Incoherent X-Ray Scattering by a Statistical Atom*

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The theory of the homogeneous interacting electron gas is used to derive a functional of the density for the form factor for incoherent scattering of x rays by a statistical atom. The results show a dramatic improvement over an early calculation of Heisenberg who used the Thomas-Fermi model. Detailed calculations of form factors are carried out for several elements (A, Cu, Ce, Na) and compared with the results of Hartree-Fock-Slater (HFS) self-consistent wave-function calculations. Whereas the Thomas-Fermi model gives incoherent cross sections which differ at low energies by orders of magnitude from those given by the HFS model, the theory of the homogeneous electron gas yields results which compare within 15% of the HFS results.

I. INTRODUCTION

In this paper we study the incoherent scattering of x rays by a statistical atom. We use the theory of the homogeneous interacting electron gas, which is density dependent. This dependence is averaged over the density distribution of the particular atom in question. The incoherent form factors resulting from our theory show a dramatic improvement over the calculation of Heisenberg,[1] who used the Thomas-Fermi statistical model. Our standard of comparison is the results of self-consistent-field calculations.

The purpose of these calculations is to extend the accuracy of the statistical model of the atom, not to provide an alternative to self-consistent-field methods.

In Sec. II, we briefly review the general theory of x-ray scattering. Following this, in Sec. III, we specialize the theory to the case of scattering by a statistical atom. Finally, in Sec. IV, the calculated results and a general discussion are presented.

II. THEORY

The formal basis for the scattering of x rays by bound electrons has been established by Waller and Hartree[2]; they derive the general equation for the intensity of the scattering of x rays by atoms in a monatomic gas. In Born approximation and for x-ray energies high compared to K-shell binding energies but small compared to mc^2, the differential cross section corresponding to a transfer of momentum $\hbar\vec{\kappa}$ from the photon to an N electron atom is given by

$$\sigma(\kappa)=\sigma_c\int|\psi|^2\left|\sum_{j=1}^{N}e^{i\vec{\kappa}\cdot\vec{r}_j}\right|^2 d\vec{\mathbf{x}}$$

$$\equiv\sigma_c\sum_{ij}\langle e^{i\vec{\kappa}\cdot(\vec{r}_i-\vec{r}_j)}\rangle, \tag{1}$$

where $\sigma_c=\sigma_c(\vec{\kappa})$ is the Thomson cross section for scattering by an unbound electron,

$$\psi=\psi(\vec{\mathbf{x}}_1\cdots\vec{\mathbf{x}}_N) \tag{2}$$

is the wave function of the ground state of the atom, the $\vec{\mathbf{x}}_j\equiv(\vec{\mathbf{r}}_j,\sigma_j)$ are the electronic space and spin coordinates, and $d\vec{\mathbf{x}}$ is the product of the $d\vec{\mathbf{x}}_j$.

The scattered radiation described by this formula consists of the coherent (elastic) and the incoherent (inelastic) scattered radiation. The coherent cross section is given by

$$\sigma_{\rm coh}=\sigma_c\left|\sum_j\langle e^{i\vec{\kappa}\cdot\vec{r}_j}\rangle\right|^2=\sigma_c F_{\rm coh}, \tag{3}$$

and the incoherent cross section by

$$\sigma_{\rm inc}=\sigma_c\left(\sum_{ij}\langle e^{i\vec{\kappa}\cdot(\vec{r}_i-\vec{r}_j)}\rangle-\left|\sum_j\langle e^{i\vec{\kappa}\cdot\vec{r}_j}\rangle\right|^2\right)$$

$$\equiv N\sigma_c F_{\rm inc}. \tag{4}$$

Van Hove[3] has shown that the scattering cross section for x rays by a system of interacting particles is expressible in terms of density distribution functions for the particles of the system. Moreover, the coherent cross section is expressible in terms of the density distribution for a single particle of the system and the total cross section (coherent plus incoherent) is expressible in terms of the correlation function which in the classical limit describes the average density distribution as seen from one particle of the system.

Following Van Hove[3] we introduce the density of the system

$$n(\vec{r}) = \sum_j \langle \delta(\vec{r} - \vec{r}_j) \rangle , \tag{5}$$

and the correlation function

$$G(\vec{r}) = (2\pi)^{-3} N^{-1} \sum_{ij} \langle \delta(\vec{r} + \vec{r}_i - \vec{r}_j) \rangle$$

$$= (2\pi)^{-3} N^{-1} \sum_{ij} \int dr' \langle \delta(\vec{r} + \vec{r}_i - \vec{r}') \, \delta(\vec{r}' - \vec{r}_j) \rangle . \tag{6}$$

From the expression

$$G(\vec{r}) = (2\pi)^{-6} N^{-1} \sum_{ij} \int d\vec{\kappa} e^{-i\vec{\kappa}\cdot\vec{r}} \langle e^{-i\vec{\kappa}\cdot(\vec{r}_i - \vec{r}_j)} \rangle , \tag{7}$$

which follows simply from the first of Eq. (6), the total scattering is related to $G(\vec{r})$ by

$$\sigma(\vec{\kappa}) = (2\pi)^3 N \sigma_c \int e^{i\vec{\kappa}\cdot\vec{r}} G(\vec{r}) \, d\vec{r} , \tag{8}$$

and the elastic scattering is related to the density by

$$\sigma_{\text{coh}}(\vec{\kappa}) = \sigma_c \int \left| e^{i\vec{\kappa}\cdot\vec{r}} n(\vec{r}) \, d\vec{r} \right|^2$$

$$= \sigma_c \int e^{i\vec{\kappa}\cdot\vec{r}} n(\vec{r}' - \vec{r}) \, n(\vec{r}') \, d\vec{r} \, d\vec{r}' \tag{9}$$

from Eqs. (3) and (5).

For systems with large numbers of particles, $G(\vec{r})$ has an especially simple asymptotic expression for large values of $\vec{r}$. For such systems, the particles in regions widely separated in space are statistically independent, so for sufficiently large $\vec{r}$,

$$\sum_{ij} \langle \delta(\vec{r} + \vec{r}_i - \vec{r}') \, \delta(\vec{r}' - \vec{r}_j) \rangle$$

$$\simeq \sum_{ij} \langle \delta(\vec{r} + \vec{r}_i - \vec{r}') \rangle \langle \delta(\vec{r}' - \vec{r}_j) \rangle$$

$$= n(\vec{r}' - \vec{r}) \, n(\vec{r}') . \tag{10}$$

Thus the coherent scattering is determined by the asymptotic part of the correlation function $G(\vec{r})$. The incoherent scattering follows from

$$\sigma_{\text{inc}}(\vec{\kappa}) = \sigma_c \int d\vec{r}' \int d\vec{r} \, e^{i\vec{\kappa}\cdot\vec{r}} \sum_{ij} [\langle \delta(\vec{r} + \vec{r}_i - \vec{r}') \, \delta(\vec{r}' - \vec{r}_j) \rangle$$

$$- \langle \delta(\vec{r} + \vec{r}_i - \vec{r}_j') \rangle \langle \delta(\vec{r}' - \vec{r}_j) \rangle] . \tag{11}$$

To summarize, we observe that Eq. (9) contains the asymptotic behavior of $G(\vec{r})$ and leads to a description of the coherent scattering in terms of the electron density distribution. The integrand in Eq. (11) describes the correlation in density fluctuations and determines the incoherent scattering.

III. INCOHERENT SCATTERING BY STATISTICAL ATOM

In the statistical model of the atom it is assumed that the potential energy $V(r)$ of an electron varies slowly with $\vec{r}$ and that at each point the system can be treated as a uniform gas of electrons. In order to evaluate the incoherent form factor, we divide the atom into boxes, neglect the density fluctuation correlations between electrons in different boxes, and in each box take the expectation value in the first term of (11) to be the one expressing the density fluctuation correlations between two points a distance r apart in a uniform gas. This will be a good approximation as long as the dimensions of a box are large compared with the range of density fluctuation correlations and as long as the potential varies only slightly over this correlation range.

In the spirit of this approximation, the second integrand of Eq. (11) is a constant so that term contributes only in the forward direction ($\vec{\kappa} = 0$); we shall henceforth ignore it. The integral over $\vec{r}$ is then evaluated as for a uniform gas at the density of electrons at the point $\vec{r}'$ in the atom.

We can now introduce the local correlation function

$$P(\vec{\kappa}, \vec{r}') \equiv \frac{1}{n(\vec{r}')} \int d\vec{r} \, e^{i\vec{\kappa}\cdot\vec{r}} \sum_{ij} \langle \delta(\vec{r} + \vec{r}_i - \vec{r}') \, \delta(\vec{r}' - \vec{r}_j) \rangle , \tag{12}$$

where now the expectation value is taken with respect to the ground state of a uniform electron gas whose density is equal to that in the atom at the point $\vec{r}'$. The incoherent scattering cross section becomes, from Eq. (11),

$$\sigma_{\text{inc}}(\vec{\kappa}) = \sigma_c \int d\vec{r}' n(\vec{r}') \, P(\vec{\kappa}, \vec{r}') . \tag{13}$$

Our first example will be the noninteracting Fermi gas, which leads to the Thomas-Fermi (TF) and Thomas-Fermi-Dirac (TFD) models of the atom. The deficiencies of the models for evaluating the incoherent form factor will then be removed by introducing the correlations brought about by the electrostatic interaction between electrons. In Sec. III C, we deal with the interacting Fermi gas by making use of the connection between the pair distribution function [Eq. (16)] and the dielectric constant of the uniform gas as described, for example, by Glick.[4]

A. Thomas-Fermi Atom

For a noninteracting Fermi gas,[5]

$$P(\vec{\kappa}, \vec{r}') = 1 - \frac{2}{n(\vec{r}')} \frac{1}{(2\pi)^3} \int d\vec{k} f_{r'}(\vec{k}) f_{r'}(\vec{k} + \vec{\kappa}) , \tag{14}$$

where

$$f_{r'}(\vec{k}) = \begin{cases} 1 & \text{for } k \le k_F \\ 0 & \text{for } k > k_F \end{cases}$$

and

$$k_F = k_F(\vec{r}') = [3\pi^2 n(\vec{r}')]^{1/3} . \tag{15}$$

Equation (14) can be evaluated explicitly to give

$$P(\vec{\kappa}, \vec{r}') = \begin{cases} \frac{3}{4}(\kappa/k_F) - \frac{3}{48}(\kappa/k_F)^3 & \text{for } \kappa \le 2k_F \\ 1 & \text{for } \kappa > 2k_F . \end{cases} \tag{16}$$

By substituting Eq. (16) into Eq. (13), and using Eq. (15) and the definition of the incoherent form factor [Eq. (4)] we have

$$F_{\rm inc} \equiv \frac{\sigma_{\rm inc}(\kappa)}{N\sigma_c} = 1 - \frac{1}{N}\int_0^{R_0} n d\vec{r}\,' + \frac{\kappa}{4\pi^2 N}\int_0^{R_0}(3\pi^2 n)^{2/3} d\vec{r}\,' - \frac{\kappa^3 R_0^3}{36N} \quad , \tag{17}$$

where the definition of R_0

$$n(R_0) = \kappa^3/24\pi^2 \tag{18}$$

follows from Eq. (15) and the condition that $P(\vec{\kappa},\vec{r}\,') \neq 1$ only for $\vec{\kappa} \leq 2k_F$.

For the Thomas-Fermi density function, a particularly simple scaling law results for $F_{\rm inc}$. Introducing the Thomas-Fermi variables $x = w^2/2 = (r/a_0) Z^{1/3} 2^{7/3} (3\pi)^{-2/3}$ and $\phi = rV/Ze^2$, where a_0 is the Bohr radius, gives

$$n = \frac{64\sqrt{2}}{9\pi^3 a_0^3}\,\frac{Z^2\phi^{3/2}}{w^3} \quad .$$

Setting N equal to the atomic number Z, we have for the neutral atom

$$F_{\rm inc} = 1 - 2^{-1/2}\int_0^{w_0} \phi^{3/2}\, w^2 dw + \frac{3}{2}\,\frac{\phi^{1/2}(w_0)}{w_0}\int_0^{w_0} \phi(w) w^3 dw - \tfrac{1}{12}\, w_0^3 \phi^{3/2}(w_0), \tag{19}$$

where w_0 is defined by

$$\kappa a_0 = 4\sqrt{2}\left(\frac{4}{3\pi}\right)^{1/3} Z^{2/3}\,\frac{\phi^{1/2}(w_0)}{w_0} \quad . \tag{20}$$

Thus, in the Thomas-Fermi model the incoherent form factor is a universal function of $\kappa Z^{-2/3}$. Equation (19) was first obtained by Heisenberg.[1]

By expanding Eq. (4) in powers of $\vec{\kappa}$ we note that $\sigma_{\rm inc}$ should be proportional to κ^2 for small κ. This dependence is lost and becomes linear in the Fermi-Thomas model because in Eq. (18), $f_{r'}(\vec{k})$ has a sharp cutoff at k_F. The proper κ dependence, as we shall see, is recovered when one takes account of electrostatic interactions in the uniform-gas model.

B. Thomas-Fermi-Dirac Atom

The next stage of sophistication in the statistical treatment of atoms is represented by the TFD model. Abrahamson[6] has calculated the density distributions for argon and copper in the TFD approximation. When these densities are substituted into Eq. (17), the results shown in Figs. 2 and 3 are obtained. Here and in other figures the abscissa is the variable $\kappa' = \sin(\frac{1}{2}\theta)/\lambda Z^{2/3}$, where θ is the angle of scattering and λ is in angstroms. The asymptotic behavior remains linear in κ, but, as seen in Figs. 2 and 3, the TFD form factor agrees more closely with the $F_{\rm inc}$ of detailed calculations than does the result of the TF model.

Exchange effects, neglected in TF approximation, but partly accounted for in the TFD model, are known to improve the electron distribution, especially in the outer regions of the atom. This may well explain the discrepancy between the TF and TFD curves which is large at small κ' but diminishes and gradually disappears at large κ'. At small κ', the scattered radiation samples mainly the outer regions of the atom, which is quite unrealistically described by the exchangeless TF model. At large κ', on the other hand, the interior of the atom is being probed, and the effective difference between the TF and TFD models is negligible.

C. Interacting Fermi Gas Model

The quantity $P(\vec{\kappa})$ (for brevity we omit the argument $\vec{r}\,'$) given in Eq. (12) can be described in terms of the dielectric constant $\epsilon(\vec{\kappa}, \omega)$:

$$P(\vec{\kappa}) = \frac{\hbar\kappa^2}{4\pi^2 ne^2}\int_0^\infty \frac{\epsilon_2(\vec{\kappa},\omega)}{|\epsilon(\vec{\kappa},\omega)|^2}\, d\omega, \tag{21}$$

where

$$\epsilon(\vec{\kappa},\omega) \equiv \epsilon_1(\vec{\kappa},\omega) + i\epsilon_2(\vec{\kappa},\omega). \tag{22}$$

The imaginary part is given by

$$\epsilon_2(\vec{\kappa},\omega) = \frac{4\pi e^2}{\kappa^2}\,\mathrm{Re}\int_0^\infty ds\, (e^{i\omega s} - e^{-i\omega s}) \times \langle e^{iHs} n^*(\vec{\kappa})\, e^{-iHs} n(\vec{\kappa})\rangle, \tag{23}$$

where H is the complete Hamiltonian, the expectation value is taken with respect to the ground state, and the subscript 1 indicates that only "single bubble" terms are to be taken in the expansion.[4] The quantity $n(\vec{\kappa})$ is the Fourier transform of the density, Eq. (5). The real part of the dielectric constant ϵ_1 is related to ϵ_2 by the Kramers-Kronig relation

$$\epsilon_1(\vec{\kappa},\omega) = 1 + \frac{2}{\pi}\, P\int_0^\infty \frac{\omega'\epsilon_2(\vec{\kappa},\omega')}{\omega'^2 - \omega^2}\, d\omega', \tag{24}$$

where P denotes the principal part.

In lowest order, i.e., the simplest bubble diagram, the dielectric constant can be evaluated explicitly[4]:

$$\epsilon_2 = \frac{1}{8 k_F a_0 z^3}\begin{cases} 4uz & \text{for } 0 < u < 1 - z \\ 1 - (u-z)^2 & \text{for } |u-z| < 1 < (u+z) \\ 0 & \text{for } |u-z| > 1 \end{cases} \tag{25}$$

and, from Eq. (24),

$$\epsilon_1 = 1 + \frac{1}{8 k_F a_0 z^3}\left([1 - (u-z)^2]\ln\left|\frac{u-z-1}{u-z+1}\right|\right.$$

$$+[1-(u+z)^2]\ln\left|\frac{u+z+1}{u+z-1}\right|+4z\Big) \quad . \quad (26)$$

In Eqs. (25) and (26), $z=k/2k_F$, $u=\hbar\omega/(2E_F z)$, $E_F=\hbar^2k_F^2/2m$, a_0 is the Bohr radius, and again $k_F=k_F(r')$, i.e., the Fermi momentum takes the values of Eq. (15) corresponding to the density at the point $\vec{r}'$ in the atom.

In a uniform gas, for small values of the wave number κ, the contributions to $P(\vec{\kappa})$ are of two kinds: the particle-hole pair excitations and the collective excitations.[7] The pair contribution comes from the frequency region in which $\epsilon_2(\vec{\kappa},\omega)$ is different from zero. The collective contribution comes from frequencies where both $\epsilon_1=0$ and $\epsilon_2=0$.

As for the case of a free-electron gas calculated in Hartree-Fock approximation, the pair excitations for the interacting gas possesses a continuous energy spectrum, but the strength of the excitation is reduced by the factor $1/|\epsilon(\kappa,\omega)|^2$. If we set this factor equal to one and calculate ϵ_2 in the HF approximation, we recover Eq. (16). Actually at small κ, $1/|\epsilon|^2$ is reduced by a factor of the order $(\kappa/k_F)^4$; this reduction is due to the screening clouds around each individual electron. We shall see that including only the pair excitations in the calculation of the incoherent atomic form factor leads to a value that is strongly depressed relative to that obtained from self-consistent atomic wave functions.

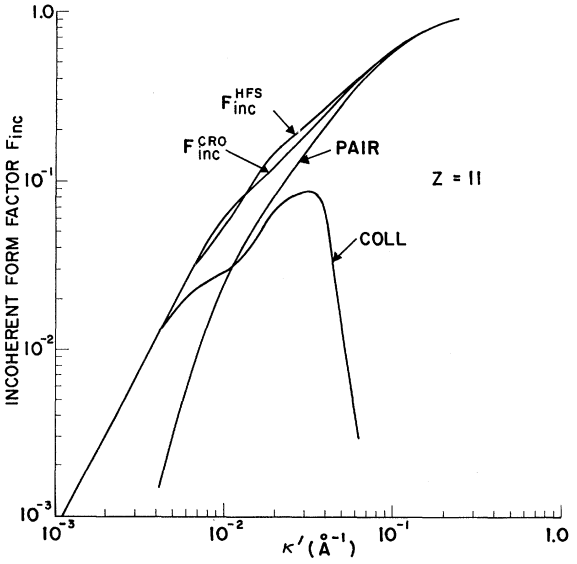

FIG. 1 Incoherent form factor F_{inc} vs the reduced momentum transfer $\kappa'=\sin(\frac{1}{2}\theta)/\lambda Z^{2/3}$ for sodium. F_{inc}^{CRO} is taken from Cromer and Mann (Ref. 9). F_{inc}^{HFS} is calculated using the statistical model and the density calculated from the wave function of Herman and Skillman (Ref. 10). Pair and collective contributions to F_{inc}^{HFS} are shown.

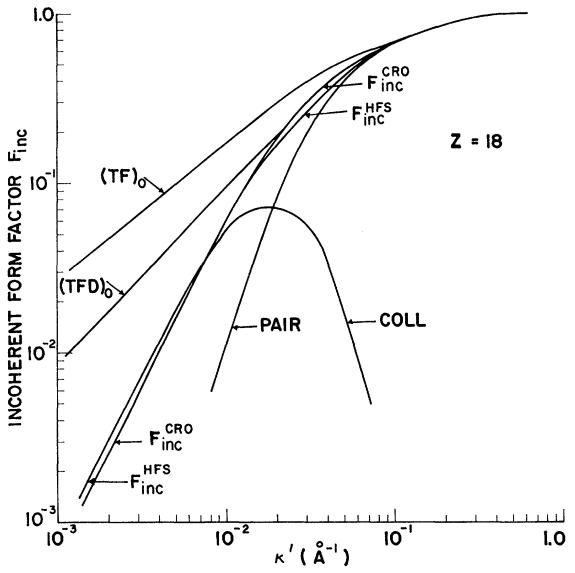

FIG. 2 Incoherent form factor F_{inc} vs κ' for argon. Notation is the same as in Fig. 1. In addition, we show the results calculated from the noninteracting gas model [Eq. (17)] using Thomas Fermi $(TF)_0$ and Thomas-Fermi-Dirac $(TFD)_0$ (Ref. 6) densities.

In the region of small κ the collective contribution to $P(\vec{\kappa})$ is, to an accuracy κ^4/k_{TF}^4,

$$P_{coll}(\kappa)\approx\hbar^2\kappa^2/2m\omega_\kappa \quad , \quad (27)$$

where ω_κ is the frequency of the collective mode with wave number κ and k_{TF} is the Thomas-Fermi screening wave number, $k_{TF}^2=(4/\pi)(k_F/a_0)$.[8] Accounting for the collective contribution within the

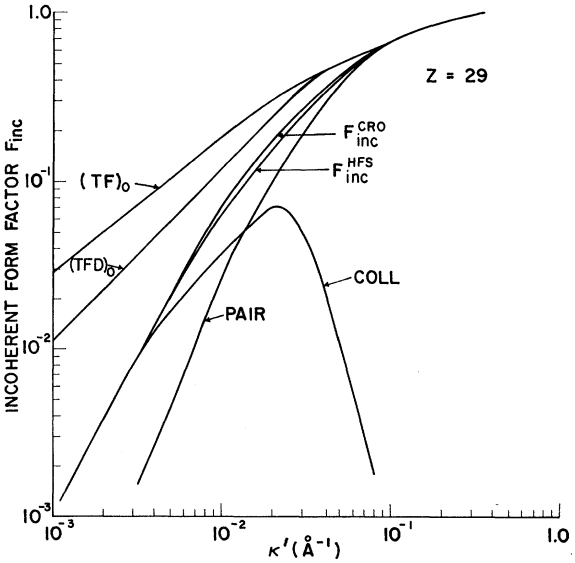

FIG. 3 Incoherent form factor F_{inc} vs κ' for copper. The notation is the same as in Fig. 2.

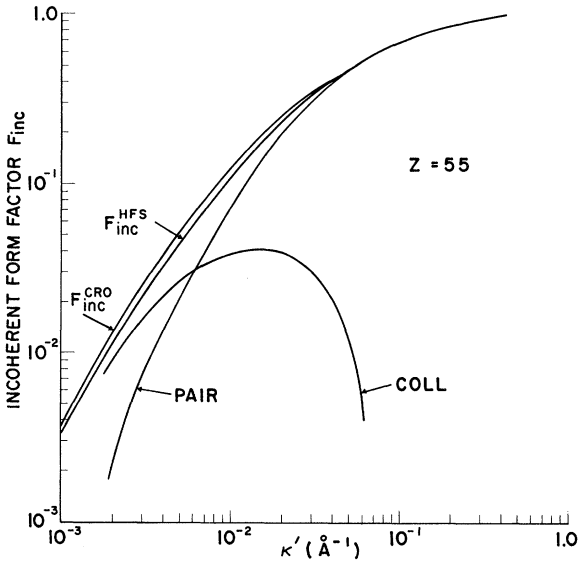

FIG. 4 Incoherent form factor F_{inc} vs κ' for cesium. Notation is the same as in Fig. 1.

framework of the statistical model adopted here, allows us to recover the κ^2 dependence of the incoherent form factor at small κ. To determine the accuracy with which the statistical model gives $F_{inc}(\vec{\kappa})$ at all κ and, in particular, the coefficient of the term proportional to κ^2 which dominates at small κ, we must perform the detailed integrations required by Eqs. (13) and (21) and compare the results with those obtained from detailed wave-function calculations.[9]

IV. RESULTS

We have carried out detailed calculations of $P(\kappa)$ [Eq. (21)], and averaged the result, as required by Eq. (13), for the atoms Na, A, Cu, and Cs. The results are shown in Figs. 1–4, respectively. The atomic densities used were those obtained from the Hartree-Fock-Slater (HFS) calculation of Herman and Skillman.[10] Comparisons are made with the results of Cromer and Mann.[9] We note the close (at worst ~15%) agreement, especially when contrasted with the results of the non-interacting TF and TFD models in Figs. 2 and 3. The particle contribution and the collective contribution which have been averaged over the density are shown separately in each graph, as well as the sum.[11]

Our calculations indicate that the functional of the density obtained by substituting Eqs. (21) and (13) can give reasonably accurate results (~15%) for incoherent form factors. They are, however, quite sensitive to the density profile in the atom, at least in the region $\kappa' \sim 0.05$. The sensitivity is apparent from Fig. 5 where we compare F_{inc} for Cu and Ar obtained from the TFD density calculated by Abrahamson[6] and the HFS density computed from the Herman-Skillman[10] wave functions. In both cases F_{inc} is computed from Eqs. (21) and (13).

While the particle and collective contributions seem to conspire in such a way as to give a smooth total result in Figs. 1–4, we point out that the smoothness is a consequence of the density-weighted integration over the volume of the atom. In Fig. 6, we show the form factors for a uniform gas at different densities; these curves exhibit gaps not characteristic of the atomic case.

V. DISCUSSION

In order to obtain the correct behavior of the incoherent form factor at small momentum transfers we were required to include two kinds of excitation in the interacting uniform gas: the shielded pair excitations and the collective excitations.[12] The shielding of the pair excitations damps the incorrect behavior of F_{inc} at low momentum transfer for the noninteracting gas (see Figs. 2 and 3). We recover the correct asymptotic behavior by including the collective effects which contribute proportionally to κ^2 for small κ.

Our statistical treatment of the incoherent form factor shares with other statistically derived quantities of the atom, the feature that it works better than we should expect.[13] In this respect, we recall that our basic approximation consisted in dividing the atom into boxes and neglecting the density fluctuation correlations between different boxes. This

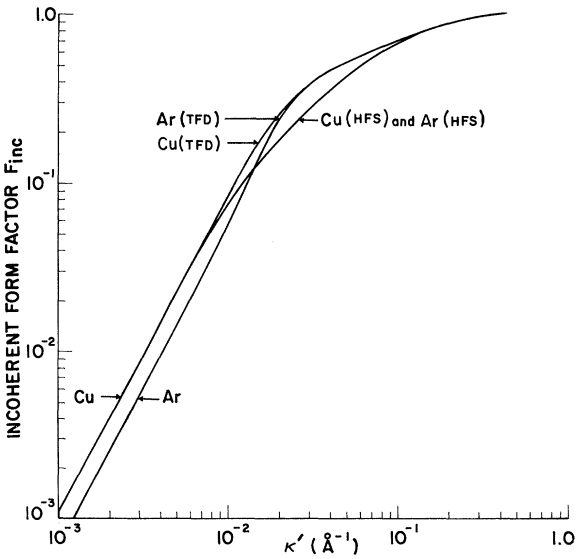

FIG. 5 Comparison of statistically derived incoherent form factors for different density distributions. TFD refers to the Thomas-Fermi-Dirac density (Ref. 6). HFS refers to the density derived from Hartree-Fock-Slater wave functions (Ref. 10).

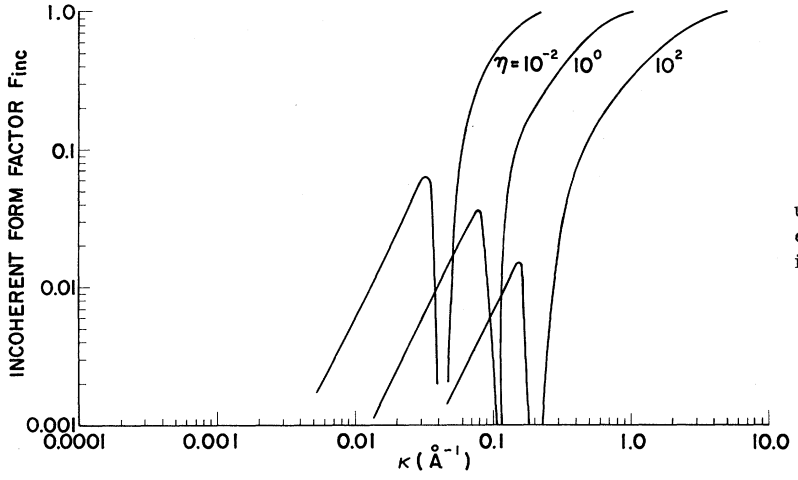

FIG. 6 Incoherent form factor for a uniform electron gas. Parameter n is the electron density in atomic units. Abscissa is $\kappa = \sin(\frac{1}{2}\theta)/\lambda$, with λ in angstroms.

requires that the correlation range k_{FT}^{-1} or κ^{-1}, whichever is smaller, be less than the dimensions of the box. Since the density should not significantly vary over the dimensions of the box, our approximations should apply if

$$\min(\kappa^{-1}, k_{FT}^{-1}) \lesssim \left(\frac{1}{\rho}\frac{\partial\rho}{\partial r}\right)^{-1} .$$

This condition, which may be too strong, is not satisfied (except for very large κ) anywhere in the atom. For $\kappa^{-1} < k_{FT}^{-1}$ the condition is satisfied, however, if, instead of the radial density gradient, we use the atomic radius as the characteristic length. This implies that for $\kappa^{-1} \lesssim R_0$, the atomic radius, the effects of unshielded pair excitations will dominate the form factor. Referring to Figs. 1–4 we see that the unshielded pair excitations dominate for $\kappa' \gtrsim 0.07$ (corresponding to $\kappa^{-1} \lesssim 0.15$ Å) which satisfies the last inequality well.

As for the small-κ behavior, we note only that the size of the physical atom (as defined, for example, as that radius R_0 which contains half the electrons in the TF atom of the same Z) is of the same order as k_{FT}^{-1} evaluated at R_0. Moreover, the two quantities scale as $Z^{-1/3}$. The relative success of the statistical model for several values of Z suggests therefore that the correct explanation of this success is connected with the near coincidence of the finite size and the corresponding fluctuation correlation length.

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