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# Analytical representation of atomic shellwise electron densities and applications*

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**Abstract.** Analytical expressions of atomic shellwise electron densities have been constructed. Our approach was based on the superposition of Yukawa potentials for the atomic electrostatic potential. The electron density distribution was then established by the Poisson equation. Parameters characterizing the shellwise electrostatic potential and the corresponding electron density distribution were obtained by a fitting procedure utilizing the Hartree-Fock-Slater (HFS) data. These parameters were determined by the atomic number and electron occupation numbers in various states. The accuracy of constructed electron density distributions was tested by comparing their various moments with the corresponding results obtained from other methods. Applications of these atomic shellwise electron densities were made for calculations of the elastic scattering cross section and the mean excitation energy.

## 1. Introduction

In a number of applications, the electrostatic potential and the radial electron density distribution of atoms are required. These applications include calculations of the momentum density and the Compton profile by a local average method (Lam and Platzman 1974, Gadre and Pathak 1981) and the generalized oscillator strength (Kwei et al 1988) and the mean excitation energy (Lindhard and Scharff 1953, Chu and Powers 1972, Tung and Kwei 1985) by a local plasma approximation. Atomic electron density distributions can be obtained by the Thomas–Fermi (TF), the Thomas–Fermi–Dirac (TFD) (Thomas 1954), the Hartree–Fock (HF) (Hartree 1957), the Hartree–Fock–Slater (HFS) (Herman and Skillman 1963) and the Dirac–Hartree–Fock–Slater (DHFS) (Kim 1967, Mayol et al 1984) methods.

Analytical expressions of the atomic potential and electron density distribution are available. An expression in terms of polynomials for the TF potential was used by Latter (1955) and by Gross and Dreizer (1979). Such an expression was rather inaccurate at large and small distances from the nucleus. Also, the superposition of three Yukawa potentials was proposed by Molière (1947) to approximate the TF potentials of atoms. Molière's expression worked better at large radial distances. The analytical form

suggested by Molière was also applied to the TFD potential (Bonham and Strand 1963), the HF potential (Strand and Bonham 1964, Boyd 1977), the DHFS potential (Salvat *et al* 1987) and the interaction of charged particles with atoms (Bethe 1953, Mott and Massey 1965, Salvat *et al* 1985, Salvat and Parallada 1984). In addition, Green *et al* (1969) introduced another analytical expression for the HFS potential. All these works have dealt with the total electron density and its corresponding electrostatic potential. Thus, their results exhibited only the overall distribution with no detailed shell structures. An earlier discussion of the shell structure of atoms is available (Boyd 1976).

In this work, we applied Molière's expressions for the analytical representation of the shellwise atomic potential and electron density distribution. With the superposition of several Yukawa potentials to approximate the HFS potential of any individual shell of an atom, we have derived analytical expressions for the shellwise electron density distributions. These expressions were in terms of parameters dependent on the atomic number and electron occupation numbers in different states. We used the HFS data of atoms to find the best fitting values of these parameters. The accuracy of electron density distributions developed in this work was tested by comparing their various moments with the corresponding results obtained from other methods. Applications of these atomic shellwise electron densities were made for calculations of the elastic scattering cross section and the mean excitation energy.

## 2. Theory

The electrostatic potential of an atom may be approximated by (Molière 1947).

$$V(r) = \frac{1}{r} \sum_i \sum_{j=1}^{n_i} Z_i \alpha_{ij} \exp(-\beta_{ij} r) \tag{1}$$

where $r$ is the radial distance from the nucleus, $Z_i$ $(i = K, L, M, \ldots)$ is the electron occupation number of the $i$th shell, and $\alpha_{ij}$ and $\beta_{ij}$ are free parameters. Note that atomic units are used throughout this paper unless otherwise specified. The electron charge density, $Q(r)$, is related to the electrostatic potential through the Poisson equation as

$$\nabla^2 V(r) = -4\pi Q(r). \tag{2}$$

Thus the charge density corresponding to the potential of equation (1) is given by

$$Q(r) = \sum_i \frac{Z_i}{4\pi r^2} \delta(r) - \sum_i \sum_{j=1}^{n_i} \frac{Z_i}{4\pi r} \alpha_{ij} \beta_{ij}^2 \exp(-\beta_{ij} r) \tag{3}$$

where the delta function term is contributed by the nucleus. Using equation (3), we obtain the radial electron density distribution of the $i$th shell as

$$\rho_i(r) = \frac{Z_i}{4\pi r} \sum_{j=1}^{n_i} \alpha_{ik} \beta_{ij}^2 \exp(-\beta_{ij} r). \tag{4}$$

Therefore, the total electron density distribution of an atom may be calculated from

$$\rho(r) = \sum_i \rho_i(r). \tag{5}$$

Note that equation (4) shows correct asymptotic behaviour at large $r$ and a divergence as $r^{-1}$ near the origin, as compared to the HFS density which decreases exponentially

at large $r$ and diverges more slowly than $r^{-1}$ near the nucleus where it is assumed to be a point charge (Mayol *et al* 1984). Although the divergence of the density may be improved by certain ways (Parr and Yang 1989), equation (4) is sufficiently accurate and general for most applications.

The zero-order moment of the electron density distribution gives the constraint

$$\sum_{j=1}^{n_i} \alpha_{ij} = 1. \tag{6}$$

In addition, various moments defined by

$$\langle r^n \rangle_i = \int_0^\infty r^n [4\pi r^2 \rho_i(r)] \, dr \tag{7}$$

may be examined by comparing their results calculated using equation (4) with those using, for instance, the HFS electron density distribution. The $n$th moment of the total electron density distribution is given by

$$\langle r^n \rangle = \sum_i \langle r^n \rangle_i. \tag{8}$$

In this work, we have fitted equation (4) to the HFS electron density distribution data to derive $\alpha_{ij}$ and $\beta_{ij}$. We chose $n_i = 2$, 3 and 5 for K, L and M shells, respectively. Parameters $\alpha_{ij}$ and $\beta_{ij}$ of the K shell can be approximated by the relations

$$\alpha_{Kj} \text{ or } \beta_{Kj'} = (A + BZ_{2s})Z^a \tag{9}$$

for $j = 1$ and $j' = 1$, 2, and

$$\alpha_{K2} = 1 - \alpha_{K1} \tag{10}$$

where $Z$ is the atomic number, $Z_{2s}$ is the number of electrons in the 2s subshell, and $A$, $B$ and $a$ are constants listed in table 1. Note that the $\beta_{Kj}$ are linearly proportional to $Z$ since $a = 1$. This can be understood from the $Z$ dependence of the exponential wavefunction for the K shell of hydrogen-like atoms. The proportional constants in the $\beta_{Kj}$ were introduced to enhance the accuracy of equation (9) by fittings.

Approximate relations for $\alpha_{ij}$ and $\beta_{ij}$ of the L shell applying to all atoms except Li and Be are

$$\alpha_{Lj} \text{ or } \beta_{Lj'} = [C + D(Z_{2p})^b + EZ_{3s} + FZ_{3p} + GZ_{3d}](Z - 2) \tag{11}$$

for $j = 1$, 2 and $j' = 1$, 2, 3, and

$$\alpha_{L3} = 1 - \alpha_{L1} - \alpha_{L2} \tag{12}$$

with all constants listed in table 2. Here $Z_{2s}$, $Z_{2p}$, $Z_{3s}$, $Z_{3p}$ and $Z_{3d}$ are the number of electrons in the 2s, 2p, 3s, 3p and 3d subshells, respectively. The parameters $\beta_{Lj}$ are proportional to $Z - 2$ except for Li and Be atoms where $Z_{2p} = 0$. This agrees with the

**Table 1.** Values of constants in equation (9).

|              | $A$     | $B$     | $a$ |
|--------------|---------|---------|-----|
| $\alpha_{K1}$ | −0.2259 | −0.0108 | 0   |
| $\beta_{K1}$  | 2.7635  | 0.224   | 1   |
| $\beta_{K2}$  | 1.1995  | 0.116   | 1   |

**Table 2.** Values of constants in equation (11).

|  | C | D | E | F | G | b |
|---|---|---|---|---|---|---|
| $\alpha_{L1}$ | 1.44 | −0.0375 | 0.036 2 | 0.091 7 | 0.018 6 | 1 |
| $\alpha_{L2}$ | −2.54 | 0.1 | −0.217 5 | −0.15 | −0.057 2 | 1 |
| $\beta_{L1}$ | 1.25 | −0.0476 | 0.051 33 | 0.005 55 | 0.003 1 | 1 |
| $\beta_{L2}$ | 0.9942 | −0.0275 | 0.017 23 | 0.006 95 | 0.001 48 | 1 |
| $\beta_{L3}$ | 0.6151 | −0.1503 | 0.036 33 | 0.008 333 | 0.004 767 | 0.298 |

rule suggested by Kregar and Weisskopf (1982) that an electron in the L shell feels a net nuclear charge $Z - 2$ owing to the shielding of nucleus by the two electrons in the K shell. This rule is no good for atoms with $Z_{2p} = 0$ since there is an appreciable probability of finding 2s subshell electrons near the nucleus. We therefore must add a term $H_j$ to $\beta_{Lj}$ to account for this effect. We found that $H_1 = 1.143\,75 - 0.321\,875Z_{2s}$, $H_2 = 0.850\,041 - 0.260\,88Z_{2s}$, and $H_3 = 0.163\,924 - 0.281\,1Z_{2s}$. It is worthwhile to mention that the above rule is different from Slater's rule (Slater 1960, Karplus and Porter 1970) in the determination of effective nuclear charge. Our approach is based on equation (4), an empirical formula containing a summation of several terms, to describe the electron density and to fit the HFS data. Not every term in this formula necessarily corresponds to a subshell composing the shell. Therefore, the dependence of effective nuclear charge defined in equation (11) on atomic number and electron occupational number is only qualitative and conceptually different from that defined in Slater's rule. This latter rule made use of a hydrogenic wavefunction by retaining only the maximum power of $r$ in the polynomial which multiplies the exponential factor. It applied reasonably well to the determination of orbital energies but not of electron densities.

Similarly, parameters $\alpha_{ij}$ and $\beta_{ij}$ for the M shell with $Z_{3p} \neq 0$ are approximated by

$$\alpha_{Mj} \text{ or } \beta_{Mj'} = [S + T(Z_{3p})^c](Z - 10)^d / (Z_M)^e \tag{13}$$

for $j = 1, 2, 3, 4$ and $j' = 3, 4, 5$,

$$\alpha_{M5} = 1 - \alpha_{M1} - \alpha_{M2} - \alpha_{M3} - \alpha_{M4} \tag{14}$$

$$\beta_{M1} = 0.9\beta_{K2} \tag{15}$$

and

$$\beta_{M2} = 0.9\beta_{L2} \tag{16}$$

where $(Z - 10)$ in equation (13) is the net nuclear charge shielded by electrons in the K and L shells and constants in this equation are listed in table 3. For atoms with

**Table 3.** Values of constants in equation (13).

|  | S | T | c | d | e |
|---|---|---|---|---|---|
| $\alpha_{M1}$ | 0 | 0.0638 | 1 | 0 | 1 |
| $\alpha_{M2}$ | 0.52 | −0.72 | 0.63 | 0 | 1 |
| $\alpha_{M3}$ | 1.81 | 0.2 | 1 | 0 | 0 |
| $\alpha_{M4}$ | −4.8 | −0.83 | 1 | 0 | 0 |
| $\beta_{M3}$ | 0.916 | −0.058 | 0.95 | 1 | 0 |
| $\beta_{M4}$ | 0.9225 | −0.362 | 0.26 | 1 | 0 |
| $\beta_{M5}$ | 0.7245 | −0.310 | 0.16 | 1 | 0 |

$Z_{3p} = 0$, we must add a term $X_j$ to $\alpha_{Mj}$ and another term $Y_j$ to $\beta_{Mj}$. We found that $X_1 = (0.032 + 0.019 Z_{3s})/Z_M$, $X_2 = (0.48 + 0.145 Z_{3s})/Z_M$, $X_3 = 0$, $X_4 = 0$ and $X_5 = -X_1 - X_2$; $Y_1 = 0$, $Y_2 = 0$, $Y_3 = 1.0469 - 0.1392 Z_{3s}$, $Y_4 = 0.7918 - 0.4547 Z_{3s}$ and $Y_5 = 0.5703 - 0.4496 Z_{3s}$. These expressions are valid for $Z$ up to 18. For atoms with greater $Z$ values, added electrons are placed in the 4s subshell before the M shell is completely filled. Taking these additional electrons into consideration, the above formulae for $\alpha_{Mj}$ and $\beta_{Mj}$ must be modified.

## 3. Results

Using the above formulae, we have calculated the shellwise electron density distribution of atoms. Figures 1, 2 and 3 show comparison of the present results with the HFS data (Herman and Skillman 1963, Mayol *et al* 1984). Good agreement is found for all cases. Figure 4 shows a comparison of the total electron density distribution for sulphur atoms calculated presently, by Salvat *et al* (1987) and using the HFS method. The present results, containing detailed shell structures, show good agreement with the HFS data, whereas those of Salvat *et al* indicate only an overall structure without shell peaks. The electrostatic potential for boron atoms is plotted in figure 5 with $ZV(r)/r$ against the radial distance $r$. The present results are also compared with the HFS data and other analytical potentials (Salvat *et al* 1987, Green *et al* 1969). It is seen that our results are in better agreement than other potentials as compared to the HFS data.

The accuracy of analytical expressions for the shellwise electron density distribution can be tested by examining the various moments of this distribution as defined in equations (7) and (8). Several values of these moments for argon atoms calculated in this work are compared with those of Cowan *et al* (1966) in table 4. Reasonably good
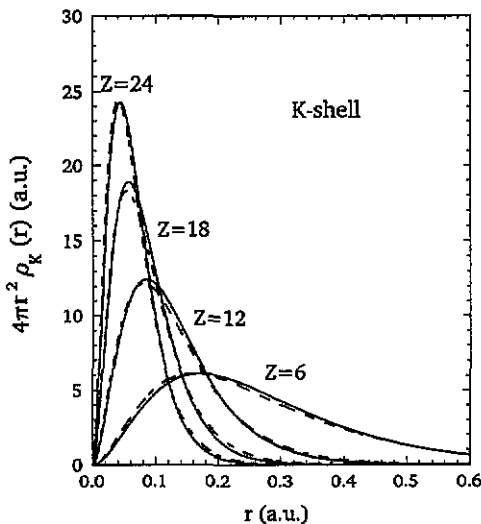


**Figure 1.** A plot of the K shell electron density distribution as a function of radial distance from the nucleus for several atoms. The full and broken curves are, respectively, results of the HFS data and this work. All quantities are in atomic units.
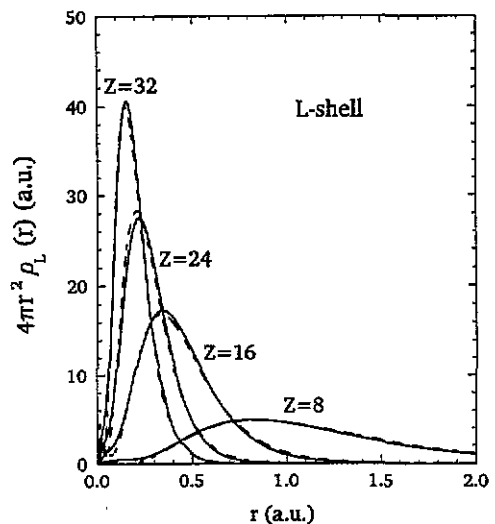
**Figure 2.** A plot of the L shell electron density distribution as a function of radial distance from the nucleus for several atoms. The full and broken curves are, respectively, results of the HFS data and this work. All quantities are in atomic units.
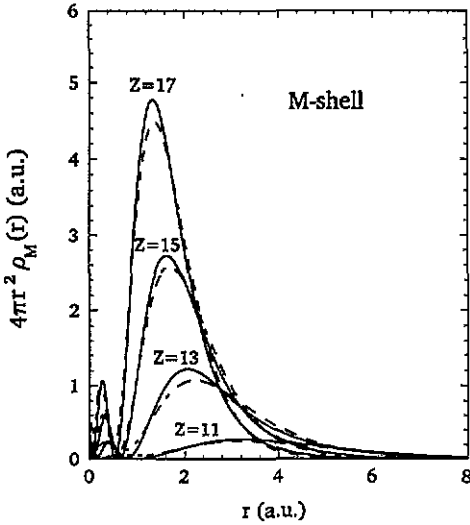
**Figure 3.** A plot of the M shell electron density distribution as a function of radial distance from the nucleus for several atoms. The full and broken curves are, respectively, results of the HFS data and this work. All quantities are in atomic units.
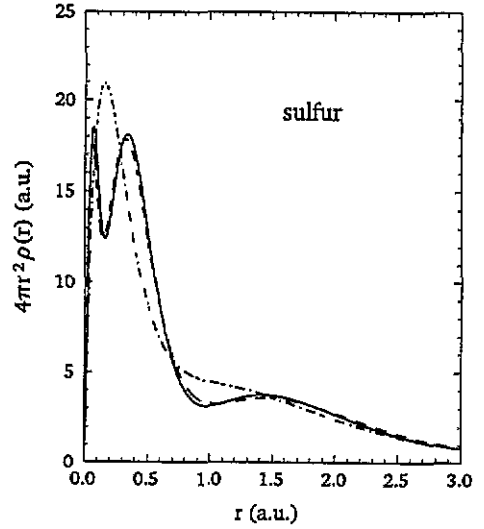
**Figure 4.** A plot of the total electron density distribution as a function of radial distance from the nucleus for sulphur atoms. The full, broken and chain curves are, respectively, results of the HFS data, this work and Salvat *et al* (1987). All quantities are in atomic units.
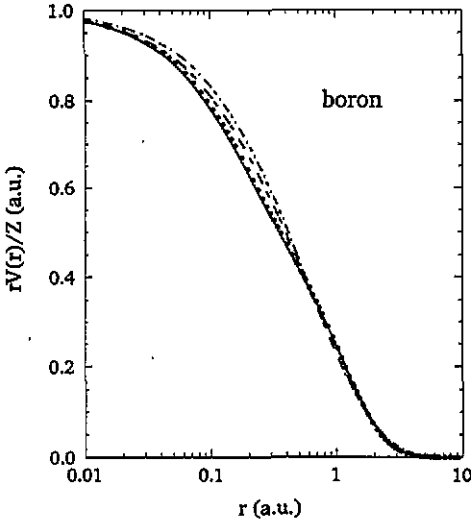


**Figure 5.** A plot of the electrostatic potential multiplying by $r/Z$ for boron atoms, where $r$ is the radial distance from the nucleus and $Z$ is the atomic number. The full circles, full, broken and chain curves are, respectively, results corresponding to the HFS data, this work, Salvat *et al* (1987) and Green *et al* (1969). All quantities are in atomic units.

agreement in this comparison ensures that the shellwise electron density distribution of equation (4) is valid over a wide range of radial distances.

## 4. Applications

The form factor for elastic interaction of an incident electron of energy $E$ with an

**Table 4.** Moments of the electron density distribution of argon atoms in atomic units.

| | | $\langle r^{-1} \rangle$ | $\langle r \rangle$ | $\langle r^2 \rangle$ | $\langle r^4 \rangle$ | $\langle r^6 \rangle$ |
|---|---|---|---|---|---|---|
| Present work | K shell | $3.57 \times 10^1$ | $1.77 \times 10^{-1}$ | $2.20 \times 10^{-2}$ | $6.74 \times 10^{-4}$ | $4.29 \times 10^{-5}$ |
| | L shell | $3.08 \times 10^1$ | $3.11 \times 10^0$ | $1.42 \times 10^0$ | $6.11 \times 10^{-1}$ | $4.59 \times 10^{-1}$ |
| | M shell | $7.76 \times 10^0$ | $1.22 \times 10^1$ | $2.24 \times 10^1$ | $1.16 \times 10^2$ | $9.93 \times 10^2$ |
| | total | $7.41 \times 10^1$ | $1.55 \times 10^1$ | $2.39 \times 10^1$ | $1.17 \times 10^2$ | $9.94 \times 10^2$ |
| Cowan *et al* | K shell | $3.52 \times 10^1$ | $1.72 \times 10^{-1}$ | $1.98 \times 10^{-2}$ | $5.02 \times 10^{-4}$ | $2.43 \times 10^{-5}$ |
| (1966) | L shell | $2.82 \times 10^1$ | $3.04 \times 10^0$ | $1.42 \times 10^0$ | $5.05 \times 10^{-1}$ | $3.11 \times 10^{-1}$ |
| | M shell | $7.28 \times 10^0$ | $1.21 \times 10^1$ | $2.19 \times 10^1$ | $1.12 \times 10^2$ | $9.96 \times 10^2$ |
| | total | $7.07 \times 10^1$ | $1.53 \times 10^1$ | $2.33 \times 10^1$ | $1.12 \times 10^2$ | $9.96 \times 10^2$ |

atom with electron density distribution, $\rho(r)$, is given by (Bethe and Jackiw 1968)

$$F(q) = \int_0^\infty \frac{\sin(qr)}{qr} 4\pi r^2 \rho(r) \, dr \tag{17}$$

where $q = 2(2E)^{1/2} \sin(\theta/2)$ is the momentum transfer and $\theta$ is the scattering angle. Substituting equations (4) and (5) into equation (17), we get

$$F(q) = \sum_i \sum_{j=1}^{n_t} Z_i \alpha_{ij} \beta_{ij}^2 / (\beta_{ij}^2 + q^2). \tag{18}$$

Thus a shellwise contribution to the form factor (Weyrich *et al* 1979) may be obtained. For incident electron energy above the Born threshold, i.e. $E \geqslant 15Z^2$ eV, the elastic scattering differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \frac{4}{q^4} [Z - F(q)]^2 \tag{19}$$

where $d\Omega = 2\pi(\sin \theta) \, d\theta$ is the differential solid angle in the direction of the scattered electron. Substituting equation (18) into equation (19) and taking the limit $q \to 0$, we obtain

$$d\sigma/d\Omega = \tfrac{1}{9} \langle r^2 \rangle^2 \tag{20}$$

where $\langle r^2 \rangle$ is the second-order moment of electron density distribution. Thus, the elastic scattering differential cross section for small $q$ may be in terms of the second order moment of electron density distribution of the interacting atoms (Ibers 1958).

In figure 6, we compare the results of our calculations using equations (17) and (18) for the form factor of neon atoms with those derived using HFS electron densities and those of Salvat *et al* (1987). It is seen that the total electron density distribution of Salvat *et al* leads to a form factor in good agreement with the HFS data only at small $q$. Our results, however, are in good agreement with the HFS data at any momentum transfer. It is also seen that $F(q)$ is contributed mainly from inner shells at large $q$ but from outer shells at small $q$. The elastic scattering differential cross section of electrons with different energies in sodium is plotted in figure 7 as a function of scattering angle. It is seen that our differential cross sections, calculated using equations (18) and (19), agree fairly well with those computed using the HFS electron densities. Furthermore, elastic scatterings are predominantly in the forward direction with smaller angle scattering for higher energy electrons.
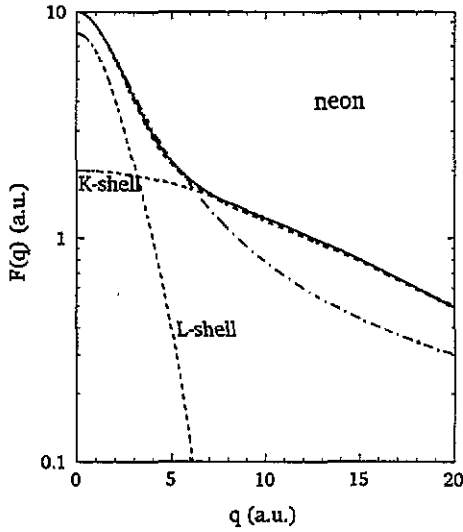
**Figure 6.** A plot of the elastic scattering form factor as a function of momentum transfer for neon atoms. The full, broken and chain curves are, respectively, results corresponding to the HFS data, this work and Salvat *et al* (1987). Shellwise contributions calculated using equation (18) are plotted separately. All quantities are in atomic units.
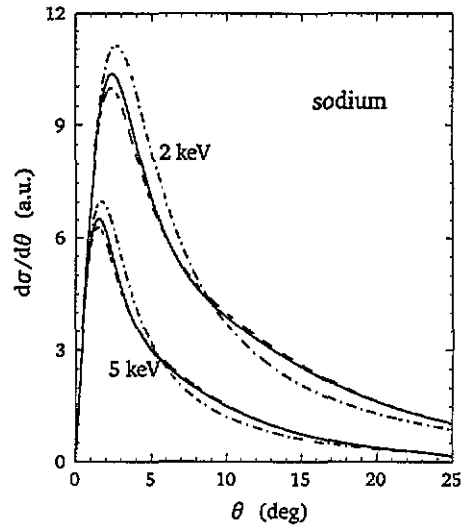
**Figure 7.** A plot of the elastic scattering differential cross section, in atomic units, as a function of scattering angle for sodium atoms and different electron energies. The full, broken and chain curves are, respectively, results corresponding to the HFS data, this work and Salvat *et al* (1987).

Another application of the electron density distribution is the mean excitation energy in the local plasma approximation. According to the Bethe theory (Bethe 1930), the stopping power for charged particles may be given in terms of the mean excitation energy, $I$, of the target material. Based on the local plasma approximation (Lindhard and Scharff 1953), we can express the mean excitation energy of the $i$th shell as (Meltzer *et al* 1990, Tung *et al* 1988)

$$\ln I_i = \frac{1}{Z_i} \int_0^\infty 4\pi r^2 \rho_i(r) \ln(\gamma_i \omega_{pi}) \, dr \tag{21}$$

where $\omega_{pi} = [4\pi \rho_i(r)]^{1/2}$ is the free electron plasma frequency and $\gamma_i$ is a parameter related to the plasma damping coefficient, both associated with the $i$th shell.

Substituting equation (4) into equation (21), we can calculate the mean excitation energy of each shell of an atom. Figure 8 is the results of these calculations for the mean excitation energy of the K, L and outermost shells as a function of atomic number. Note that we have taken $\gamma_i = 1$ in these calculations in order to compare our results with those of Meltzer *et al* (1990) using the same approximation. It is seen that our results are in good agreement with those of Meltzer *et al*, however, discrepancies exist for results between the local plasma approximation and the oscillator strength method (Oddershede and Sabin 1984). These discrepancies are understood as due to the adoption of $\gamma_i = 1$ which neglects the contribution from revolution frequencies. By the assumption of plasma oscillation frequency equal to the revolution frequency, it was found that (Lindhard and Scharff 1953) $\gamma_i = 1.414$. The actual value of $\gamma_i$ is mostly between (Tung *et al* 1988) 1 and 2.
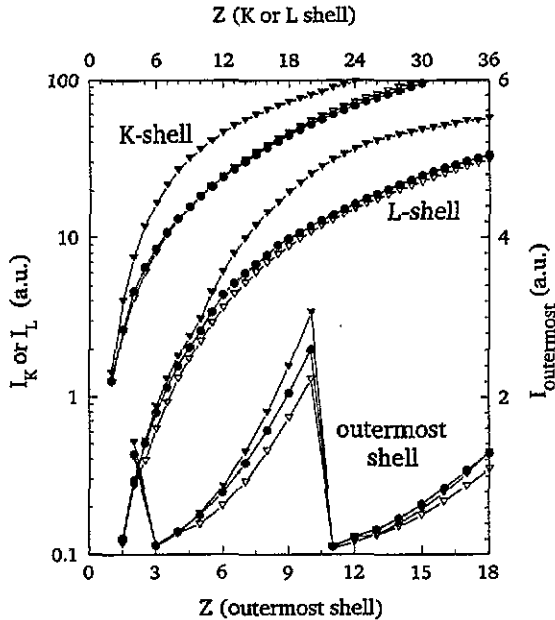
**Figure 8.** A plot of the mean excitation energy, in atomic units, for K, L and outermost shells as a function of atomic number. Data are from calculations using the oscillator strength method (Oddershede and Sabin 1984), ▼; the local plasma approximation (Meltzer *et al* 1990), ▽; and equations (4) and (21), ●.

## 5. Conclusions

Analytical expressions of atomic shellwise electron densities and electrostatic potentials of the present work are quite accurate in comparison with the HFS data. The accuracy of these expressions was confirmed by comparing their various moments with the corresponding results obtained from other methods. Applications of these expressions were made for calculations of the elastic scattering cross section and the mean excitation energy.

For solid atoms, our electron density distributions can still be applied to inner shells due to the negligible influence of neighbouring solid atoms. For outer shell electrons, one must take this influence into consideration. The extension of this work to electron density distributions of solid atoms is under way.

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