

tion of the Franck-Condon principal to the well-known potential-energy curves²¹ of the N_2 and N_2^+ systems suggests that the emission of the N_2^+ first negative and the N_2 second positive systems are the most likely results of the collisions. In electron impact, the cross sections are comparable.^{14,20} However, for proton impact there is the additional consideration that the excitation of the $N_2(C^3\Pi_u)$ state is forbidden by the Wigner spin-conservation rule, and this is confirmed by our observa-

²¹ F. R. Gilmore, J. Quant. Spectry. Rad. Trans. 5, 369 (1965).

tion that the second positive band system of N_2 is only weakly excited by direct proton impact. Theoretical values of overlap integrals give a reasonable prediction of the relative population of the two vibrational levels of $N_2^+(B^2\Sigma)$ that we have investigated.

ACKNOWLEDGMENT

The construction of the apparatus used in this work was assisted by a "Small Equipment Grant" from the Western Electric Company.

Atomic Form Factor and Incoherent-Scattering Function of the Helium Atom*

YONG-KI KIM AND MITIO INOKUTI

Argonne National Laboratory, Argonne, Illinois

(Received 21 July 1967)

The atomic form factor and the incoherent-scattering function of the helium atom have been calculated from several wave functions of differing accuracies. The form factor calculated from the Hartree-Fock wave function is in very close agreement with that from the 20-term Hylleraas wave function for all values of the momentum transfer. For small momentum transfers (<3 atomic units), the incoherent-scattering function is sensitive to the wave function used, but it becomes insensitive for large momentum transfers. Correlated wave functions give values of the incoherent-scattering function, at small momentum transfers, approximately 5% lower than the Hartree-Fock wave function does. Consequences of the above results in the calculation of x-ray and electron-scattering cross sections are discussed.

I. INTRODUCTION

THE atomic form factor $F(K)$ and the incoherent-scattering function $S_{\text{inc}}(K)$ for a neutral atom of atomic number Z are defined as follows:

$$F(K) = \sum_{j=1}^Z \langle \exp(i\mathbf{K} \cdot \mathbf{r}_j) \rangle, \quad (1)$$

$$S_{\text{inc}}(K) = Z^{-1} \left[\sum_{j,k=1}^Z \langle \exp[i\mathbf{K} \cdot (\mathbf{r}_j - \mathbf{r}_k)] \rangle - |F(K)|^2 \right], \quad (2)$$

where $\langle \rangle$ denotes an expectation value in the ground state, \mathbf{K}/\hbar is the momentum transfer, and \mathbf{r}_j the radial vector from the nucleus to the j th electron. Both $F(K)$ and $S_{\text{inc}}(K)$ are even functions of K .

The functions $F(K)$ and $S_{\text{inc}}(K)$ play important roles in the theory of scattering of x rays and electrons by atoms.¹⁻³ When the energy of an incident photon is much smaller than the rest energy mc^2 of an electron, the cross section $d\sigma_{\text{coh}}$ for coherent scattering of the

photon by an atom into the solid-angle element $d\Omega$ is

$$d\sigma_{\text{coh}} = \frac{1}{2} r_0^2 (1 + \cos^2\theta) |F(K)|^2 d\Omega, \quad (3)$$

where $r_0 = e^2/mc^2$ is the classical electron radius, and θ , the angle between the initial and final momenta of the photon, is twice the Bragg angle. In Eq. (3), $I_{\text{Th}} = \frac{1}{2} r_0^2 (1 + \cos^2\theta)$ is the Thomson cross section for scattering by a free electron, and we may interpret $|F(K)|^2$ as the effective number of atomic electrons contributing to the coherent scattering. In x-ray scattering, the variable $\sin(\theta/2)/\lambda = K/4\pi$ is commonly used in place of K , with λ the wavelength of the incident photon. The total incoherent-scattering cross section $d\sigma_{\text{inc}}$ of x rays is⁴

$$d\sigma_{\text{inc}} = I_{\text{Th}} Z S_{\text{inc}}(K) d\Omega. \quad (4)$$

Coherent and incoherent scattering of x rays correspond respectively to elastic and inelastic scattering of fast electrons. The differential cross section $d\sigma_{\text{el}}$ for the elastic scattering of electrons by an atom, in the first Born approximation, is

$$d\sigma_{\text{el}} = 4a_0^2 / (Ka_0)^4 |Z - F(K)|^2 d\Omega, \quad (5)$$

⁴ A relativistic correction is necessary for high-energy photons, particularly at large angles. In such cases, I_{Th} in Eq. (4) should be replaced by the Klein-Nishina cross section.

* Work performed under the auspices of the U. S. Atomic Energy Commission.

¹ M. H. Pirene, *The Diffraction of X-Rays and Electrons by Free Molecules* (Cambridge University Press, London, 1946).

² A. T. Nelms and I. Oppenheim, J. Res. Natl. Bur. Std. (U. S.) 55, 53 (1955).

³ G. W. Grodstein, Natl. Bur. Std. (U. S.) Circ. No. 583 (1957).

TABLE I. Atomic form factor $F(K)$ of the helium atom.

$\frac{\sin(\frac{1}{2}\theta)}{\lambda} (\text{\AA}^{-1})$	Ka_0	3-term HF ^a	2-term HY ^b	3-term HY	6-term HY	20-term HY
0	0	2	2	2	2	2
0.025	0.166243	1.9892	1.9901	1.9890	1.98905	1.98906
0.050	0.332485	1.9571	1.9609	1.9567	1.95681	1.95682
0.075	0.498728	1.9057	1.9136	1.9046	1.90496	1.90500
0.100	0.664971	1.8372	1.8503	1.8354	1.83613	1.83620
0.125	0.831214	1.7551	1.7734	1.7524	1.75352	1.75365
0.150	0.997456	1.6626	1.6858	1.6589	1.66065	1.66085
0.200	1.32994	1.4604	1.4902	1.4546	1.45785	1.45816
0.300	1.99491	1.0602	1.0881	1.0519	1.05819	1.05842
0.400	2.65988	0.7383	0.7531	0.7303	0.73804	0.73785
0.500	3.32485	0.5089	0.5113	0.5025	0.50995	0.50948
0.600	3.98983	0.3529	0.3478	0.3482	0.35449	0.35404
0.700	4.65480	0.2481	0.2398	0.2447	0.24965	0.24936
0.800	5.31977	0.1772	0.1683	0.1748	0.17862	0.17851
0.900	5.98474	0.1288	0.1204	0.1280	0.12993	0.12996
1.000	6.64971	0.09523	0.09893	0.09387	0.096078	0.096185
1.100	7.31468	0.07152	0.06522	0.07048	0.072166	0.072308
1.200	7.97965	0.05453	0.05926	0.05371	0.055011	0.055162
1.300	8.64462	0.04216	0.03777	0.04150	0.042516	0.042662
1.400	9.30959	0.03302	0.02938	0.03248	0.033283	0.033416
1.500	9.97456	0.02617	0.02315	0.02573	0.026366	0.026483

^a HF: Hartree-Fock wave function (Ref. 11).^b HY: Hylleraas wave function (Ref. 12).

where $a_0 = \hbar^2/me^2$ is the Bohr radius. In this case, we may interpret $F(K)$ as representing the effective shielding of the nuclear charge Z . The differential cross section $d\sigma_{\text{inel}}$ of electrons summed over all inelastic collisions with an atom, also in the first Born approximation and when the momentum of the incident electron is very large compared to the momentum transfer, is^{5,6}

$$d\sigma_{\text{inel}} = \frac{4a_0^2}{(Ka_0)^4} Z S_{\text{inc}}(K) d\Omega. \quad (6)$$

Knowledge of $S_{\text{inc}}(K)$ for a wide range of K is essential for application of a sum rule for the Bethe cross sections for inelastic scattering of fast charged particles.⁷ The functions $F(K)$ and $S_{\text{inc}}(K)$ are also used in the calculation of the effect of the atomic electrons on the pair-production and bremsstrahlung cross sections.^{8,9} Still another application of $S_{\text{inc}}(K)$ is found in the theory of multiple scattering.¹⁰

In this work, we present the values of $F(K)$ and $S_{\text{inc}}(K)$ calculated from available wave functions with varying accuracy for the ground state of the helium

⁵ N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, London, 1965), 3rd ed., p. 495.

⁶ The kinematic part of the relativistic correction is given by multiplying the right-hand sides of Eqs. (5) and (6) by $(1 - v^2/c^2)^{-1}$, with v the velocity of the incident electron. There are, however, other relativistic effects such as spin effect and retardation which must also be considered. For the relativistic corrections in elastic scattering, see J. W. Motz, H. Olsen, and H. W. Koch, *Rev. Mod. Phys.* **36**, 881 (1964).

⁷ M. Inokuti, Y.-K. Kim, and R. L. Platzman, *Phys. Rev.* **164**, 55 (1967).

⁸ H. A. Bethe and J. Ashkin, *Experimental Nuclear Physics*, edited by E. Segrè (John Wiley & Sons, Inc., New York, 1953), Vol. I, p. 166.

⁹ J. A. Wheeler and W. E. Lamb, Jr., *Phys. Rev.* **55**, 858 (1939).

¹⁰ U. Fano, *Phys. Rev.* **93**, 117 (1954).

atom. Apart from the practical significance of the results in the many applications cited above, the calculations reveal the dependence of the expectation values on the wave functions, and, in particular, on the description of the electron correlation in the atom. The wave functions used here are a 3-term analytic Hartree-Fock (HF) wave function¹¹ and four (2-, 3-, 6-, and 20-term) Hylleraas (HY) wave functions.¹² Similar subjects have been discussed by several authors¹³⁻¹⁸ but the most accurate wave function used so far is the 6-term HY wave function or those with the same order of accuracy in terms of energy.

II. ATOMIC FORM FACTOR AND INCOHERENT-SCATTERING FUNCTION

Derivations of analytic expressions for $F(K)$ and $S_{\text{inc}}(K)$ for the HF and HY wave functions are straight-

¹¹ P. S. Bagus and T. L. Gilbert (unpublished). The analytic HF wave function we have used is $\psi(r_1, r_2) = (4\pi)^{-1} \phi(r_1) \phi(r_2)$, where $\phi(r) = 4.75657e^{-1.460r} - 1.40361re^{-2.641r} - 1.26842re^{-1.722r}$. This is believed to be one of the most accurate HF wave functions currently available, and is of comparable accuracy to that published by E. Clementi, *IBM J. Res. Develop., Suppl.* **9**, 2 (1965).

¹² The Hylleraas wave functions were taken from the following literature: two- and three-term HY wave functions: L. C. Green *et al.*, *Phys. Rev.* **112**, 1187 (1958); six-term HY wave function: A. L. Stewart and T. G. Webb, *Proc. Phys. Soc. (London)* **82**, 532 (1963); 20-term HY wave function: J. F. Hart and G. Herzberg, *Phys. Rev.* **106**, 79 (1957).

¹³ S. Huzinaga, *Progr. Theoret. Phys. (Kyoto)* **23**, 562 (1960).

¹⁴ M. Inokuti, *Progr. Theoret. Phys. (Kyoto)* **25**, 717 (1961).

¹⁵ W. Kołos and K. Pecul, *Ann. Phys. (N. Y.)* **16**, 201 (1961); W. Kołos, *Bull. Acad. Polon. Sci. Série Sci. Math. Astron. Phys.* **8**, 67 (1960).

¹⁶ R. P. Hurst, *Acta Cryst.* **13**, 634 (1960).

¹⁷ M. L. Rustgi, M. M. Shukla, and A. N. Tripathi, *Acta Cryst.* **16**, 926 (1963).

¹⁸ L. S. Bartell and R. M. Gavin, Jr., *J. Chem. Phys.* **43**, 856 (1965).

TABLE II. Incoherent scattering function of the helium atom. [Values listed below are $ZS_{\text{inc}}(K)$ with $Z=2$.]

$\frac{\sin(\frac{1}{2}\theta)}{\lambda} (\text{\AA}^{-1})$	Ka_0	3-term HF ^a	2-term HY ^b	3-term HY	6-term HY	20-term HY
0	0	0	0	0	0	0
0.025	0.166243	0.02163	0.01788	0.02043	0.020691	0.020637
0.050	0.332485	0.08480	0.07124	0.07995	0.080913	0.080716
0.075	0.498728	0.1843	0.1557	0.1735	0.17546	0.17509
0.100	0.664971	0.3123	0.2659	0.2938	0.29674	0.29621
0.125	0.831214	0.4598	0.3953	0.4322	0.43599	0.43540
0.150	0.997456	0.6178	0.5367	0.5802	0.58457	0.58406
0.200	1.32994	0.9336	0.8297	0.8765	0.88094	0.88102
0.300	1.99491	1.4380	1.3337	1.3593	1.36108	1.36273
0.400	2.65988	1.7274	1.6526	1.6558	1.65524	1.65689
0.500	3.32485	1.8705	1.8241	1.8186	1.81719	1.81772
0.600	3.98983	1.9377	1.9105	1.9043	1.90286	1.90245
0.700	4.65480	1.9692	1.9533	1.9487	1.94762	1.94682
0.800	5.31977	1.9843	1.9748	1.9719	1.97109	1.97027
0.900	5.98474	1.9917	1.9859	1.9842	1.98358	1.98290
1.000	6.64971	1.9955	1.9918	1.9908	1.99038	1.98985
1.100	7.31468	1.9974	1.9950	1.9945	1.99418	1.99379
1.200	7.97965	1.9985	1.9969	1.9966	1.99636	1.99608
1.300	8.64462	1.9991	1.9980	1.9978	1.99766	1.99745
1.400	9.30959	1.9995	1.9987	1.9986	1.99844	1.99829
1.500	9.97456	1.9997	1.9991	1.9990	1.99894	1.99882

^a HF: Hartree-Fock wave function (Ref. 11).

^b HY: Hylleraas wave function (Ref. 12).

forward but tedious.¹⁹ The atomic form factors are given in Table I, and the incoherent-scattering functions in Table II. Table III contains the values of $[Z-F(K)]/(Ka_0)^2$, which appears in Eq. (5) for $d\sigma_{\text{el}}$. The expectation value

$$X^2 = \langle r_1^2 + r_2^2 \rangle / (3a_0^2), \quad (7)$$

which is closely related to $d\sigma_{\text{el}}$ in the zero-angle limit [see Eq. (8)] and also is proportional to the diamagnetic susceptibility, is listed in Table IV. The energy expectation values computed from various wave functions are also listed in Table IV and indicate the relative merit of the wave functions according to this criterion.

Several points are evident in Table I. The values of $F(K)$ computed from the HF wave function are in very good agreement with those of the 20-term HY wave function, and the deviation is about $\frac{1}{2}\%$ or less for all values of Ka_0 . The values of $F(K)$ from the HF wave function are closer to those of the 20-term HY wave function than the values given by the 2- and 3-term HY wave functions, and are comparable to those of the 6-term HY wave function. In the range $Ka_0 > 3$, the HF values are smaller than the 20-term HY values, and vice versa in the range $Ka_0 < 3$.

The fact that less correlated wave functions tend to overestimate $F(K)$ for smaller values of Ka_0 and vice versa has been pointed out by Hurst.¹⁶ His explanation was that the dependence of $F(K)$ on the factor $\exp(i\mathbf{K}\cdot\mathbf{r})$ is such that the variation of charge density near the nucleus affects $F(K)$ for large values of K , and vice versa. This tendency is observed in all the wave functions listed in Table I.

The excellent agreement of $F(K)$ given by the HF

¹⁹ These expressions are included in the Argonne National Laboratory Report No. ANL-7220, 1966, p. 13 (unpublished).

wave function and the 20-term HY wave function can be taken as an evidence that the independent-particle model is a good approximation for a closed-shell atom. It should also be noted that $F(K)$ is the expectation value of the sum of one-electron operators, and in general, the HF wave functions are known to produce reasonable expectation values of one-electron operators.^{20,21} We may therefore safely expect that the HF wave functions for the closed-shell atoms will give good form factors. It may not, however, be true for atoms with open-shell ground-state configurations.^{22,23}

Table II shows that the values of $S_{\text{inc}}(K)$ calculated from the HF wave function are larger than those given by the HY wave functions. The deviation is of the order of 5% for $Ka_0 < 2.5$ and becomes much less for larger Ka_0 . This is understandable partly because $S_{\text{inc}}(K)$ contains the expectation value of a two-electron operator. Other evidence has already suggested that the HF wave functions do not give as reliable expectation values of two-electron operators as those of one-electron operators.²³

Fairly accurate tables of $F(K)$ are available in the literature.^{17,18,24} As to the incoherent-scattering function, however, only a few references are available.^{18,25}

²⁰ M. Cohen and A. Dalgarno, Proc. Phys. Soc. (London) 77, 748 (1961).

²¹ J. Goodisman and W. Klemperer, J. Chem. Phys. 38, 721 (1963).

²² R. McWeeny, Acta Cryst. 4, 513 (1951).

²³ For instance, J. W. Cooper and J. B. Martin [Phys. Rev. 131, 1183 (1963)] show that some expectation values for the three-electron system are more sensitive to the electron correlation than the corresponding values for the two-electron system.

²⁴ International Tables for X-Ray Crystallography (Keynote Press, Birmingham, England, 1962), Vol. III.

²⁵ A. H. Compton and S. K. Allison, X-Rays in Theory and Experiment (D. Van Nostrand Company, Inc., New York, 1935), Appendix IV.

TABLE III. Amplitude $[Z-F(K)]/(Ka_0)^2$ for elastic scattering of an electron by the helium atom.^a

$\frac{\sin(\frac{1}{2}\theta)}{\lambda}$ (\AA^{-1})	Ka_0	3-term HF ^b	2-term HY ^c	3-term HY	6-term HY	20-term HY
0	0	0.3949	0.3589	0.3991	0.39787	0.39778
0.025	0.166243	0.3932	0.3576	0.3973	0.39606	0.39596
0.050	0.332485	0.3879	0.3536	0.3920	0.39071	0.39059
0.075	0.498728	0.3794	0.3472	0.3835	0.38209	0.38194
0.100	0.664971	0.3681	0.3386	0.3721	0.37060	0.37043
0.125	0.831214	0.3545	0.3280	0.3584	0.35674	0.35656
0.150	0.997456	0.3391	0.3158	0.3428	0.34108	0.34089
0.200	1.32994	0.3051	0.2883	0.3084	0.30652	0.30634
0.300	1.99491	0.2362	0.2291	0.2382	0.23665	0.23660
0.400	2.65988	0.1783	0.1762	0.1795	0.17837	0.17840
0.500	3.32485	0.1349	0.1347	0.1355	0.13479	0.13483
0.600	3.98983	0.1035	0.1038	0.1038	0.10337	0.10340
0.700	4.65480	0.08086	0.08124	0.08101	0.080784	0.080797
0.800	5.31977	0.06441	0.06473	0.06449	0.064360	0.064364
0.900	5.98474	0.05224	0.05248	0.05229	0.052212	0.052211
1.000	6.64971	0.04308	0.04324	0.04311	0.043057	0.043055
1.100	7.31468	0.03604	0.03616	0.03606	0.036031	0.036029
1.200	7.97965	0.03055	0.03064	0.03057	0.030546	0.030543
1.300	8.64462	0.02620	0.02626	0.02621	0.026194	0.026192
1.400	9.30959	0.02270	0.02274	0.02270	0.022692	0.022691
1.500	9.97456	0.01984	0.01987	0.01984	0.019837	0.019836

^a Values in this table must be multiplied by $2a_0 = 1.05833 \text{ \AA}$ to be compared with those in Table 3, 3A(1) of Ref. 24.

^b HF: Hartree-Fock wave function (Ref. 11).

^c HY: Hylleraas wave function (Ref. 12).

Although $F(K)$ is comparatively insensitive to the accuracy of the wave function, $S_{\text{inc}}(K)$ is sensitive, especially for small K . For instance, $S_{\text{inc}}(K)$ of Compton and Allison²⁵ for $Ka_0 \cong 0.665$ is as much as 20% smaller than our HF and the 20-term HY values. Bartell and Gavin¹⁸ calculated both $F(K)$ and $S_{\text{inc}}(K)$ for $\sin(\theta/2)/\lambda \leq 1.0$. They used the "closed-shell correlated wave function" of Roothaan and Weiss,²⁶ and the result is comparable to ours from the 6-term HY wave function.

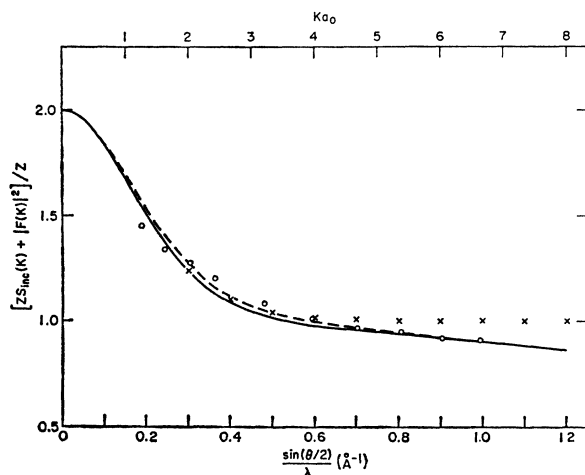


FIG. 1. Total x-ray scattering by the helium atom. The solid line is the result computed from the 20-term Hylleraas wave function (Ref. 12) with the relativistic correction (Ref. 1, p. 34), and the crosses (x) indicate the same without the relativistic correction. The broken line is the result computed from the Hartree-Fock wave function (Ref. 11), and the circles (o) indicate the experimental values of E. O. Wollan (Ref. 27).

²⁶ C. C. J. Roothaan and A. W. Weiss, Rev. Mod. Phys. **32**, 194 (1960). The wave function used in Ref. 18 is the "closed-shell correlated" one tabulated in Tables VI and VII of this reference.

III. SCATTERING CROSS SECTIONS

The results of the preceding section show that HF wave functions cannot be depended on to give accurate cross sections of the inelastic processes for small momentum transfers. In the case of the x rays, the small-angle incoherent-scattering cross section depends on the accuracy of wave functions. However, the total cross section (coherent plus incoherent) for the small-angle x-ray scattering does not depend very appreciably on wave functions, because for small momentum transfers the contribution from the coherent part is so large as to mask any difference in the incoherent part due to wave functions. In Fig. 1 we show the total x-ray scattering cross section of the helium atom calculated from the HF wave function, 20-term HY wave function, and the experimental result of Wollan.²⁷ Although the 20-term HY wave function, gives slightly better agreement with experiment at small scattering angles, the over-all performance of the HF wave function is comparable. The disagreement in the intermediate range of Ka_0 (2~5) is not understood. It can be seen also from Fig. 1 that the relativistic correction is necessary for large-angle scattering to obtain agreement with experiment.

The electron elastic-scattering cross section for small momentum transfers depends on the accuracy of the wave function more strongly than $F(K)$ itself. In particular, the behavior of $[Z-F(K)]/(Ka_0)^2$ is more sensitive to the wave function in the outer region of the atom because the leading term in the power-series expansion of $F(K)$ is cancelled by Z . As seen in Table III, the HF values of $[Z-F(K)]/(Ka_0)^2$ are different from

²⁷ E. O. Wollan, Phys. Rev. **37**, 862 (1931).

the 20-term HY values only for very small K , and the deviation is about 1% or less for $Ka_0 < 1$.

A useful quantity in this context is the zero-angle limit ($K \rightarrow 0$) of the elastic-scattering differential cross section,

$$d\sigma_{el}(\theta \rightarrow 0) = (X^2)^2 a_0^2 d\Omega, \quad (8)$$

which is given in terms of the expectation value X^2 defined by Eq. (7) and listed in Table IV. The data there indicate that, as the wave function steadily improves in terms of the energy, the value of X^2 follows an erratic trend until an accuracy corresponding to about the 6-term HY wave function is attained. The good agreement of our value of X^2 from the 20-term HY wave function with the best value by Pekeris²⁸ (cf. Table IV) gives an encouraging support to the accuracy of our $F(K)$ and $S_{inc}(K)$ obtained from the 20-term HY wave function.

The Eckart (ECK) type, or the open-shell type, wave functions are known to give too large a value of X^2 (cf. Table IV) and hence too large a value of $d\sigma_{el}(\theta \rightarrow 0)$.¹⁴ It is also interesting to note that the 3-term HY wave function gives very good values of $S_{inc}(K)$ compared to those from the 20-term HY wave function, as well as the value of X^2 . Experience with the 2-term HY wave function, however, was alarmingly discouraging. It gives values of $S_{inc}(K)$ almost 10% lower than those of the 20-term HY wave function for small Ka_0 , though the accuracy of $F(K)$ is comparable to that of the HF wave function. This may be interpreted as indicating that effects of the electron correlation are not adequately represented by the single r_{12} term.

In summary, we conclude that all cross sections for large momentum transfers are not very sensitive to the wave functions. For small momentum transfers, however, the incoherent-scattering cross section of x rays and the inelastic-scattering cross section of electrons according to the Born approximation are sensitive to the accuracy of the wave functions, and the HF wave function gives cross sections in error by about 5%. The electron elastic-scattering cross section for small momentum transfers depends moderately on the accuracy of wave functions, and the HF values will be in error by about 2%.²⁹ Various numerical data indicate that the 2-term HY and ECK wave functions are not dependable for cross-section calculations. The above features may serve as a guide for investigation of other atoms, although caution is required in generalizing our conclusions.²³

²⁸ C. L. Pekeris, Phys. Rev. **115**, 1216 (1959).

TABLE IV. Expectation values of the total energy and X^2 for the helium atom. (a.u. = atomic units.)

Wave function	Total energy (a.u.)	X^2 (a.u.)
Experimental Pekeris ^e	2.903387 ($\pm 1.1 \times 10^{-6}$) ^a	0.803 \pm 0.009 ^b
(extrapolated)	2.903724376	0.79565533
Exponential ^d	2.847656	0.7023
3-term HF ^e	2.861680	0.7899
ECK ^f	2.8757	0.8252
2-term HY ^g	2.89112	0.7179
Correlated closed-shell ^h	2.90039	0.7894
3-term HY ^g	2.90243	0.7982
Correlated open shell ^h	2.90319	0.7947
6-term HY ^g	2.90332	0.79574
10-term HY ⁱ	2.9036027	0.79554
14-term HY ^j	2.9037009	0.79512
18-term HY ^k	2.9037150	0.79530
20-term HY ^g	2.9037179	0.79555

^a This value is the sum of the total energy of He⁺ and the experimental ionization potential of He [G. Herzberg, Proc. Roy. Soc. (London) **A248**, 309 (1958)]. This value includes relativistic effects, whereas calculated values are nonrelativistic.

^b Deduced by W. F. Miller and R. L. Platzman (unpublished) from re-examination of diamagnetic susceptibility measurements both of L. G. Hector [Phys. Rev. **24**, 418 (1924)] and of G. G. Havens [Phys. Rev. **43**, 992 (1933)]. H. A. Bethe and E. E. Salpeter [*Quantum Mechanics of One- and Two-Electron Atoms*] (Springer-Verlag, Berlin, 1957), p. 357, using Haven's measurement only, give a slightly larger value with smaller error limits. The Pekeris value lies outside these limits.

^c Reference 28.

^d $\psi = (\zeta^3/\pi) \exp[-\zeta(r_1+r_2)]$, $\zeta = (27/16)a_0^{-1}$.

^e Reference 11.

^f R. P. Hurst *et al.*, Mol. Phys. **1**, 189 (1958).

^g Reference 12.

^h Reference 26.

ⁱ S. Chandrasekhar, D. Elbert, and G. Herzberg, Phys. Rev. **91**, 1172 (1953).

^j S. Chandrasekhar and G. Herzberg, Phys. Rev. **98**, 1050 (1955).

^k T. Kinoshita, Phys. Rev. **105**, 1490 (1957).

Note added in proof. Recently $S_{inc}(K)$ computed from a numerical HF wave function was published by D. T. Cromer and J. B. Mann [J. Chem. Phys. **47**, 1892 (1967)]. Their result is in close agreement with our HF values.

ACKNOWLEDGMENTS

The authors wish to express their gratitude to Professor R. L. Platzman for reviewing the manuscript, to Professor U. Fano for continued interest and encouragement, and to Dr. P. S. Bagus for supplying his unpublished results.

²⁹ Experimental results are often normalized to a theoretical value at a particular angle. For example, J. Geiger [Z. Physik **175**, 530 (1963)] normalized his 25-keV data at $\theta = 9.4 \times 10^{-3}$ radian, using the theoretical cross section obtained from an ECK wave function. Had he used the Pekeris value of X^2 , his cross sections would have been reduced by about 4%. On the other hand, the relativistic kinematic correction (see Ref. 6) will increase his cross sections by about 10% at this incident energy. Other relativistic corrections have not been evaluated.