Analytic atomic form factors for atoms and ions with $Z \leq 54$*

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The independent-particle model of Green, Sellin, and Zachor (GSZ) with parameters fixed by an *ab initio* variational procedure is used to obtain approximate atomic form factors for all atoms and ions with $Z \leq 54$. For convenience of application we replace the electron density obtained using Poisson's equation from the GSZ potential by an approximating sum of Debye or Yukawa functions. This sum implies a corresponding approximating sum of Debye or Yukawa potentials for the GSZ potential. These steps lead to convenient analytic form factors whose parameters may all be fixed in terms of the two GSZ parameters. In this way, we can define approximate form factors for any of the 1485 species with $Z \leq 54$. For most of these (~ 1300 ionic species), no previous form-factor calculations have been reported.

I. INTRODUCTION

As a result of four recent studies,[1-4] the two parameters characterizing the independent-particle-model (IPM) potential of Green, Sellin, and Zachor[5] (GSZ) have been determined for the 1485 atoms and positive ions having 54 or fewer protons in the nucleus. These potential parameters were obtained by an *ab initio* variational procedure[1,3] in which the two potential parameters are varied so as to minimize the expectation value of the exact Hamiltonian of the particular species in question. In the present work we use electronic densities associated with these GSZ-IPM potentials to obtain the atomic form factor of each of these species. For convenience of application we represent these form factors in analytic forms whose parameters can be readily obtained from those listed in Ref. 4.

II. GSZ-IPM POTENTIAL

The GSZ-IPM potential can be written in atomic units as

$$V(r) = 2\{(N-1)[1-\Omega(r)] - Z\}/r, \tag{1}$$

with the screening function $\Omega(r)$ given by

$$\Omega(r) = [(\eta/\xi)(e^{\xi r} - 1) + 1]^{-1}, \tag{2}$$

and where N is the total number of electrons in the atom or ion, Z is the number of protons in the nucleus of the species in question, and r is the distance from the center of the atom or ion. The parameters η and ξ are determined by the variational procedure[1,3] mentioned above.

If we assume an atom or ion has a spherically symmetric electron density $\rho(r)$, we can write the elastic form factor $F(q)$ as

$$F(q) = 4\pi \int_0^\infty \rho(r) \frac{\sin qr}{qr} r^2 \, dr \tag{3}$$

where q is the magnitude of the momentum transferred in an elastic collision in which the atom or ion was initially at rest. Knowing $V(r)$, the average potential an electron experiences at a distance r from the atomic center, we can determine $\rho(r)$ and, therefore, $F(q)$. We have a choice of two methods for obtaining $\rho(r)$. Using $V(r)$, given by Eq. (1), as the atomic potential, we can solve the Schrödinger equation to obtain the single-electron wave functions. The electron density is then given by

$$\rho(\vec{\mathbf{r}}) = \sum_{i=1}^{N} \psi_i^*(\vec{\mathbf{r}}) \psi_i(\vec{\mathbf{r}}), \tag{4}$$

where $\psi_i(\vec{\mathbf{r}})$ is the wave function of the ith electron. Alternatively, we can obtain $\rho(r)$ from Poisson's equation. The potential in Eq. (1) consists of a contribution from the electron-nucleus interaction and a contribution due to the interaction between an electron at r and the other $N-1$ electrons. From Eq. (1) we see that we can represent the contribution *per electron* which this latter interaction makes to $V(r)$ as

$$v(r) = 2[1 - \Omega(r)]/r. \tag{5}$$

Using $v(r)$ in Poisson's equation we can obtain the average density per electron. We find that

$$\rho(r)/N = (1/4\pi r)\, d^2\Omega/dr^2$$

$$= (\eta\xi e^{-\xi r}/4\pi r) p(\xi r), \tag{6}$$

where

$$p(\xi r) = \frac{H + (H-1)e^{-\xi r}}{[H - (H-1)e^{-\xi r}]^3} \tag{7}$$

and

$$H = \eta/\xi. \tag{8}$$

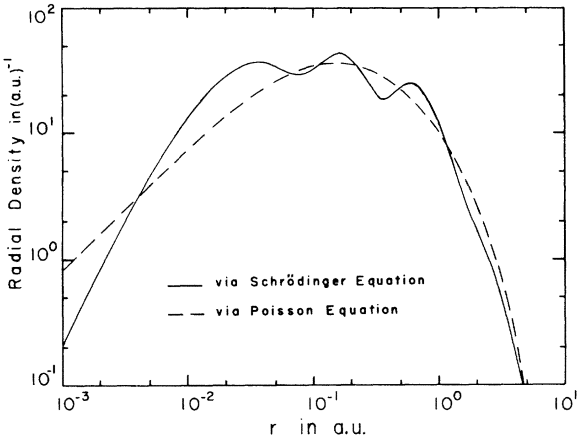

FIG. 1. Radial potential for the neutral zinc atom obtained from Schrödinger's equation (solid line) and Poisson's equation (dashed line).

The GSZ potential is not self-consistent and, consequently, the two densities of Eqs. (4) and (6) are not identical. In particular, the density of Eq. (4) shows shell structure, but the density of Eq. (6) does not. In Fig. 1, we show the radial densities, $4\pi r^2\rho(r)$, of neutral zinc obtained by both methods. The solid line, which represents the radial densities obtained from the wave functions, shows obvious shell structure, and it agrees very closely with the radial density for zinc obtained by Herman and Skillman.[6] The dashed line, which represents the radial density obtained using Poisson's equation, evidences no shell structure, but represents a reasonable "smooth average" of the solid curve which could be useful for many purposes. Furthermore, as we shall see, such functions can be accurately represented in a way which leads to an analytic expression for the form factor [Eq. (3)]. In this way, we can obtain an analytic form factor for any of the 1485 species for which the GSZ potential parameters are known.

III. ANALYTIC FORM FACTOR

Substituting Eq. (6) into Eq. (3) and with $R = \xi r$, we can express the form factor as

$$F_{\xi,\eta}(q) = \frac{N\eta}{q}\int_0^\infty e^{-R}p(R)\sin(qR/\xi)\,dR, \tag{9}$$

where we have indicated explicitly the dependence of the form factor on ξ and η. The integral in Eq. (9) cannot be performed analytically with $p(R)$ given by Eq. (7). However, $p(R)$ can be accurately approximated by a sum of exponentials which leads to an analytic form factor. Thus, if we approximate Eq. (7) by

$$p_E(R) = Ae^{-\alpha R} + Be^{-\beta R} + Ce^{-\gamma R}, \tag{10}$$

the integral in Eq. (9) becomes

$$F_{\xi,\eta}(q) = N\eta\xi\left(\frac{A}{q^2+\xi^2(1+\alpha)^2} + \frac{B}{q^2+\xi^2(1+\beta)^2} + \frac{C}{q^2+\xi^2(1+\gamma)^2}\right). \tag{11}$$

It should be noted that the density function $\rho(r)$ corresponding to $p(r)$ [see Eq. (6)] is the well-known Debye function or Yukawa function and that the corresponding potential function is also a Debye or Yukawa function.

To reduce the number of parameters in Eq. (10) and to ensure a good fit, we demand that

$$\lim_{R\to\infty} p_E(R) = \lim_{R\to\infty} p(R) = 1/H^2,$$

$$p_E(0) = p(0) = 2H - 1, \tag{12}$$

and

$$\int n_E(R)\,d^3r = \int n(R/\xi)\,d^3(R/\xi) = 1,$$

where $n_E(R) = Hp_E(R)e^{-R}/4\pi R$. These conditions can be satisfied if we choose

$$A = \left(\frac{1}{H} - \frac{1}{H^2} - \frac{2H-1-1/H^2}{(1+\beta)^2}\right)/D, \tag{13}$$

$$B = \left(\frac{2H-1-1/H^2}{(1+\alpha)^2} - \frac{1}{H} + \frac{1}{H^2}\right)/D, \tag{14}$$

$$C = 1/H^2, \tag{15}$$

$$\gamma = 0 \tag{16}$$

with $D = 1/(1+\alpha)^2 - 1/(1+\beta)^2$.

For the 1485 atoms and positive ions with $Z \leq 54$, the values of ξ and η, presented in Ref. 4, yield values of H which range between 0.5 and 5.5. By nonlinear least-squares fitting of $p_E(R)$ to $p(R)$, we determined the two remaining unfixed parameters, α and β, for $0.5 \leq H \leq 6.0$ and $0 \leq R \leq 5.0$. The values of α and β we obtained are presented in Table I along with the corresponding values of H. The fits we obtained are excellent for values of H such that $0.7 \leq H \leq 1.5$. For this range of H, with the values of α and β in Table I, $p_E(R)$ is usually well within 1% of $p(R)$ in the range of R we considered. The quality of the fits gradually degrades as H increases from 1.5 or decreases from 0.7. Nevertheless, they are still very good. This can be seen in Fig. 2, where we have plotted

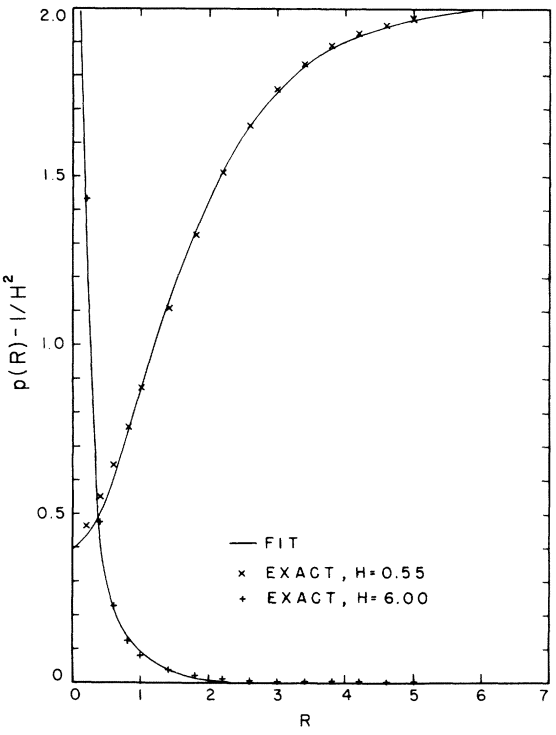

FIG. 2. The solid lines are plots of $p_E(R)-1/H^2$ vs R for $H=0.55$ and $H=6.0$ obtained with the appropriate values of α and β from Table I. The ×'s and +'s are the values of $p(R)-1/H^2$ plotted vs R for $H=0.55$ and $H=6.0$, respectively.

$p(R)-1/H^2$ and $p_E(R)-1/H^2$ against R for $H=0.55$ and for $H=6.00$. These plots represent the two poorest fits we obtained, with the largest meaningful differences ($<12\%$) occurring for $R\approx 0.2$ to 0.4.

As a further check on the quality of the fits, using Eq. (6), we took the antiderivative of $He^{-R}p_E(R)$ twice with respect to R and compared the resulting screening function with the initial GSZ function [see Eq. (2)]. In this comparison we found that for $0.5\leq H\leq 3.5$, there is always less than a 2% difference and usually less than a 1% difference between the two functions for all values of R for which the screening function is non-negligible. For $3.5\leq H\leq 6.0$, the percent differences are always less than 10%. Thus, over the range of H of interest to us, our fit gives an adequate representation of both the density and potential as sums of Yukawa or Debye functions.

IV. CONCLUSIONS

The potential function corresponding to our analytic form factor is

$$V_E(r)=2[N-1-Z-(N-1)\Omega_E(r)]/r \qquad (17)$$

with

$$\Omega_E(r)=\frac{Ae^{-(1+\alpha)\xi r}}{(1+\alpha)^2}+\frac{Be^{-(1+\beta)\xi r}}{(1+\beta)^2}+Ce^{-\xi r}. \qquad (18)$$

This representation of the GSZ potential as a sum of Coulomb and Yukawa potentials may, of itself, be a useful by-product of our study. These potentials **have** been subjected to a great variety of analyses **in** nuclear and particle physics, some of which might be adapted to atomic physics. Since the density we are attempting to fit is itself a smoothed version of the actual density, we feel the quality of the fits we present here are more than adequate for most purposes. When more accurate results are needed, the density obtained from Eq. (4) should be used and the desired form factors calculated numerically.[8]

With $F_{\xi,\eta}(q)$ given by Eq. (11), A, B, C, and γ given by Eqs. (13)–(16), and α and β obtained by interpolation from Table I, we have an analytic expression for the form factor of all atoms and positive ions with $Z\leq 54$. The required values of η and ξ and, therefore, of H can be readily obtained from Ref. 4. In Figs. 3 and 4 we have plotted samples of $F_{\xi,\eta}(q)$ obtained from Eq. (11) for several different species against $X=q/4\pi=\sin(\theta/2)/\lambda$ where θ is the scattering angle and λ is the wavelength of the scattered particle. We have included in these two figures corresponding plots of $F(q)$ obtained from Hartree-Fock (HF) wave functions[9,16] and Thomas-Fermi (TF) potentials,[10,11] where such results exist.

The relationships between the HF, TF, and GSZ form factors illustrated in these graphs are fairly typical. Neither the plots of the TF nor those of

TABLE I. Values of α and β obtained by fitting $p_E(R)$ to $p(R)$, along with the corresponding values of H.

H	α	β	H	α	β
0.500	1.0949	1.0954	1.050	2.1091	1.0008
0.525	1.1158	1.1036	1.100	2.2271	1.0038
0.550	1.1271	1.1212	1.150	2.3397	1.0080
0.575	1.1477	1.1346	1.300	2.6701	1.0256
0.600	1.1489	1.1442	1.500	3.1041	1.0560
0.625	1.1612	1.1555	2.000	4.1915	1.1497
0.650	1.1764	1.1591	2.500	5.2712	1.2556
0.675	1.1709	1.1798	3.000	6.3233	1.3666
0.700	1.1910	1.1735	3.500	7.3406	1.4808
0.750	1.2981	1.1105	4.000	8.3223	1.5983
0.800	1.4863	1.0427	4.500	9.2732	1.7209
0.854	1.6302	1.0182	5.000	10.189	1.8462
0.900	1.7599	1.0066	5.500	11.074	1.9756
0.950	1.8831	1.0013	6.000	11.931	2.1090

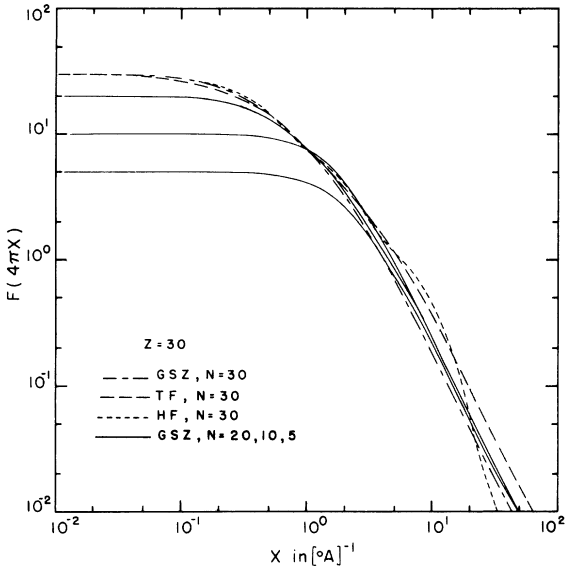

FIG. 3. Plots of the GSZ from factor vs $X = \sin(\theta/2)\lambda$ for various species with $Z = 30$. The appropriate values of N can be found on the graph. Plots of the TF and HF form factors for the neutral are also shown.

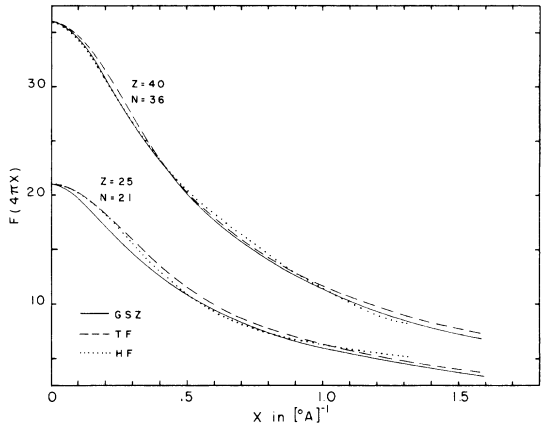

FIG. 4. Plots of the form factors for two ionic species calculated by the GSZ, TF, and HF methods.

the GSZ form factors have any of the undulations resulting from shell structure in the electron density which the plots of the HF form factors evidence. Nevertheless, both the TF and GSZ form factors represent rather good smoothed averages of the HF form factors for $X \lesssim 13$ Å^{-1}. Since the parameter variation of the GSZ potential reflects the shell structure of the periodic table, the $F(q)$ of GSZ is usually in better agreement with that of HF than is the $F(q)$ of TF for $1.0 \leq X < 10.0$ Å^{-1}. For large $X > 15$ Å^{-1} both the TF and GSZ form factors are too large. Several workers[12,13] have shown that at large values of X, the form factor should go as X^{-4}, but the GSZ form factor in Eq. (11) goes as X^{-2} for large X and, using Molière's[7] fit to the TF potential, we can obtain an expression for $F(q)$ similar to Eq. (11) with the corresponding large-X behavior. This behavior of the IPM and TF form factors at large X is to be expected since the large-X behavior of the form factor is determined by the small-r behavior of the electron density, and both the GSZ-IPM and the TF model yield densities via Poisson's equation which are singular at the origin (GSZ as r^{-1} and TF as $r^{-3/2}$). Furthermore, for such large values of X, the dominant contribution to the form factor comes from inner-shell electrons, particularly K-shell electrons. Except for species with small Z, the K-shell electrons should be handled relativistically. Since this work is based upon the nonrelativistic Schrödinger equation, caution should be exercised on their use for $X > 10$–13 Å^{-1}.

For $X < 10$–13 Å^{-1} the analytic form factors presented here, which are very simple to obtain, are rather good approximations to the results of the more sophisticated and accurate calculations which are available for neutral[14,15] and some ionized species.[16–19] More importantly, the form factors encompassed by this work can be used to represent many (~1300) ionic species for which no such previous calculations are available.

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