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High-accuracy Compton profile of molecular hydrogen from explicitly correlated Gaussian wave function

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The electron momentum distribution for molecular hydrogen is calculated from an explicitly correlated Gaussian wave function corresponding to the total energy of − 1.17442 a.u. and accounting for 99.9% of the correlation energy. The high-accuracy Compton profile obtained confirms the results of recent high-energy electron-impact spectroscopy measurements of Lee, but disagrees in the region of very small momentum with earlier x-ray Compton-scattering data.

I. INTRODUCTION

It has been known for a long time[1,2] that the spectrum of the Compton-scattered photons is closely related to the distribution of the electronic momentum in atoms, molecules, or solids. However, it was not until 1970 that Eisenberger and Platzman[3] showed rigorously that for $k^2 \gg 2E_B$ (where k is the momentum transfer and E_B is the binding energy of the scattering electron[4]) the shape of the shifted Compton line (the Compton profile) is independent of the momentum transfer and scattering angle, and, for randomly oriented systems is determined solely by the radial momentum distribution function $I(p)$

$$J(q)=\frac{1}{2}\int_{|q|}^{\infty} p^{-1}I(p)\,dp\,. \tag{1}$$

Hughes and Mann[5] showed that the Compton profile $J(q)$ can also be measured by electron scattering. The validity of Eq. (1), i.e., the validity of the so-called impulse approximation (IA), is in this case also limited[6] to large values of the momentum transfer k.

The first quantitative test of Eq. (1) has been made by Eisenberger[7] who measured the He and H_2 Compton profiles applying the x-ray scattering technique and compared them with the theoretical profiles calculated by Henneker[8] using the Hartree-Fock self-consistent-field (HFSCF) or the multiconfiguration self-consistent-field (MCSCF) wave functions. While the agreement between the theory and the experiment was excellent for helium, the theoretical profiles for H_2 were at small q substantially higher than the experimental one. This disagreement was somewhat disturbing, since, due to the weaker binding of electrons, Eq. (1) should be more accurate for H_2 than for He. Moreover, it has been found[9] that the vibrational correction to the theoretical Compton profile raises it by approximately 1% in the low-momentum region and thereby increases the disagreement between theory and experiment. To clear up the reason for the observed discrepancy, Brown and Smith[10] calculated the Compton profile of H_2 using the Liu[11] 39-term configuration interaction (CI) function accounting for 98% of the correlation energy. It turned out that the resulting profile is lower than the HFSCF one but still gives for $J(0)$ an error of about 2% (including the vibrational correction), which is greater than the experimental error of ±0.7%. Brown and Smith[10] conclude that the expected corrections to the theoretical profile with more correlation should largely remove this discrepancy.

Very recently, however, Lee[6] has determined the H_2 and D_2 Compton profiles by means of the high-energy electron impact spectroscopy (HEEIS) and has found them to be about 2% higher than the x-ray profile of Eisenberger. Thus, the Lee value of $J(0)$ has been very close to the theoretical result of Brown and Smith corrected for the vibrational effect but not corrected for the lacking correlation correction. The main purpose of our paper is to find whether the latter correction is large enough to confirm the x-ray scattering data or is negligible and thereby corroborates the recent electron scattering measurements.

With this end in view, a high-accuracy Gaussian wave function containing explicitly the interelectronic distance r_{12} and giving 99.9% of the correlation energy is transformed into momentum space and the radial momentum distribution $I(p)$ is calculated from it without recourse to any numerical quadrature. The Compton profile of H_2, resulting from $I(p)$ via single numerical integration, turns out to be very close to the theoretical profile of Brown and Smith and thereby confirms the HEEIS data of Lee. In particular, the height of our theoretical profile amounting to 1.5465 a.u. (including the vibrational correction) is in excellent agreement with the HEEIS value of 1.540 ± 0.010 a.u.

The other purpose of our paper is to present a high-accuracy radial momentum distribution for H_2 that could be used to test the various scattering techniques employed to study the electron density of molecules or solids.

II. METHOD

Among many ground-state wave functions for H_2 available in the literature, the most accurate one is that of Kołos and Wolniewicz.[12] Unfortunately, owing to the presence of the odd powers of the interelectronic distance r_{12}, this wave function seems to be extremely difficult to transform into momentum space. Since the explicit dependence of a wave function upon the interelectronic distance is essential to obtain the correlation energy with a very high accuracy, we decided to apply in our calculations the basis set of explicitly correlated Gaussian functions (CGF). We shall show that this basis set, employed for the first time by Longstaff and Singer,[13] enables one to obtain very accurate values of the correlation energy and permits the Fourier transformation to be carried out analytically. The explicit form of our wave function is

$$\psi(\vec{r}_1, \vec{r}_2) = \tfrac{1}{4}(1+P_{12})(1+I)\sum_{k=1}^{N} c_k \chi_k(\vec{r}_1, \vec{r}_2), \tag{2}$$

$$\chi_k(\vec{r}_1, \vec{r}_2) = \exp(-\alpha_k r_{A1}^2 - \beta_k r_{B1}^2 - \alpha_k' r_{A2}^2 - \beta_k' r_{B2}^2 - \gamma_k r_{12}^2), \tag{3}$$

where the operator P_{12} interchanges the electronic coordinates, the operator I inverts the wave function through the midpoint of the internuclear axis, and r_{A1}, r_{A2}, r_{B1}, r_{B2}, r_{12} are distances between the electrons (1 or 2) and nuclei (A or B) specified by the respective subscripts. The linear c_k and nonlinear α_k, β_k, α_k', β_k', γ_k parameters have been determined in the following way. For the first 42 of $N=101$ terms in Eq. (2), we have set $\gamma_k=0$ and the parameters α_k, β_k, α_k', and β_k' have been obtained by expanding the HFSCF function of Schwartz and Schaad[14] according to Eqs. (2) and (3). All the linear and remaining nonlinear parameters have been determined by minimizing the total energy $\epsilon = (\psi|H\psi)/(\psi|\psi)$. The resulting total and correlation energies are shown in Table I, where they are also compared with the results of other accurate calculations for H_2. It is seen that our wave function is almost as accurate as that of Kołos and Wolniewicz and predicts the correlation energy of H_2 with an error of two orders of magnitude smaller than the previous best CGF function of Handy.[15]

The Fourier transformation of $\psi(\vec{r}_1, \vec{r}_2)$ can be written in the following way:

$$\tilde{\psi}(\vec{p}_1, \vec{p}_2) = \tfrac{1}{4}(1+P_{12})(1+\tilde{I})\sum_{k=1}^{N} c_k \tilde{\chi}_k(\vec{p}_1, \vec{p}_2), \tag{4}$$

where

$$\tilde{\chi}_k(\vec{p}_1, \vec{p}_2) = (2\pi)^{-3} \int\int \exp(-i\vec{p}_1\vec{r}_1 - i\vec{p}_2\vec{r}_2) \times \chi_k(\vec{r}_1, \vec{r}_2)\, d\vec{r}_1\, d\vec{r}_2 \tag{5}$$

and $\tilde{I}$ is the Fourier transform of the operator I

$$\tilde{I}\varphi(\vec{p}_1, \vec{p}_2) = e^{-i(\vec{A}-\vec{B})(\vec{p}_1+\vec{p}_2)}\varphi(-\vec{p}_1, -\vec{p}_2). \tag{6}$$

The vectors $\vec{A}$ and $\vec{B}$ specify here the positions of nuclei A and B, respectively. The sixfold integral in Eq. (5) can be solved analytically and after some tedious algebra one gets

$$\tilde{\chi}_k(\vec{p}_1, \vec{p}_2) = C_k \exp\left\{-i(\vec{p}_1\vec{S}_k + \vec{p}_2\vec{T}_k) - \frac{1}{4\mu_k}\left[\tau_k' p_1^2 + \tau_k p_2^2 + \gamma_k(\vec{p}_1+\vec{p}_2)^2\right]\right\}, \tag{7}$$

where

TABLE I. Comparison of total energies of H_2 obtained by using various basis sets.[a]

	Basis[b]	$E_{\rm var}$	$\%E_{\rm corr}$[c]
Longstaff and Singer (Ref. 13)	CGF	−1.168 1	84.4
Das and Wahl (Ref. 16)	STO	−1.169 8	88.6
Handy (Ref. 15)	CGF	−1.170 0	89.1
Liu (Ref. 11)	STO	−1.173 63	97.9
This work	CGF	−1.174 42	99.9
Kołos and Wolniewicz (Ref. 12)	KWB	−1.174 47	100.0

[a] Energies in a.u.; internuclear separation is 1.4 a.u.

[b] Specification of basis set: CGF—correlated Gaussian functions; STO—Slater-type orbitals; KWB—the Kołos and Wolniewicz basis of functions in eliptic coordinates.

[c] $\%E_{\rm corr} = 100\% \times (E_{\rm var} - E_{\rm SCF})/(E_{\rm exact} - E_{\rm SCF})$, where $E_{\rm SCF} = -1.133\,63$ a.u. (Ref. 17) and $E_{\rm exact} = -1.174\,47$ a.u. (Ref. 12).

$$C_k=\left(\frac{1}{4\mu_k}\right)^{3/2}\exp\left[-\left(\frac{\alpha_k\beta_k}{\tau_k}+\frac{\alpha_k'\beta_k'}{\tau_k'}\right)(\vec{\mathrm{A}}-\vec{\mathrm{B}})^2-\frac{\tau_k\tau_k'\gamma_k}{\mu_k}(\vec{\mathrm{P}}_k-\vec{\mathrm{Q}}_k)^2\right] \tag{8a}$$

and the following notation is used:

$$\tau_k=\alpha_k+\beta_k,\quad \tau_k'=\alpha_k'+\beta_k',\quad \mu_k=\tau_k\tau_k'+\gamma_k(\tau_k+\tau_k')\,, \tag{8b}$$

$$\vec{\mathrm{P}}_k=(\alpha_k\vec{\mathrm{A}}+\beta_k\vec{\mathrm{B}})/\tau_k,\quad \vec{\mathrm{Q}}_k=(\alpha_k'\vec{\mathrm{A}}+\beta_k'\vec{\mathrm{B}})/\tau_k'\,, \tag{8c}$$

$$\begin{aligned}\vec{\mathrm{S}}_k&=[\tau_k(\tau_k'+\gamma_k)\vec{\mathrm{P}}_k+\tau_k'\gamma_k\vec{\mathrm{Q}}_k]/\mu_k\,,\\ \vec{\mathrm{T}}_k&=[\tau_k'(\tau_k+\gamma_k)\vec{\mathrm{Q}}_k+\tau_k\gamma_k\vec{\mathrm{P}}_k]/\mu_k\,.\end{aligned} \tag{8d}$$

The momentum-space wave function $\tilde{\psi}(\vec{\mathrm{p}}_1,\vec{\mathrm{p}}_2)$ can now be used to calculate the diagonal element of the first-order density matrix. This is given by

$$\rho(\vec{\mathrm{p}})=2\int|\psi(\vec{\mathrm{p}},\vec{\mathrm{p}}\,')|^2\,d\vec{\mathrm{p}}\,'=\sum_{kl}^{N}c_kc_l\,\rho_{kl}(\vec{\mathrm{p}})\,, \tag{9}$$

where

$$\rho_{kl}(\vec{\mathrm{p}})=\frac{1}{8}\int[(1+P_{12})(1+\tilde{I})\tilde{\chi}_k(\vec{\mathrm{p}},\vec{\mathrm{p}}\,')]^*(1+P_{12})\times(1+\tilde{I})\tilde{\chi}_l(\vec{\mathrm{p}},\vec{\mathrm{p}}\,')\,d\vec{\mathrm{p}}\,'\,. \tag{10}$$

In evaluating Eq. (10), one obviously cannot make use of the Hermiticity of P_{12} and $\tilde{I}$; hence all the 16 integrals resulting from (10) are different. Thus the result of the integration over $\vec{\mathrm{p}}\,'$ can be written

$$\rho_{kl}(\vec{\mathrm{p}})=\sum_{m=1}^{16}d_{klm}\exp(i\vec{\mathrm{p}}\vec{\mathrm{v}}_{klm}-\epsilon_{klm}p^2)\,, \tag{11}$$

where d_{klm}, $\vec{\mathrm{v}}_{klm}$, and ϵ_{klm} are constants that can easily be obtained from Eqs. (7)–(10). The explicit expressions for these constants are somewhat too involved to be reported here. The radial momentum distribution function to be used in Eq. (1) is obtained by averaging $\rho(\vec{\mathrm{p}})$ over all orientations of the vector $\vec{\mathrm{p}}$. The integration resulting from the averaging procedure is elementary and its result is

$$I(p)=4\pi p\sum_{kl}^{N}\sum_{m=1}^{16}c_kc_l\frac{d_{klm}}{v_{klm}}\sin(v_{klm}p)\times\exp(-\epsilon_{klm}p^2)\,, \tag{12}$$

where $v_{klm}=|\vec{\mathrm{v}}_{klm}|$. We see that for the wave function of Eqs. (2) and (3) the radial momentum distribution $I(p)$ can simply be expressed via elementary functions. This makes the basis set of the correlated Gaussian functions to be especially useful for the calculation of high-accuracy Compton profiles. When the numerical values of $I(p)$ are calculated, the single integral in Eq. (1) can easily be carried out numerically by using, e.g., Simpson quadrature.

III. RESULTS AND DISCUSSION

The high-accuracy radial momentum distribution function for H_2 obtained by using Eq. (12) is tabulated in Table II, whereas in Table III are presented: the Compton profile calculated from our $I(p)$, Eq. (12), the HFSCF and MCSCF profiles of Henneker,[8] the CI profile of Brown and Smith,[10] the CI profile of Smith *et al.*,[18] this same profile corrected for the vibration-rotation motion of nuclei[18] and the experimental profiles obtained by using the x-ray[7] and the electron[6] scattering techniques. In Table IV we report the values of $\rho(0)$, $\langle p^0\rangle$, $\langle p^1\rangle$, $\langle p^2\rangle$, $\langle p^3\rangle$, and $\langle p^4\rangle$ calculated from our $I(p)$. The numerical integrations were carried out using a suitable 271-point Simpson quadrature. We have checked that, to the number of digits quoted, the errors of these integrations have no effect on our results. Since our radial momentum density dies out as $p\exp(-cp^2)$ while the correct[20] behavior is p^{-6}, it might be expected that our values of $J(q)$ are inaccurate at large q. However, we have verified that the exponential decay of $I(p)$ manifests itself only for $p>60$ a.u. This fact is, of course, due to the high quality of our basis set. Comparison of our Compton profile with that of Brown and Smith[10] (the latter dies out like q^{-6}) shows also that the improper large-q behavior of our $J(q)$ is not relevant at physically interesting values of q.

In order to illustrate the high effectiveness of our basis set, it is worthwhile to report here some position-space properties of H_2 calculated recently

TABLE II. Electron momentum density of H_2. Internuclear separation is 1.4 a.u. All values in a.u.

p	$I(p)$ [a]	p	$I(p)$ [a]
0.00	0.000 00	1.1	0.595 66
0.05	0.018 22	1.2	0.494 13
0.10	0.071 17	1.3	0.404 67
0.15	0.153 99	1.4	0.328 45
0.20	0.259 32	1.5	0.264 96
0.25	0.378 33	1.6	0.212 83
0.30	0.501 75	1.7	0.170 46
0.35	0.620 96	1.8	0.136 25
0.40	0.728 70	1.9	0.108 80
0.45	0.819 62	2.0	0.086 84
0.50	0.890 38	2.2	0.055 46
0.55	0.939 61	2.4	0.035 72
0.60	0.967 57	2.6	0.023 34
0.75	0.942 89	2.8	0.015 55
0.80	0.907 62	3.0	0.010 61
0.85	0.863 70	4.0	0.002 36
0.90	0.813 80	5.0	0.000 82
0.95	0.760 28	6.0	0.000 31
1.00	0.705 08	10.0	$0.000\,01_5$

[a] $I(p)$ is normalized to unity.

TABLE III. Comparison of theoretical and experimental Compton profiles of H_2.[a]

q	HFSCF[b]	MCSCF[b]	CI1[c]	CI2[d]	CIV[e]	CGF[f]	X-ray[g]	HEEIS[h]
0.0	1.558	1.573	1.529	1.5322	1.5467	1.5319	1.513	1.540
0.1	1.520	1.532	1.493	1.4962	1.5096	1.4958	1.475	1.501
0.2	1.413	1.416	1.393	1.3946	1.4050	1.3939	1.378	1.392
0.3	1.257	1.249	1.245	1.2444	1.2508	1.2435	1.240	1.233
0.4	1.074	1.060	1.069	1.0677	1.0702	1.0670	1.065	1.051
0.5	0.887	0.871	0.888	0.8858	0.8850	0.8855	0.887	0.868
0.6	0.713	0.699	0.717	0.7149	0.7118	0.7151	0.712	0.699
0.7	0.560	0.551	0.566	0.5646	0.5603	0.5651	0.561	0.553
0.8	0.433	0.429	0.440	0.4388	0.4340	0.4394	0.435	0.431
0.9	0.331	0.330	0.337	0.3372	0.3324	0.3377	0.334	0.333
1.0	0.250	0.253	0.257	0.2571	0.2528	0.2575	0.255	0.255
1.2	0.142	0.147	0.147	0.1478	0.1447	0.1481	0.150	0.149
1.4	0.080	0.085	0.084	0.0849	0.0828	0.0850	0.089	0.087
1.6	0.045	0.049	0.049	0.0491	0.0479	0.0492	0.051	0.051
1.8	0.026	0.029	0.029	0.0289	0.0281	0.0289	0.030	0.030
2.0	0.015	0.017	0.017	0.0173	0.0169	0.0173	0.015	0.018

[a] All values reported here are in a.u. Theoretical profiles have been calculated at the equilibrium separation of nuclei, $R = 1.4$ a.u.

[b] Henneker results reported by Eisenberger (Ref. 7); SCF function of Cade (unpublished), and MCSCF function of Das and Wahl (Ref. 16).

[c] Brown and Smith (Ref. 10) results; CI function of Liu (unpublished).

[d] Smith *et al.* (Ref. 18) results, CI function of Liu (Ref. 19).

[e] Profile CI2 corrected for the vibration-rotation motion of nuclei (Ref. 18).

[f] This work.

[g] Eisenberger (Ref. 7) experimental results. Experimental errors are ±0.7%, ±1%, ±3%, and ±10% at $q = 0.0$, 0.6, 1.2, and 1.8, respectively.

[h] Lee (Ref. 6) experimental results obtained by HEEIS. Displayed numbers are evaluated using Eq. (10) of Ref. 6 with coefficients from Table VII of Ref. 6. The experimental error is reported by Lee only at $q = 0.0$. It amounts to ±0.7%.

by using our CGF wave function. The calculated value of the parallel component of H_2 polarizability is 6.372 a.u.,[21] whereas the exact result amounts to 6.380 a.u.[22] The quotient $V/2E$ (the virial theorem) calculated at $R = 1.4$ a.u. turns out to be equal to 1.000 26 while the exact value is 1.000 24.[12] For the dispersion energy of H_2 at the distance of the Van der Waals minimum ($R = 8$ a.u.) we obtained the value of -3.659×10^{-5} a.u.,[23] whereas the previous best result of Kołos[24] is -3.658×10^{-5} a.u. The above results demonstrate the high accuracy of our wave function and are supplementary to the information contained in Table I.

Table IV shows that our values of $\rho(0)$, $\langle p^0 \rangle$, $\langle p^1 \rangle$, $\langle p^2 \rangle$, $\langle p^3 \rangle$, and $\langle p^4 \rangle$ are in good agreement with values obtained by Lee,[6] lying well within the experimental error limits. In the case of $\langle p^{-1} \rangle$, $\langle p^0 \rangle$, and $\langle p^1 \rangle$ our results are very close to those obtained from the CI STO calculations[10] but for higher powers of momentum we have obtained significant improvement. For $\langle p^2 \rangle$ we have obtained excellent agreement with the exact result of Kołos and Wolniewicz.[12] On the other hand our value of $\langle p^4 \rangle$, though closer to the exact one[25] than any other result quoted in Table IV, is still by about 0.5 a.u. too small. The reason for this is the above-mentioned too-fast decay of our $I(p)$ for large p. This is clearly seen if we note that the contribution to $\langle p^4 \rangle$ from the high-momentum region $p > 60$ a.u. [i.e., from that area where our $I(p)$ dies out too fast], estimated by using the hydrogen atom density amounts to about 0.4 a.u. The same effect can also enter $\langle p^2 \rangle$ and $\langle p^3 \rangle$ but at the last digit quoted in Table IV.

Comparison of the fourth and seventh columns of Table III shows that, in spite of using a much better wave function, giving 99.9% of the correlation energy, our Compton profile is very close to that of Brown and Smith, obtained with the wave function giving only 98% of the correlation energy. Thus, our values of $J(q)$ cannot be expected to change when the remaining 0.1% of the electron correlation is allowed for. We can conclude then, that the Compton profile calculated by us is the ultimate nonrelativistic IA Compton profile for H_2. It is worthwhile to add here that our value of $J(0)$, contrary to what one might intuitively expect, is slightly higher than the value obtained by Brown and Smith. However, in later papers[18,26] Smith *et al.* quote a different value for $J(0)$ obtained with

TABLE IV. Expectation values of some powers of momentum and the momentum density at $p=0$ for H_2 molecule. All values in a.u.[a]

	$\rho(0)$	$\frac{1}{2}\langle p^{-1}\rangle$	$\langle p^0\rangle$	$\langle p^1\rangle$	$\langle p^2\rangle$	$\langle p^3\rangle$	$\langle p^4\rangle$
Experiment (Ref. 6)	1.254 ± 0.251	1.540 ± 0.010	1.993 ± 0.020	1.854 ± 0.028	2.346 ± 0.094	4.048 ± 0.405	10.58 ± 5.29
CI STO[b]	1.149	1.529 (1.532 21)[c]	2.000	1.857	2.342	4.126	12.02
This work	1.169 06	1.531 94	2.000	1.856 89	2.350 06	4.218	12.75
Exact	···	···	2.0	···	2.350 07[d]	···	13.25[e]

[a] Theoretical values do not include vibrational corrections.

[b] Values other than $\langle p^{-1}\rangle$ were obtained in Ref. 6 by fitting the results of Brown and Smith (Ref. 10).

[c] Reference 18.

[d] Reference 12.

[e] Reference 25.

a slightly different Liu CI function[19] and equal to 1.5322. This value as well as the whole profile of Ref. 18 (cf. Table III) are almost identical with ours, thereby confirming the high, limiting accuracy of our Compton profile.

Comparison of the second and seventh columns of Table III clearly shows that the electron correlation correction to the Hartree-Fock profile is small, ranging from −1.7% for $q=0$ to +3% for $q=1$ and +13% for $q=2$. It is difficult to say whether the correlation contribution to $J(q)$ behaves similarily for other molecules. For H_2O for instance, this contribution has been found[27] to be positive at $q=0$. However, it should be noted that while for $q>1$ even a moderately correlated wave function can describe adequately the correlation correction to $J(q)$, a high-accuracy wave function is required to predict a correct sign of this correction at small values of q. For example, the MCSCF wave function of Das and Wahl[16] accounting for 89% of the correlation energy of H_2 predicts a wrong (positive) sign for the correlation contribution to $J(0)$.

To compare the theoretical profile with an experiment one should add the correction for the vibration-rotation motion of nuclei.[9,18] Owing to the slight anharmonicity of this motion the average internuclear distance $\langle R\rangle$ is somewhat larger than the equilibrium separation $R_e=1.4$ a.u. Thus the vibrationally averaged profile should be more similar to the profile of two H atoms, i.e., should be slightly higher and more contracted than that calculated at $R=1.4$ a.u. It has been found,[9,18] that the vibrational correction to $J(0)$ is really positive and increases $J(0)$ by about 1%. The corrected value equal to 1.546 is in excellent agreement with the experimental value of Lee[6] obtained by using high-energy electron scattering but disagrees with the earlier x-ray Compton scattering data of Eisenberger.[7]

It should be noted, however, that our profile cannot be in a complete agreement with Lee's profile for the whole range of the variable q. The reason for this is that the latter profile is normalized to 0.9965 rather than to unity. Lee argues that his profile should not be renormalized and that his method of normalizing the experimental data leads to very accurate values of $J(q)$ near the peak of the profile. Therefore, his values of $J(q)$ must be smaller than curs at some larger values of q. This is clearly observed at $0.3 \leq q \leq 0.8$. In this region, however, our profile corrected according to Ref. 18 lies well within the error limits of the x-ray experiment. The same would occur for the HEEIS profile provided that the experimental error limits were in that case about twice as large as the x-ray profile error limits. Unfortunately, experimental error is reported by Lee only at $q = 0$.

The low-momentum disagreement between the x-ray Compton profile on the one hand and the HEEIS and theoretical ones on the other is much larger than the experimental error bounds. Unless the multiple-scattering effects[28] are considerably stronger for H_2 than for helium, this disagreement is difficult to explain at the moment.

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