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Compton profiles of Ne, Ar, and Kr

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Compton profiles of Ne, Ar, and Kr are calculated from ground-state energies and wave functions with full correlation contributions included. The latter is carried out by regarding atoms as inhomogeneous interacting electron-gas systems using the Kohn-Sham self-consistent scheme in the local-density approximation. The calculated values are brought closer to the experimental values from Hartree-Fock results. There are numerical problems for large atoms.

I. INTRODUCTION

Improved techniques in Compton scattering measurements have induced numerous experimental and theoretical investigations of electron momentum distributions.[1] Tables of calculated Compton profiles of atoms based on the available Hartree-Fock wave functions[2,3] have been published and deposited.[4-6] Compton profile measurements can be useful as a probe into many-body interactions in an electron liquid, as well as for Fermi surfaces in the case of metals.[7-9] It is therefore of great interest to calculate the effect of correlations on Compton profiles. Lam and Platzman[10] (LP) formulated a general approach to determine the momentum density and Compton profile of an inhomogeneous interacting electron system. Their method is based on a combination of Feynman's theorem[11] and the Hohenberg-Kohn formulation[12] of inhomogeneous electron gas. In their original paper,[10] several approximate practical calculation methods have been suggested. One of these, the locally averaged method, has been applied to rare-gas atoms[13] and to alkali metals.[14-16] The other more systematic way, also suggested by LP, in incorporating correlation effects in inhomogeneous gas systems makes use of the Kohn-Sham self-consistent scheme.[17] This is the method used here to study rare-gas atoms. The local-density approximation is made. The local-density approximation is expected to be good for slowly varying density systems like those for metals. Previous experience indicates that, even for atoms, it has been fairly successful.[18] In Sec. II we shall summarize the LP method. The reader is referred to the original papers[10,12,17] for the detailed derivation and careful reasoning involved.

For closed-shell atoms, correlation effects are relatively small. Since accurate experimental results[19-21] and several theoretical estimates[22-24] are available, rare-gas atoms are studied here for comparison. Our results are closer to the best-measured values, but numerical uncertainties are present in larger atoms, the radial wave functions of which have long tails. These will be presented and discussed in Sec. III.

II. METHOD

In x-ray or γ-ray scattering experiments from an electron gas, when both the energy and momentum transfers are large, the electrons are scattered into the continuum. The impulse approximation is applicable.[25] In this approximation the differential cross section is found to be linearly proportional to $J(q)$, where

$$J(q)=\int\int dp_x\,dp_y\,(N_{\vec{p}})_{p_z=q} \tag{2.1}$$

and the momentum density $N_{\vec{p}}$ is defined by

$$N_{\vec{p}}=\langle\Phi|a_{\vec{p}}^{\dagger}\,a_{\vec{p}}|\Phi\rangle\,. \tag{2.2}$$

$|\Phi_0\rangle$ is the exact ground-state wave function of the electronic system and $a_{\vec{p}}$ and $a_{\vec{p}}^{\dagger}$ are the annihilation and creation operators of the free-electron state $|p\rangle=e^{i\vec{p}\cdot\vec{r}}$. To calculate the Compton profile $J(q)$, we must first calculate the exact ground state $|\Phi_0\rangle$ of the interacting electron system. This is carried out by using the Kohn-Sham self-consistent scheme based on the Hohenberg-Kohn theorems. If we define the energy functional $E(n)$ as (we use units of $\hbar=e^2=m=1$)

$$E(n)=\int V(\vec{r})\,n(\vec{r})\,d\vec{r}+\frac{1}{2}\int\int\frac{n(\vec{r})\,n(\vec{r}')}{|(\vec{r}-\vec{r})|}\,d\vec{r}\,d\vec{r}'+G[n] \tag{2.3}$$

for the system of inhomogeneous nonrelativistic interacting electrons under the influence of an external potential $V(\vec{r})$ and the mutual Coulomb repulsion, $G[n]$ is shown by using the first Hohenberg-Kohn theorem to be a universal unique functional of the true ground-state density.[12] By writing $G[n]$ as

$$G[n]=T_s[n]+E_{xc}[n], \tag{2.4}$$

where $T_s[n]$ is the kinetic energy of a noninteracting electron gas of density $n(\vec{r})$, and $E_{xc}[n]$ is, by definition, the exchange and correlation energy functional of an interacting electron gas with density $n(\vec{r})$. Kohn and Sham[17] used the stationary nature of $E[n]$ (second Hohenberg-Kohn theorem) to obtain a self-consistent set of one-electron equations:

$$[\tfrac{1}{2}\nabla^2+V_{\mathrm{eff}}(\vec{r})]\Psi_i(\vec{r})=E_i\Psi_i(\vec{r}), \tag{2.5}$$

where

$$V_{\mathrm{eff}}(\mathrm{r})\equiv V(\mathrm{r})+\int\frac{n(\vec{r})}{|\vec{r}-\vec{r}'|}\,d\vec{r}'+V_{xc}(\vec{r}') \tag{2.6}$$

and

$$V_{xc}(\mathrm{r})\equiv\delta E_{xc}[n]/\delta n(\vec{r}), \tag{2.7}$$

$$n(\vec{r})=\sum_{i=1}^{N}|\Psi_i(\vec{r})|^2. \tag{2.8}$$

This system of equations is formally exact.

To find a connection between the above and the momentum density $N_{\vec{p}}$, LP[10] considered a modified Hamiltonian of the form

$$H(\lambda)=H+\lambda a^\dagger_{\vec{p}}a_{\vec{p}}, \tag{2.9}$$

where H is the true Hamiltonian of the interacting electron system, and λ, a parameter. Feynman's theorem states

$$\frac{\partial E_p(\lambda)}{\partial\lambda}=\left(\phi(\lambda),\frac{\partial H(\lambda)}{\partial\lambda}\phi(\lambda)\right), \tag{2.10}$$

giving [from Eq. (2.2)],

$$N_p=\left(\frac{\partial E_p(\lambda)}{\partial\lambda}\right)_{\lambda=0}. \tag{2.11}$$

The modification in $H(\lambda)$ only affects the ground-state energy E through the explicit dependence of $G_\lambda[n]$ in λ [Eq. (2.3)] and the contribution from the dependence in $n(\vec{r})$ can be neglected because of the stationary properties of E with respect to $n(\vec{r})$ (see the detailed arguments given in LP[10]). Consequently,

$$N_p=\left(\frac{\partial G_\lambda[n]}{\partial\lambda}\right)_{\lambda=0}=\left(\frac{\partial T_p[n]}{\partial\lambda}\right)_{\lambda=0}+\left(\frac{\partial E_{xc}[n]}{\partial\lambda}\right)_{\lambda=0}. \tag{2.12}$$

The kinetic energy operator T_p of noninteracting electrons can be written in terms of creation and annihilation operators for plane waves

$$T_p=\sum\epsilon_k(p)a_k^\dagger a_k, \tag{2.13}$$

where

$$\epsilon_k(p)=\epsilon_k+\lambda\,\delta_{p,k}\quad\text{and}\quad\epsilon_k=\tfrac{1}{2}k^2. \tag{2.14}$$

Equation (2.12) then becomes

$$\begin{aligned}N_p&=\frac{\partial T_p}{\partial\epsilon_p}+\frac{\partial E_{xc}[n]}{\partial\epsilon_p}\\&=\sum_{i=1}^{N}|\langle p|\psi_i\rangle|^2+\frac{\delta E_{xc}[n]}{\delta\epsilon_p}.\end{aligned} \tag{2.15}$$

$E_{xc}[n]$ is the defined exchange and correlation energy functional of an interacting electron gas. Its exact form is not known. Previous experiences indicate that the local approximation is good in solving ground-state problems of metals and fairly good even in atomic problems.[18,26,27] In this approximation,

$$E_{xc}[n]\simeq\int\epsilon_{xc}(n(\vec{r}))n(\vec{r})\,d\vec{r}, \tag{2.16}$$

where $\epsilon_{xc}(n)$ is the exchange and correlation energy per electron of an interacting electron gas at uniform density n equal to the local density $n(\vec{r})$ of the given system at $\vec{r}$. Then V_{xc} of Eq. (2.7) has the explicit form

$$V_{xc}\equiv\mu_{xc}=\mu_x+\mu_c, \tag{2.17}$$

where

$$\mu_x=-(3n/\pi)^{1/3} \tag{2.18}$$

and μ_c is obtained from interpolating between the low-density formula of Wigner and the high-density result of Gell-Mann and Brueckner.[28] For explicit values of μ_c, see Fig. 1 of Ref. 18.

The second term of Eq. (2.15) becomes

$$\begin{aligned}\frac{\delta E_{xc}[n]}{\delta\epsilon_p}&=\int\frac{\delta\epsilon_{xc}}{\delta\epsilon_p}n(\vec{r})d\vec{r}\\&=\int[N_p^0(n(\vec{r}))-N_p^F(n(\vec{r}))]n(\vec{r})\,d\vec{r},\end{aligned} \tag{2.19}$$

where $N_p^F(n)$ is the free-electron Fermi distribution, and $N_p^0(n)$ is the momentum density of an uniform electron liquid with local density $n(\vec{r})$. Explicit values of N_p have been calculated by Daniel and Vosko[29,30] (DV) and by Lundqvist.[31,32] At high metallic densities the deviations between the two are small. At lower densities the deviations become significant, and the former method breaks down.[32,33] The Lundqvist calculation emphasizes the coupling of electrons to plasmons. We used the Lundqvist values (Table I) in the following calculation.

Here we have a slight inconsistency in calculat-

TABLE I. Momentum distribution by Lundqvist (Ref. 31).

k r_s	$r_s=2$	$r_s=3$	$r_s=4$	$r_s=5$
0	0.98	0.96	0.94	0.93
0.20	0.98	0.96	0.94	0.93
0.4	0.97	0.95	0.94	0.92
0.6	0.97	0.94	0.92	0.90
0.8	0.94	0.92	0.88	0.86
0.9	0.92	0.88	0.85	0.83
0.96	0.90	0.85	0.82	0.80
1−	0.87	0.82	0.78	0.75
1+	0.10	0.12	0.14	0.15
1.04	0.06	0.09	0.11	0.11
1.1	0.04	0.06	0.07	0.08
1.2	0.02	0.03	0.04	0.05
1.4	0.01	0.01	0.02	0.02
1.6	0.003	0.005	0.007	0.009
1.8	0.001	0.002	0.003	0.005
2.0	0.0006	0.001	0.002	0.002
2.2	0.0003	0.0006	0.0009	0.001
2.4	0.0001	0.0003	0.0004	0.0006

ing correlation effects. Lundqvist's values are used in Eq. (2.19) to give us the correction term [second term of Eq. (2.15)]. The Fourier transforms [first term in Eq. (2.15)] of the Kohn-Sham one-electron wave functions are obtained from using the interpolated form μ_{xc} in Eq. (2.17). This is one source of error in our present calculation, as will be seen in the results. In the low-density tail regions of large atoms, the second term in Eq. (2.15) over corrects. It is especially noticeable at small q.

Now we have one complete calculation scheme. Adding (2.17) and (2.18) to Eqs. (2.5)–(2.8), we have an explicit self-consistent set of equations from which we obtain the one-electron wave functions. The Fourier transform of these gives the first term of Eq. (2.15). The second term is obtained from evaluating Eq. (2.19). From $N_{\vec{p}}$, we then can calculate $J(p_z)$ using Eq. (2.1). In practice, it is found more advantageous to evaluate $J(p_z)$ directly without passing through the $N_{\vec{p}}$ eval-

TABLE II. Compton profile $J(q)$ of atomic Ne.

			Present work					
q	HF[a]	CI[b]	$J^{(1)}$	+ $J^{(2)}$	= $J(q)$	J_{HF}[c] (1s)	J_E[d]	J_{expt}
0.0	2,725 67	2.724 46	2.789	−0.050	2.739	0.0899	2.582	2.762
0.1	2.717 97	2.716 71	2.782	−0.042	2.740	0.0899	2.574	2.754
0.2	2.694 31	2.692 86	2.755	−0.031	2.723	0.0898	2.558	2.738
0.3	2.653 23	2.651 48	2.709	−0.022	2.687	0.0897	2.519	2.698
0.4	1.593 22	2.591 04	2.641	−0.012	2.629	0.0894	2.451	2.630
0.5	2.513 52	2.510 83	2.550	−0.010	2.540	0.0892	2.359	2.537
0.6	2.414 80	2.411 54	2.438	−0.005	2.433	0.0888	2.249	2.427
0.7		2.295 46	2.309	−0.004	2.305	0.0884	2.124	2.301
0.8	2.170 45	2.166 13	2.168	−0.003	2.162	0.0879	1.986	2.162
0.9		2.027 87	2.020	−0.002	2.018	0.0874	1.839	2.014
1.0	1.890 10	1.885 13	1.869	−0.002	1.867	0.0868	1.685	1.859
1.2	1.606 97	1.602 00	1.577	0.000	1.577	0.0855	1.394	1.565
1.4	1.345 36	1.341 02	1.316	0.003	1.319	0.0840	1.140	1.308
1.6	1.117 64	1.114 35	1.092	0.002	1.094	0.0823	0.921	1.086
1.8	0.926 91	0.924 87	0.906	0.003	0.909	0.0804	0.749	0.910
2.0	0.770 92	0.770 12	0.755	0.004	0.759	0.0784	0.608	0.765
2.5	0.501 43	0.502 93	0.498	0.004	0.502	0.0729	0.355	0.501
3.0	0.345 82	0.348 20	0.346	0.003	0.349	0.0668	0.225	0.359
3.5	0.252 82	0.255 11	0.257	0.003	0.260	0.0605	0.156	0.277
4.0	0.193 73	0.195 55	0.195	0.002	0.197	0.0542	0.102	0.210
5.0	0.124 50	0.125 40	0.126	0.001	0.127	0.0424	0.041	0.126
6.0	0.085 11	0.085 52	0.086	0.001	0.087			
7.0	0.059 72	0.059 92	0.060	0.000	0.060			
8.0	0.042 42	0.042 54	0.042	0.000	0.042			
9.0	0.030 36	0.030 45	0.030	0	0.030			
10.0	0.021 88	0.021 95	0.022	0	0.022			
15.0	0.004 79	0.004 81	0.005	0	0.005			
20.0			0.001	0	0.001			
25.0	0.000 43	0.000 43	0.000	0	0.000			
30.0				0	0			

[a] Calculated from Clementi functions by Smith and Brown (Ref. 23).

[b] Second-order configuration-interaction calculation by Smith and Brown (Ref. 23).

[c] Calculated from Clementi 1s wave functions by Weiss *et al.* (Ref. 4).

[d] Measurement by Eisenberger (Ref. 20) with the 1s core contribution subtracted out.

uation. In the correction term it is more accurate to do the $\vec{p}$ integrations before the $\vec{r}$ integrations.

For closed-shell atoms, Eq. (2.15) combined with Eq. (2.1) can be explicitly written

$$J(p_z)=J^{(1)}(p_z)+J^{(2)}(p_z)\,. \tag{2.20}$$

Here

$$J^{(1)}(p_z)=4\sum_{n,l}(2l+1)\int_0^\infty |K_{nl}(p)|^2(p^2-p_z^2)^{1/2}\times d[(p^2-p_z^2)^{1/2}], \tag{2.21}$$

$$K_{nl}(p)=\int P_{nl}(r)j_l(pr)r\,dr\,, \tag{2.22}$$

where $P_{nl}(r)$ is the radial wave function obtained from the self-consistent solution of Eqs. (2.5)–(2.8): $\Psi_i\equiv[P_{nl}(r)/r]Y_l^m(\theta,\phi)$. And the correction term

$$J^{(2)}(p_z)=\int dr\,I(r)n(r)\,, \tag{2.23}$$

with

$$I(r)=\tfrac{3}{2}\frac{1}{p_F}(r)\int_0^\infty[N_k^0(\vec{r})-N_k^F(\vec{r})](k^2-k_z^2)^{1/2}\times d[(k^2-k_z^2)^{1/2}]\,, \tag{2.24}$$

III. RESULTS

Calculated Compton profiles of Ne, Ar, and Kr are presented below. To help us to understand and appraise the results, we should keep the limitations of the method in mind.

The local-density approximation is supposedly better in ground-state properties for larger atoms. However, radial electron wave functions of larger atoms have longer tails. Local approximation is poor in the tail regions. Correlation expressions used are strictly valid only in high and medium electron densities ($r_s\leqslant 6$, where $\frac{4}{3}\pi r_s^3=1/n$) regions. Extrapolations to larger r_s become uncertain. N_p values in Table I are given only to two

TABLE III. Compton profile of atomic Ar.

q	Expt. (1)[a]	Expt. (2)[b]	HF[a]	LAM[a]	Present work		
					$J^{(1)}$ +	$J^{(2)}$ =	$J(q)$
0.0	5.058	5.118	5.052	5.378	5.157	−0.097	5.060±0.020
0.1	5.022	5.082	5.028	5.299	5.133	−0.084	5.049±0.020
0.2	4.917	4.976	4.950	5.044	5.026	−0.058	4.968±0.020
0.3	4.749	4.806	4.812	4.727	4.851	−0.039	4.812±0.020
0.4	4.526	4.581	4.608	4.405	4.637	−0.027	4.610±0.005
0.5	4.259	4.310	4.369	4.090	4.359	−0.017	4.342±0.005
0.6	3.960	4.007	4.028	3.787	4.030	−0.008	4.022±0.005
0.7	3.643	3.686	3.690	3.499	3.673	−0.005	3.668±0.005
0.8	3.319	3.357	3.328	3.226	3.312	−0.001	3.311±0.005
0.9	3.000	3.034	2.982	2.970	2.962	−0.001	2.961±0.005
1.0	2.697	2.726	2.658	2.729	2.639	−0.000	2.639±0.005
1.2	2.164	2.184	2.108	2.295	2.101	0.006	2.107±0.005
1.4	1.753	1.765	1.701	1.920	1.707	0.007	1.714
1.6	1.461	1.467	1.417	1.601	1.426	0.011	1.437
1.8	1.264	1.266	1.221	1.336	1.229	0.010	1.239
2.0	1.129	1.128	1.084	1.122	1.091	0.011	1.102
2.5	0.924	0.899	0.873	0.812	0.878	0.008	0.886
3.0	0.744	0.737	0.736	0.685	0.736	0.004	0.740
3.5	0.634	0.626	0.621	0.591	0.621	0.002	0.623
4.0	0.534	0.525	0.520	0.512	0.518	0.001	0.519
5.0	0.366	0.357	0.351	0.379	0.358	0.001	0.359
6.0	0.260	0.252	0.249	0.274	0.249	0.001	0.250
7.0	0.181	0.174	0.177	0.192	0.178	0.001	0.179
8.0	0.137	0.131	0.130	0.131	0.131	0.001	0.132
9.0	0.104	0.099	0.098	0.089	0.098	0.000	0.098
10.0	0.078	0.074	0.075	0.064	0.076	0.000	0.076
15.0	0.025	0.023	0.025	0.026	0.025	0.000	0.025
20.0					0.010	0.000	0.010
25.0					0.004	0.000	0.004
30.0					0.002	0.000	0.002

[a] Reference 13.

[b] Reference 21. Revised values after relativistic effects have been corrected.

significant figures. $J(q)$, as $q \rightarrow 0$, is especially sensitive to wave functions at large r. Tail regions having densities as low as to give $r_s \gtrsim 10$, still contribute significantly to $J(q)$ for small q. Other numerical difficulties will be discussed below as we encounter them.

A. Ne

Column 2 of Table II lists the Fourier-transform results of the Clementi Hartree-Fock wave functions as calculated by Smith and Brown.[23] Other similar calculations on Hartree-Fock wave functions also give the same values at least to the first three figures. Full second-order configuration-interaction correlated functions of Viers, Harris, and Schaeffer[34] have been used by Smith and Brown[23] to calculate the third-column numbers. They also evaluated L-shell correlation using Ahlrich-Hinze multiconfiguration Hartree-Fock wave functions and obtained slightly larger $J(q)$ for small q, namely, $J(0) = 2.737\,13$, $J(0.5) = 2.518\,68$. Our results are presented in the next three columns, the first of which gives the first term $J^{(1)}(q)$ of Eq. (2.20), followed by the correction term $J^{(2)}(q)$. The full $J(q)$ is the sum of $J^{(1)}$ and $J^{(2)}$. The last column of Table II gives the experimental values obtained by Eisenberger[20] with the 1s core contribution[4] (Hartree-Fock) added to them.

By comparing the various columns, we see that the configuration-interaction results do not differ from the Hartree-Fock values significantly. Our fully correlated values as a whole are slightly closer to the experimental values. As expected, correlation effects are not large.

It is interesting to compare our $J^{(1)}(q)$ with the reported values of $J(q)$ by Sabin and Trickey[35] using Hedin and Lundqvist[36] correlation energy instead of our μ_c. Their $J(q)$ values $[J(0) = 2.7833$, $J(.5) = 2.5467$, $J(1.0) = 1.8730$, $J(2.0) = 0.7572]$ are quite close to $J^{(1)}(q)$ in Table II. Though it was claimed to be a local-density functional calculation, the second term $J^{(2)}(q)$ which should appear in the theory has not been included in their work.

In Ne atom, the electron-density tail is short.

TABLE IV. Compton profile of atomic Kr.

q	Expt. (1)[a]	Expt. (2)[b]	HF[a]	LAM[a]	Present work $J(q)$
0.0	7.025	7.312	7.228	7.240	7.25 ±0.08
0.1	7.152	7.260	7.194	7.182	7.24 ±0.08
0.2	7.022	7.109	7.085	7.013	7.16 ±0.08
0.3	6.767	6.871	6.888	6.735	6.97 ±0.08
0.4	6.459	6.559	6.595	6.360	6.68 ±0.08
0.5	6.098	6.191	6.216	5.968	6.28 ±0.05
0.6	5.701	5.787	5.776	5.590	5.82 ±0.05
0.7	5.289	5.367	5.309	5.230	5.34 ±0.05
0.8	4.880	4.950	4.848	4.891	4.87 ±0.02
0.9	4.491	4.552	4.420	4.574	4.42 ±0.02
1.0	4.133	4.185	4.039	4.277	3.96 ±0.02
1.2	3.540	3.577	3.441	3.747	3.411
1.4	3.122	3.146	3.037	3.299	3.047
1.6	2.850	2.863	2.769	2.927	2.804
1.8	2.670	2.676	2.583	2.629	2.628
2.0	2.533	2.535	2.441	2.399	2.487
2.5	2.219	2.213	2.144	2 024	2.179
3.0	1.898	1.886	1.857	1.764	1.850
3.5	1.597	1.582	1.578	1.551	1.561
4.0	1.338	1.271	1.326	1.343	1.309
5.0	0.937	0.916	0.934	1.008	0.925
6.0	0.683	0.673	0.678	0.741	0.677
7.0	0.522	0.503	0.512	0.534	0.516
8.0	0.399	0.382	0.400	0.384	0.405
9.0	0.316	0.301	0.319	0.294	0.324
10.0	0.254	0.240	0.259	0.243	0.263
15.0	0.095	0.091	0.104	0.111	0.101
20.0	0.044		0.049	0.047	0.050
25.0	0.022		0.026	0.023	0.026
30.0	0.009		0.015	0.014	0.016

[a] Reference 13.

[b] Reference 21. Revised values after relativistic effects have been corrected.

The difficulties we mentioned above do not significantly affect the values. Our estimate of various errors, including other numerical problems is about ±0.005 for $q = 0$ and less for larger q. The over correction of $J^{(2)}(q)$ for small q can be seen by comparing $J(0)$ and $J(0.1)$ values (column 7). The calculated $J(0)$ should have a value larger than 2.739.

B. Ar

The second[13] and third columns[21] of Table III give the experimental values of Compton profiles. The third column gives the revised values after relativistic effects have been corrected. The column labeled LAM lists the results obtained by the locally averaged method.[13] Our present calculation is expected to be better than LAM.

In Ar, the tail effect starts to show. With various values for the cutoff of the tail, this error can be estimated. In the calculation of the Kohn-Sham one-particle equation, [Eq. (2.5)], Herman-Skillman[37] mesh has been used. The mesh has a basic periodicity in it. Fourier transform of the wave functions gives fictitious oscillations at high q. Troubles in the Fourier transforms for small and large arguments have not been properly eliminated. Such and other numerical difficulties which most significantly affect $J(q)$ for small q, do not occur in Ne-atom analysis. They start to appear in the Ar calculation, and become serious in Kr. When oscillations occur at high $q(>70p_F)$, the tail is cut off, and $J(q)$ is renormalized[35] to the atomic number Z. For Ar, the integral of $J(q)$ before normalization is 17.96. The error limits given in the table include both the intrinsic tail problem and various numerical difficulties. Again, the values of $J(q)$ for small q should be larger than those listed in the table because of the over correction of $J^{(2)}$.

C. Kr

The Kr results are listed in Table IV. The columns are similar to those in Table III. Here, our results become less reliable. Estimated errors are shown in the table.

IV. CONCLUSION

As expected, correlation effects in rare-gas atoms are small. Our results do consistently agree with the measured values. Correlation contributions to Kohn-Sham self-consistent calculation should be consistent to that used in the second term of Eq. (2.20). For large atoms, $J(q)$ at small q, are troubled by the presence of long low-density tails. Such difficulties are not present in metals.

This second method proposed by LP is consistently better than the local average method in including correlation effects. It is fairly successful when applied to rare-gas atoms. Most of the numerical difficulties associated with the low-density-tail regions of large atoms should not appear in metals.

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