRPA, and the RRPARA models are nearly identical and are shown as a single curve in figure 2.

4. Conclusion

For the innermost subshell of neon, the RRPA results (with experimental threshold) give a good estimation of the total cross section, with a slight deviation from experiment at higher energies. We determined that if relaxation effects are included in calculations, it is also important to include the effects of the Auger decay. Esteva et al's [7] measurements near threshold exhibit a slope that differs from theoretical predictions. It is hoped that this work will encourage further experimentation in the near threshold region of the 1s subshell of neon.
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References