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Abstract. A simple procedure for obtaining 1s electron wavefunctions in complex atoms is presented which takes into account many body, relativistic and finite nuclear size effects.

In recent years there have been a number of solutions to the Hartree–Fock problem in complex atoms. Perhaps the most widely used solutions are those given by Herman and Skillman (1963, to be referred to as HS). HS give numerical solutions to the Hartree–Fock equations for most atoms in the periodic table. These solutions are obtained in the Slater free electron approximation (Slater 1960). Finite nuclear size effects are ignored and relativistic corrections to the single particle energies are obtained in first order perturbation theory.

In heavy atoms the inner shell electron wavefunctions (in particular those of the 1s shell) may be substantially modified by the finite nuclear size and relativistic effects. These modifications are of significance in the calculation of electron capture cross sections. We report here on our results for K shell electrons based upon the HS compilations.

Suppose H is the full relativistic single particle Hamiltonian for the 1s electronic state Ψ. Then Ψ is the proper eigenfunction to use in calculating electron capture cross sections. The Hamiltonian H_0 and eigenfunctions Ψ_0 of the relativistic hydrogenic problem (nucleus of charge Z) are well known. We may construct a Foldy–Wouthuysen (FW) transformation F_0 (Rose 1961) such that Φ_0 is the classical limit of Ψ_0

$$\Phi_0 = F_0\Psi_0. \tag{1}$$

Similarly we can define F such that Φ is the classical limit of Ψ. Then if

$$\Phi = \mathscr{A}\Phi_0 \tag{2}$$

we may write

$$\Psi = F^{-1}\mathscr{A}F_0\Psi_0. \tag{3}$$

It may be shown that

$$\mathscr{A}(r, Z) = \frac{\Phi_{\mathrm{HS}}(Z, r)}{\Phi_0(Z, r)} + \mathrm{O}(\alpha(\alpha Z)). \tag{4}$$

To lowest order we find for nuclei with a closed L shell an excellent representation of $\mathscr{A}$ to be (with r in natural units)

$$\mathscr{A}(r, Z) = \exp\left(Z\eta\alpha^2 r^2 + \frac{\zeta}{Z}\right) \tag{5}$$

where $\eta = 0{\cdot}122$ and $\zeta = -0{\cdot}40$. In figure 1 we illustrate $\ln \mathscr{A}$ for a number of atoms.

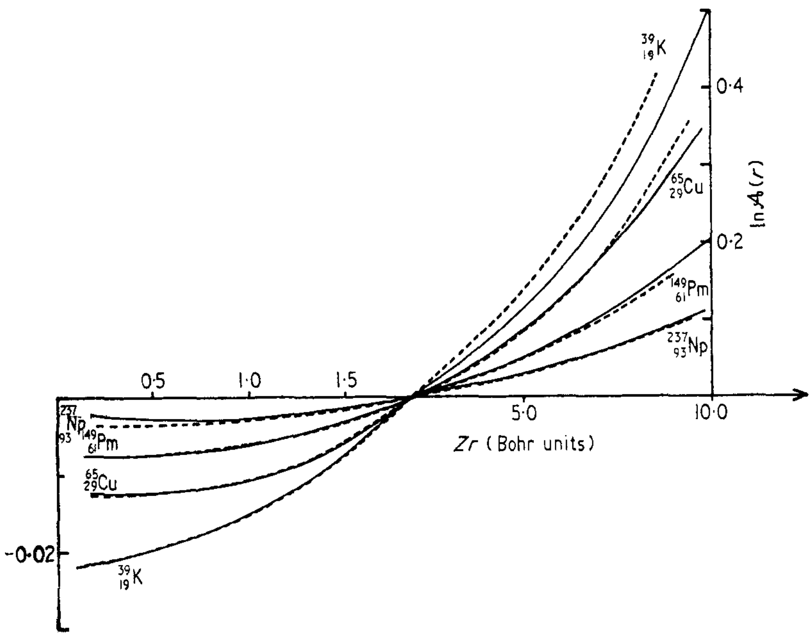

Figure 1. A plot of $\ln \mathscr{A}$ against Zr. The full curves denote exact numerical values, the broken curve is the function $\mathscr{A}$ given in equation (5). Note the change in scale in the negative region.

The FW transformations may be written in the form

$$F = \prod_{n=0}^{\infty} \exp(-\mathrm{i}S^{(n)}) \tag{6}$$

where Bjorken and Drell (1964) give

$$S_0^{(1)} = S^{(1)} = \frac{i\beta}{2m}\left(-\mathrm{i}\alpha_r \frac{\partial}{\partial r}\right).$$

Here α_r and β are Dirac matrices. Thus

$$F^{-1}\mathscr{A}F_0 = \sum_{n=0}^{\infty} \left(\frac{\mathrm{i}\beta\alpha_r}{2m}\right)^n \frac{1}{n!} \frac{\partial^n \mathscr{A}}{\partial r^n} (1+\mathrm{O}(\alpha^2 Z)) \tag{8}$$

which is the Taylor expansion for $\mathscr{A}(r+\frac{1}{2}\mathrm{i}\beta\alpha_r, Z)$. Thus equation (3) for the relativistic 1s wavefunction in a complex atom may be written simply in terms of the corresponding relativistic hydrogenic wavefunctions, to the lowest order, as

$$\Psi = \mathscr{A}(r+\tfrac{1}{2}\mathrm{i}\beta\alpha_r, Z)\Psi_0. \tag{9}$$

To take account of finite nuclear size effects it is only necessary to modify Ψ_0 in equation (9). This is particularly trivial in the case of a uniform charge distribution. To the order we are working to the operator $\mathscr{A}$ is not affected.

Of course, the simple representation of Ψ given in equation (9) is not asymptotically correct as $r \to \infty$ if equation (5) is used. However since $\mathscr{A}$ has only risen to approximately 3 even in the heaviest atoms by the time Ψ_0 has fallen to about 10^{-4} of its maximum value and hence the wavefunction remains normalized and behaves properly over the physically significant region.

Both the many body and finite nuclear size effects tend to reduce the amplitude of the electron wavefunction at the nuclear radius below its hydrogenic value. Relativistic effects tend in the opposite direction and for $Z \geqslant 20$ the relativistic effects win and the amplitude is enhanced compared to its hydrogenic value. Work is in progress to analyse the significance of these effects on K capture cross sections.

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