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ONE-ELECTRON EXCITATIONS, LOCAL POTENTIALS AND MANY-ELECTRON EFFECTS

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A continuum photoionization cross section studied over a large range of energies gives information about the dynamical behaviour of atomic electrons, and theoretical calculations have to account for the whole range between very slow and very fast electrons. Such processes, in the outer and intermediate shells in heavy atoms, have been described as approximate one-electron excitations, in which an electron-hole pair in the final state becomes strongly modified by its interaction with the surrounding atomic medium[1,2]. In this paper we construct an effective "local" potential, which incorporates many-electron effects treated in the HF (Hartree-Fock) and Random Phase Approximations (RPAE, E stands for Exchange). Such a potential gives a clearer insight into the dynamics of excitation processes.

First, we mention strict one-electron models (Herman-Skillman[3], Kohn-Sham[4], local density scheme[5]). In these models one calculates the ground-state electronic density and potentials for an atom and then the excited one-electron states using the same local potential. Starting from a HF description of the ground state (HF potential operator con-

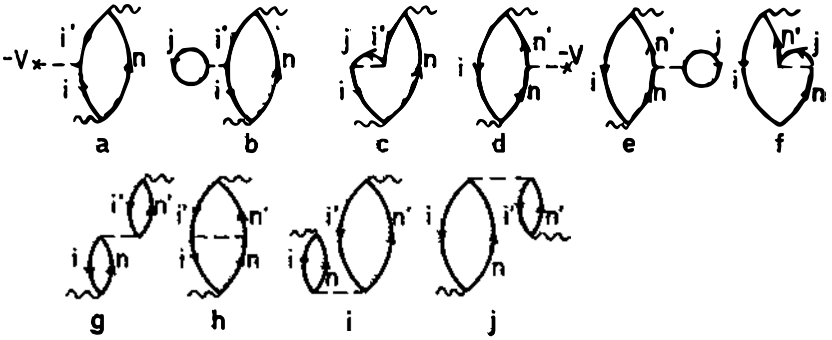

Fig. 1. Polarization (Goldstone time-ordered) diagrams, first order in perturbation expansion.

sisting of diagrams a+b+c), we still have a one-electron picture, but the potential for an excited electron, HFav (diagrams d+c+f), is now non-local; it is constructed so that the electron feels the spherically averaged potential of the HF ground state with the initial one-electron orbital removed$^{2)}$. Consequently, in both cases, an excited electron sees the same potential as it moves in the ground state. Physically, this means that the electronic density of the rest of the system is not perturbed by the excitations of an electron-hole pair. The polarizability of the remaining electrons is, therefore, considered to be zero and that the potential does not include many-body effects. All effects of the dynamical interaction are transferred to the perturbation expansion and have to be accounted for explicitly.

By coupling the electron-hole excitation to a state of angular momentum ^{1}p (HF^{1}p, potential operator for excited states consists of diagrams d+e+f+diagonal parts of diagrams g and h), one includes very important effects of the dipole polarizability of the medium$^{2)}$.

Inclusion of Fermi-sea correlations (ground-state correlations, diagrams i+j+corresponding exchange diagrams summed to infinite order in perturbation expansion) lead to the RPAE scheme. The difference in the potential HFav versus the potentials HF^{1}p and RPAE is actually a measure of many-body effects.

Wave functions and "local"potentials

The idea is to construct a local potential in the following way: First, the effective one-electron wave function and energy should be found within a certain approximation (HFav, HF^{1}p, RPAE) and then a local potential producing the same wave function$^{6)}$ should be obtained from the Schrödinger equation, whose solutions are these wave functions and energies.

The Schrödinger equation with a local one-electron potential becomes

$$\left[-\frac{d^2}{dr^2} + V^{eff}_{n\ell}(r) - E\right]P_{n\ell}(r) = 0$$

Knowing the wave function, one obtains the corresponding local potential

$$V^{eff}_{n\ell}(r,E) = (\frac{d^2}{dr^2} - E)\ P_{n\ell}(r)/P_{n\ell}(r) ,$$

$$V^{eff}_{n\ell}(r,E) = V_{n\ell}(r) + \frac{\ell(\ell+1)}{r^2} .$$

Naturally, the resulting local potential is singular at the nodes of the wave function. The singularity is a consequence of the non-locality and is characteristic of a particular wave function and energy. Supposing an energy-independent potential, one can produce other functions at other energies by means of the Schrödinger equation, but one has to remove the singularity and make the potential smooth.

Application to one-electron excitations in Kr and Ba

We shall present some results for the 4p→d excitation in Kr and the 4d→f excitation in Ba. A full account of the results will appear elsewhere$^{6)}$.

(i) Kr

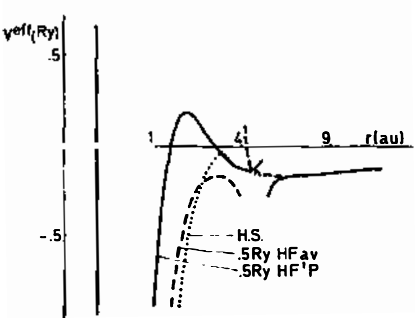

Fig. 2

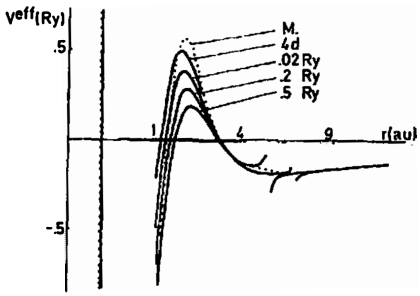

Fig. 3

Fig. 2. Local potentials for atomic Kr.

Fig. 3. Energy dependence of the 4pεd HF^{1}P local potential for atomic Kr. The figure also shows the parametrized energy inddpendent local potential for Kr by Miller et al.$^{7)}$.

Fig. 2 shows a comparison of the (4p^{5}εd)HFav and (4p^{5}εd)HF^1 results for the continuum energy ε=0.5 Ry (the 4p^5 core is frozen), together with the Herman-Skillman potential$^{3)}$. The results of the Kr 4p photoabsorption cross section$^{1,8,9)}$ have shown that the HF^{1}p oscillator strength (both discrete and continuum), compared with the HFav case, is shifted to higher energies. The reason for this is the prominent barrier which appears in the HF^1p potential. This could be explained as the weakly attractive HFav exchange potential becomes strongly repulsive in the HF^1p scheme. Physically, the barrier is a result of the dynamical interaction between the electron-hole excitation and the remaining electrons in the 4p subshell. As the barrier does not exist for the HFav effective potential, even if it is a mixture of the true potential and the angular momentum potential, we would phrase it a collective barrier. It is a consequence of the strong dipole polarizability of the 4p subshell and is really due to many-electron effects. The effect of including Fermi-sea correlations, leading to the RPAE shows a barrier which is somewhat higher and pulled in. As a result, the RPAE oscillator strength is lower, shifted to lower energies in comparison with the HF^1p one, and is in rather good agreement with experiment.

ii) Ba

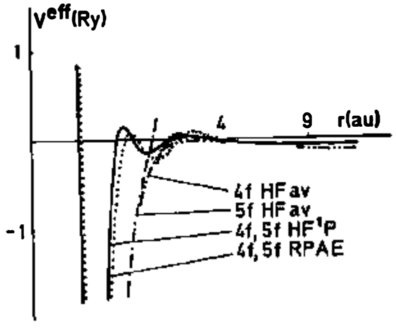

Fig. 4

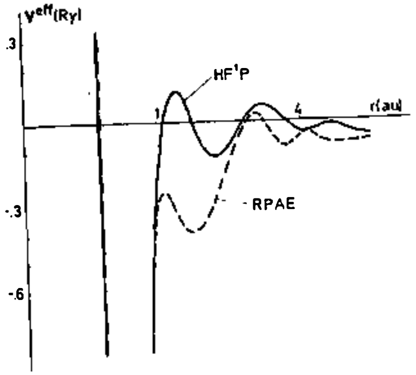

Fig. 5

In Fig. 4 we compare the $(4d^9nf)$HFav and $(4d^9nf)$ HF^1p results for n=4,5. There is now an angular momentum barrier in the HFav potential, but in the HF^1p potential there is also a collective barrier. We have plotted the potential corresponding to $(4d^9nf)\,^1p$ RPAE excitations for n=4,5.

In Fig. 5 we show the HF^1p and RPAE results for 0.1 Ry continuum energy. In the discrete as well as in the continuum state the barrier is lowered and the effect on the photoabsorption cross section is quite appreciable[1,2]. The modification of the effective potential by Fermi-sea correlations is, therefore, of crucial importance. Finally, let us mention that the RPAE breaks down completely in the region of 0-15 eV above the 4d threshold

A consequence of the inclusion of relaxation effects is that at low kinetic energies screening effects will make the 4d-hole less attractive.
This will raise the collective barrier and keep the f-electron from penetrating into the deep core region until the energy is considerably increased. As a result,the photoabsorption cross section will be considerably lowered in the threshold region.

References

1. M.Ya. Amusia and N.A. Cherepkov, Case Studies in Atomic Physics 5, 47 (1976).
2. a) G. Wendin, in Photoionization and Other Probes of Many-Electron Interactions (ed. Wuilleumier F.), NATO A.S.I. series, Plenum 1976, p. 83.
6. G. Wendin and Ž. Crljen (to be published).
7. D.L. Miller and J.D. Dow, Phys. Lett. 60A, 16 (1977).
3. F. Herman and S. Skillman, Atomic Structure Calculations, Prentice Hall Inc. 1963.
4. W. Kohn and L.J. Sham, Phys. Rev. 140, A1133 (1965).
5. O. Gunnarsson and B.I. Lundqvist, Phys. Rev. B13, 4274 (1976).
8. J.W. Cooper, Phys. Rev. 128, 681 (1962).
9. M.Ya. Amusia, N.A. Cherepkov and L.V. Chernysheva, Sov.Phys. -JETP 33, 90 (1971).