Comment on independent-particle-model form factors for atoms and ions with $Z \leq 54$

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Using single-electron wave functions associated with the independent-particle-model potential of Green, Sellin, and Zachor, with parameters obtained by an *ab initio* variational procedure, one can obtain accurate atomic form factors for any atom and positive ion with $Z \leq 54$. Sample results are found to compare favorably with available Hartree-Fock results. However, for most positive ions with $Z \leq 54$, Hartree-Fock or Hartree-Fock-Slater calculations of the form factors do not presently exist.

I. INTRODUCTION

The independent-particle-model (IPM) potential of Green, Sellin, and Zachor[1] (GSZ) was used recently[2] in conjunction with the Poisson equation to obtain approximate, analytic atomic form factors for all neutral and positively ionized species with 54 or fewer protons in the nucleus. The two parameters characterizing the GSZ potential for each of these species have previously been obtained by an *ab initio* variational method.[3-6] Although these analytic form factors should be adequate for many applications, if more accurate form factors are required, the GSZ potential may readily be used to obtain quantum-mechanical form factors comparable in accuracy with those obtained from more elaborate atomic models.

II. QUANTUM-MECHANICAL ELASTIC ATOMIC FORM FACTORS

We assume each species has a spherically symmetric electron density $\rho(r)$ which corresponds to the elastic form factor

$$F(q) = 4\pi \int_0^\infty \rho(r) \frac{\sin(qr)}{qr} r^2 \, dr, \qquad (1)$$

where q is the magnitude of the momentum transferred in an elastic collision to the atom or ion which is assumed to be initially at rest. In contrast to our recent work, in which $\rho(r)$ and $F(q)$ were obtained using Poisson's equation, we here determine $\rho(r)$ in terms of single-electron radial wave functions obtained from the Schrödinger equation for a single electron in a GSZ potential. Thus

$$\rho(r) = \sum_s \omega_s R_s^2(r), \qquad (2)$$

where the sum is over all occupied shells s, specified by the quantum numbers n and l, $R_s(r)$ is the single-electron radial wave function for the sth shell, and ω_s is the number of electrons occupying the shell s.

The single-electron radial wave functions are obtained using a modified version of the Schrödinger-equation–solving subroutine of the Herman and Skillman[7] program. Here we replace the Hartree-Fock-Slater-Latter numerical potential by the analytical GSZ potential, and, in addition, we alter the spatial grid to permit more accurate numerical integration of the integral in Eq. (1) at large q. The integration was performed at each value of q by using a modified Simpson's rule very similar to that suggested by Pohler and Hanson[8]
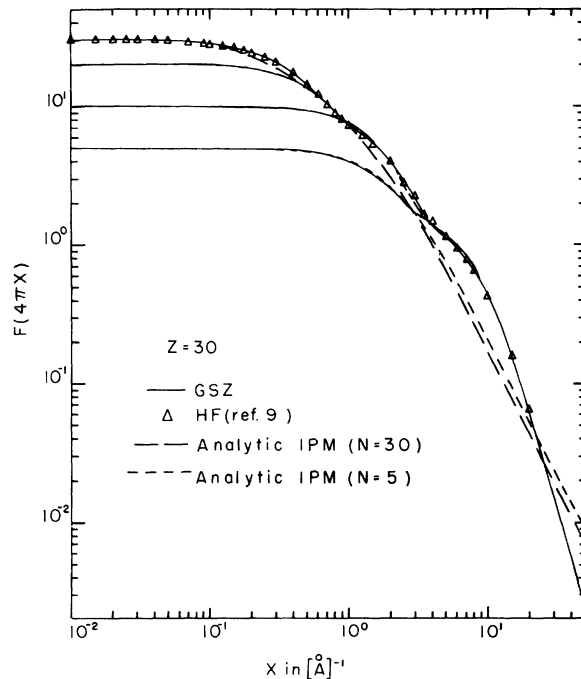

FIG. 1. Form factor $F(4\pi X)$ vs X for neutral zinc ($Z = 30$) and several of the positive ions of zinc. The symbols represent values of the HF form factors (Ref. 10), the solid line represents the values of the GSZ-Schrödinger form factors, and the dashed lines are the GSZ-Poisson form factors for zinc, with $N = 30$ and 5.
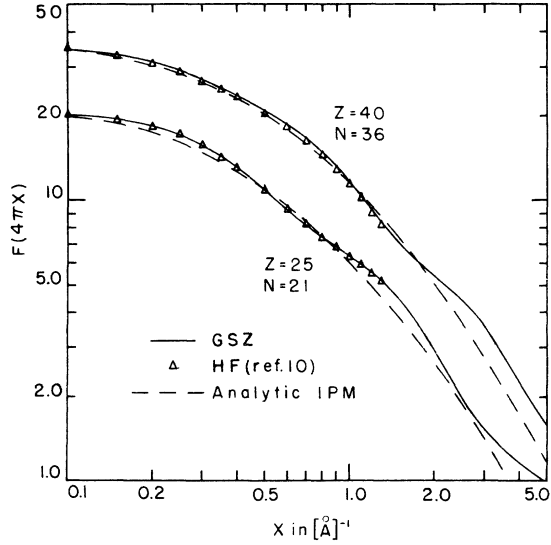
FIG. 2. Form factor $F(4\pi X)$ vs X for sample ions whose Z and N values are indicated on the graph. The symbols represent values of the HF form factors (Ref. 11), the solid lines are the values of the GSZ-Schröding-er form factors, and the dashed lines are the corresponding GSZ-Poisson form factors.

to accommodate the rapid oscillations in $\sin(qr)$ in the integrand of Eq. (1).[9]

We present examples of the results of our quantum-mechanical form-factor calculations in Figs. 1 and 2 and in Table I. The two figures contain graphs of the form factors we obtained for several neutral and ionic species plotted against the variable $X = q/4\pi = \sin\theta/\lambda$, where θ is the scattering angle and λ is the wavelength of the scattered particle in Å. We have included in these figures, for purposes of comparison, corresponding plots of $F(q)$ vs X, obtained from Hartree-Fock (HF) calculations[10,11] and the analytic form factors of Ref. 2. As these figures indicate, the agreement between the GSZ-IPM form factors obtained here and the HF form factors is excellent. Comparisons with Hartree-Fock-Slater (HFS) form factors also lead to qualitatively similar results, although differences at small values of q might be expected because of the characteristic weakness of the HFS potential in the valence-shell region. This weakness exists even when one uses the Latter device to correct the large-r behavior of the HFS potential, which goes to zero rather than $-2/r$ (for neutral species).[12]

III. DISCUSSION AND CONCLUSIONS

In using form factors obtained from the GSZ potential by this Schrödinger-equation procedure, certain limitations should be kept in mind. First,

the behavior of these form factors is somewhat suspect for $X \geq 10$ Å^{-1}, since, in this range, the dominant contribution to $F(q)$ comes from the density of the K-shell electrons. Except for species with low Z, these electrons should be described relativistically, instead of by the nonrelativistic Schrödinger equation we have used. Second, the GSZ potentials found in Refs. 3–6 were obtained with a view toward seeking possible systematic behavior of the two potential parameters with respect to Z for a given electronic configuration. Eventually, linear dependences for both GSZ parameters were discerned for isoelectronic systems which maintain the same electronic configuration. We essentially assumed that the various shells were filled successively in the order $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6$. On the other hand, experiment and Hartree-Fock-Roothaan calculations[13] indicate that the filling order of the $4s$ and $3d$ shells fluctuates for neutrals with $19 \leq Z \leq 28$, as does the filling order for the $5s$ and $4d$ shells when $37 \leq Z \leq 48$. One must consider and allow for these competitions between orbitals if strictly ground-state form factors are desired.

From the sample results presented in Sec. II, it is clear that the GSZ potential with parameters determined by the *ab initio* variational procedure described in Refs. 3–6 is capable of yielding elastic atomic form factors whose accuracy is competitive with that of HF calculations. However, for most positive ions with $Z \leq 54$, HF or even

TABLE I. GSZ-Schrödinger form factors and corresponding values of X for neutral zinc ($Z = 30$). The format A (B) means $A \times 10^B$.

X (Å^{-1})	$F(4\pi X)$	X (Å^{-1})	$F(4\pi X)$
1.0000 (−2)	29.978	1.0000	7.3583
1.2589 (−2)	29.965	1.2589	6.2109
1.5849 (−2)	29.944	1.5849	5.2051
1.9953 (−2)	29.912	1.9953	4.0480
2.5119 (−2)	29.862	2.5119	2.8566
3.1623 (−2)	29.782	3.1623	1.9365
3.9811 (−2)	29.658	3.9811	1.4037
5.0119 (−2)	29.465	5.0119	1.1173
6.3096 (−2)	29.172	6.3096	8.9116 (−1)
7.9433 (−2)	28.733	7.9433	6.5239 (−1)
1.0000 (−1)	28.094	1.0000 (1)	4.2430 (−1)
1.2589 (−1)	27.197	1.2589 (1)	2.4548 (−1)
1.5849 (−1)	25.988	1.5849 (1)	1.2831 (−1)
1.9953 (−1)	24.430	1.9953 (1)	6.1865 (−2)
2.5119 (−1)	22.489	2.5119 (1)	2.8031 (−2)
3.1623 (−1)	20.144	3.1623 (1)	1.2178 (−2)
3.9811 (−1)	17.412	3.9811 (1)	5.1579 (−3)
5.0119 (−1)	14.432	5.0119 (1)	2.1893 (−3)
6.3096 (−1)	11.520	6.3096 (1)	9.1476 (−4)
7.9433 (−1)	9.0797	7.9433 (1)	3.8588 (−4)
		1.0000 (2)	2.1907 (−4)

HFS form-factor calculations do not exist. Since the two GSZ potential parameters per species have already been determined for the 1485 species with $Z \leq 54$, anyone with a need of such form factors can use a simple Schrödinger-equation–solving code and the integration procedure described herein to obtain, quickly and inexpensively, accurate, numerical form factors for any of these species. This approach is not only economical in computer time, but also provides an alternative way of communicating form factors which avoids voluminous journal tabulation.

Finally, we call attention to the recent work of Talman and Shadwick,[14] who used a numerical energy minimization technique almost identical in philosophy with our *ab initio* analytic variational procedure. An analysis by Green and Kutcher[15] shows that the two variational potentials agree very accurately, thus suggesting that the basis of this work is very close to a best smooth analytic representation of an IPM atomic potential.

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