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LETTER TO THE EDITOR

Application of the relativistic random-phase approximation to the photoionisation of atoms

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Abstract. Exploratory calculations of atomic photoionisation cross sections including both relativistic and correlation effects are undertaken using the relativistic random-phase approximation (RRPA). In these preliminary calculations we examine the photoionisation of He and Be atoms. The cross sections and asymmetry parameters for these light elements agree precisely with non-relativistic RPA values. Elastic phaseshifts for the $e^- + He^+$ and $e^- + Be^+$ systems are obtained and agree with non-relativistic calculations in the ^1P eigenchannel; our ^3P phaseshifts have no counterpart in non-relativistic theory.

Recent experimental and theoretical studies of the atomic photoionisation process have uncovered several interesting features of the structure of atoms. Prominent among these features are:

(i) the important role of correlations in accurate theoretical predictions of photoelectric cross sections σ near threshold (Amusia and Cherepkov 1975, Kelly and Simons 1973);

(ii) the importance of relativistic (spin–orbit) effects in explaining branching ratios of cross sections for different atomic subshells (Samson *et al* 1975, Shannon *et al* 1977); and

(iii) the significance of both relativity and correlation in determining the asymmetry parameter β for heavy atoms (Dehmer and Dill 1976).

It is apparent from the work of Amusia and Cherepkov (1975) and others (Kelly 1975, Cooper 1975) that correlation effects for closed-shell atoms are well described by the non-relativistic RPA. Since the calculations of Amusia and Cherepkov (1975), Amusia *et al* (1976) are completely non-relativistic they do not address the important problems mentioned under items (ii) and (iii) above. Relativistic calculations (Pratt *et al* 1973), on the other hand, have been successful in treating the high-energy photoeffect where correlation is unimportant. In recent years relativistic treatments have been specialised to the low-frequency region of the spectrum by Walker and Waber (1973a,b, 1974) to describe features of the spectrum sensitive to spin–orbit interaction. These relativistic calculations have omitted correlation and therefore have been of limited value in explaining cross section ratios and asymmetry parameters (Dehmer and Dill 1976).

It is our proposal to undertake a comprehensive study of the low-frequency photoeffect including both correlations and relativity by employing the RRPA (Johnson *et al* 1976, Lin *et al* 1977). Below we give a brief outline of the theory and describe the results of some preliminary applications of RRPA to studies of the photoeffect in He and Be.

The photoelectron angular distribution is described by the differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{\sigma}{4\pi}(1 - \tfrac{1}{2}\beta P_2(\cos\theta))$$

where θ is the angle between the electron and photon directions, σ is the scattering cross section, and β is the electron asymmetry parameter. Both σ and β depend on the photon frequency ω. In the non-relativistic theory σ and β depend on the quantum numbers n and l of the subshell from which the electron is photo-ejected; in the relativistic theory there is a further dependence on the subshell quantum number $j = l \pm \frac{1}{2}$.

In our preliminary studies we have considered photoemission from the 1s shell of He and from the 2s shell of Be. For either case there are two possible continuum states for the ejected electron $\epsilon_{p_{1/2}}$ and $\epsilon_{p_{3/2}}$. The expressions for σ and β in these cases can be written

$$\sigma = \frac{12\pi\alpha p\epsilon}{\omega}(\tfrac{1}{3}|R_1|^2 + \tfrac{2}{3}|R_2|^2)$$

and

$$\beta = 2 - \frac{2|R_1 - R_2|^2}{|R_1|^2 + 2|R_2|^2}.$$

Here p is the electron momentum, ϵ the electron energy and α is the fine-structure constant. The radial transition matrix elements R_1 and R_2 are taken between the bound s state and the continuum $\epsilon_{p_{1/2}}$ and $\epsilon_{p_{3/2}}$ states, respectively. In the calculations of Walker and Waber (1973a,b, 1974) single-particle matrix elements are determined using Dirac–Hartree–Fock–Slater radial wavefunctions. In RRPA calculations the corresponding radial matrix elements are determined by solving the coupled radial RRPA equations. Each radial matrix element involves correlation corrections from the final-state interactions between the electron in the $\epsilon_{p_{1/2}}$ and $\epsilon_{p_{3/2}}$ channels as well as ground-state correlations. For the He photoeffect the radial RRPA equations are written down in Johnson and Lin (1976) while the corresponding Be equations are written out in Lin and Johnson (1977).

We solve the radial RRPA equations numerically, demanding solutions which behave asymptotically as an outgoing wave in the $p_{1/2}$ channel and an incoming wave in the $p_{3/2}$ channel or vice versa. The boundary conditions lead to a two-channel S matrix which is diagonalised to give scattering eigenphases for electron–ion P-wave scattering.

Graphs of the singlet and triplet P-wave eigenphases determined from the RRPA equations are presented in figure 1. The ^{1}P phase for He agrees closely with the non-relativistic RPA values determined by Jamieson (1969) while the ^{1}P phase for Be corresponds closely with that predicted by Stewart (1975). The ^{3}P phaseshifts have no counterpart in non-relativistic RPA; they arise in the present calculation because spin–orbit coupling mixes ^{3}P into the final (essentially pure ^{1}P) excited state.

The radial matrix elements in each of the two channels are determined using the RRPA matrix elements including ground-state correlation terms. In the Be example it is necessary to include inner-shell excitations in order to bring 'length-gauge' and 'velocity-gauge' cross sections into precise numerical agreement.

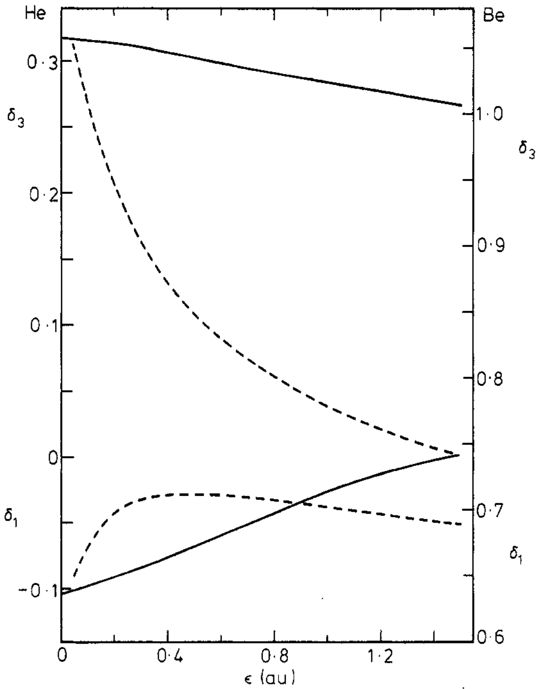

Figure 1. Elastic p-wave phaseshifts for e–He$^+$ and e–Be$^+$ scattering plotted against continuum electron energy ϵ. The full curves give RRPA values for e–He$^+$ scattering; δ_1 refers to the singlet phaseshift and δ_3 refers to the triplet phaseshift. The broken curves give RRPA values for e–Be$^+$ scattering. The right-hand scale refers to Be. For all cases the Coulomb phaseshift has been removed.

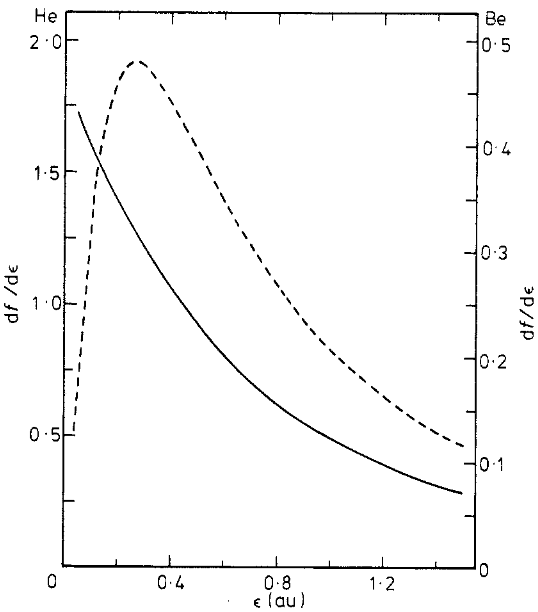

Figure 2. Oscillator strength distributions for He and Be photoionisation. The full curve describes He while the broken curve refers to Be. The photoionisation cross section is $\sigma(\mathrm{Mb}) = 4{\cdot}03\ \mathrm{d}f/\mathrm{d}\epsilon$.

Graphs of the final results of our exploratory calculations are presented for Be and He in figure 2, where we give the dimensionless quantity $\mathrm{d}f/\mathrm{d}\epsilon$ plotted against the electron energy ϵ. The quantity $\mathrm{d}f/\mathrm{d}\epsilon$ is related to the cross section by

$$\sigma = 4{\cdot}03 \frac{\mathrm{d}f}{\mathrm{d}\epsilon}(\mathrm{Mb}).$$

Again the relativistic results for He are in close agreement with the non-relativistic RPA results of Jamieson (1969) and with Amusia *et al* (1976), while the present Be results agree well with the non-relativistic calculations of Stewart (1975) and with Amusia *et al* (1976).

The asymmetry parameter β deviates from two by only a small amount ($\sim 10^{-6}$) for the cases considered. We expect, however, that in systems where relativistic effects are more important, such as photoemission from the 5s shell of Xe, the departure of β from two will be significant.

Our preliminary calculations were all designed to test RRPA procedures for simple systems where detailed non-relativistic comparisons were already available. Studies are underway for more complex systems where relativistic effects are expected to play a significant role.

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