Electron-impact excitation cross sections for allowed transitions in atoms

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We present semiempirical Gaunt factors for the widely used Van Regemorter formula [Astrophys. J. **136**, 906 (1962)] for allowed transitions from $l=0$ or $l=1$ levels in atoms with the LS coupling. Cross sections calculated using these Gaunt factors agree with measured cross sections to within experimental error.

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I. INTRODUCTION

Interpretation of spectroscopic measurements and simulation of kinetic and transport processes in nonequilibrium plasmas requires knowledge of many electron-impact excitation cross sections for atoms and ions. In general, any excitation cross section may be calculated by computer codes designed for this purpose (see, for example, Refs. [1–7]). Hundreds of cross sections are already calculated or determined experimentally for some intervals of incident electron energy. These results can be found in atomic data bases [7]. However, published cross sections are often insufficient for detailed simulation of experiments, since data on many cross sections are missing or do not cover the entire energy range required for calculation of excitation rates, especially for non-Maxwellian plasmas.

In such a situation, it is desirable to have an easy-to-use formula of known accuracy applicable to various classes of transitions. Estimates of electron-impact excitation cross sections are frequently based on the Van Regemorter formula [8–10]

$$\sigma_{qq'}^{\mathrm{exc}}(x)=\frac{8\pi}{\sqrt{3}}\pi a_0^2 f_{qq'}\frac{\mathscr{R}^2}{E_{qq'}^2}\frac{G_{qq'}(x)}{x}, \qquad (1)$$

which is derived for single-electron electric dipole transitions (in other words, for optically allowed transitions) [11–13]. Here $\sigma_{qq'}^{\mathrm{exc}}(x)$ is the electron-induced excitation cross section from the lower state q into the upper state q', $x=\varepsilon/E_{qq'}$, ε is the kinetic energy of relative motion between projectile electron and target atom (ion), $E_{qq'}$ is the transition energy, a_0 is the Bohr radius, $\mathscr{R}$ is the Rydberg energy unit, $f_{qq'}$ is the absorption oscillator strength, and $G_{qq'}(x)$is the Gaunt factor (which may be treated as a fitting function of order unity). It is known that formula (1) provides a better fit to experimental data if different expressions for the Gaunt factor are used when applied to atoms, singly charged ions, or multiply charged ions; and to transitions with $\Delta n=0$ or $\Delta n>0$ [4,8–10,14–16]. Probably, the fit may be improved further if a dependence on other transition parameters is introduced in the Gaunt factor, for example, dependence on the orbital quantum number of the optical electron l, as is found for multiple ions [17] using high-accuracy theoretical results.

After the first publication by Van Regemorter in 1962 [8], there were a few attempts to infer reasonably accurate Gaunt factors for various classes of transitions including nondipole and intercombination ones [9,10,14–16] . The Gaunt factors obtained do not provide an accuracy of about 10–30%, which is expected from atomic codes, and there is some criti-

TABLE I. Experimentally studied allowed transitions with $\Delta n=0$ in atoms with the LS coupling.

Atom	Transition	ΔE (eV)	Ref.	Number of experimental values	Projectile electron energy range (eV)	$f_{qq'}$
He	$1s2s\ ^3S-1s2p\ ^3P$	1.144	[20]	35	1.3–2000	0.539 [49]
	$1s2s\ ^1S-1s2p\ ^1P$	0.602	[20]	37	0.7–2000	0.376 [49]
Li	$2s\ ^2S-2p\ ^2P$	1.848	[21]	22	2.1–1400	0.745 [50]
			[19]	94 (33)	2–300	
Na	$3s\ ^2S-3p\ ^2P$	2.104	[22]	17	5–1000	0.99 [49]
			[19]	95 (35)	2–300	
Mg	$3s^2\ ^1S-3s3p\ ^1P$	4.346	[23]	26	4.6–1400	1.9 [49]
K	$4s\ ^2S-4p\ ^2P$	1.617	[24]	3	6–60	1.09 [49]
			[19]	96 (32)	1.5–300	
Rb	$5s\ ^2S-5p\ ^2P$	1.579	[19]	94 (32)	1.5–300	0.99 [49]
Cs	$6s\ ^2S-6p\ ^2P$	1.432	[19]	100 (34)	1.5–300	1.07 [49]
Ba	$6s^2\ ^1S-6s6p\ ^1P$	2.239	[25]	29	2.3–1500	1.6 [49]

TABLE II. Experimentally studied allowed transitions with $\Delta n>0$ in atoms with the *LS* coupling.

Atom	Transition	ΔE (eV)	Ref.	Number of experimental values	Projectile electron energy range (eV)	$f_{qq'}$
H	$1s-2p$	10.199	[26]	13	11–199.1	0.416 [49]
H	$1s-3p$	12.088	[27]	5	29–506	0.0791 [49]
He	$1s^2\ ^1S-1s2p\ ^1P$	21.218	[28]	36	40–2000	0.276 [49]
			[29]	3	29.2–48.2	
			[30]	1	200	
			[31]	1	23.2	
			[32]	5	200–7000	
			[33]	15	22.4–196.1	
			[34]	26	30–2000	
			[35]	25	30–2000	
			[36]	17	50–3000	
			[37]	3	30–100	
			[38]	2	60,80	
			[39]	15	22.03–400	
			[20]	15	30–500	
He	$1s^2\ ^1S-1s3p\ ^1P$	23.09	[30]	1	200	0.0734 [49]
			[28]	38	40–2000	
			[40]	5	100–800	
			[34]	26	30–2000	
			[41]	28	25–2000	
			[42]	2	50,100	
			[33]	15	23.74–207.8	
			[35]	25	30–2000	
			[36]	23	50–6000	
He	$1s^2\ ^1S-1s4p\ ^1P$	23.74	[43]	5	60–2400	0.0302 [49]
			[30]	1	200	
			[40]	1	200	
			[34]	25	30–2000	
			[28]	35	30–2000	
			[36]	23	50–6000	
He	$1s^2\ ^1S-1s5p\ ^1P$	24.05	[36]	23	50–6000	0.0153 [52]
			[40]	1	200	
He	$1s2s\ ^1S-1s3p\ ^1P$	2.474	[20]	31	2.6–2000	0.1514 [49]
He	$1s2s\ ^1S-1s4p\ ^1P$	3.124	[20]	31	3.283–2525	0.0507 [52]
He	$1s2s\ ^3S-1s3p\ ^3P$	3.19	[20]	31	3.2–2000	0.0645 [49]
			[44]	4	4.5–16	
He	$1s2s\ ^3S-1s4p\ ^3P$	3.89	[20]	31	3.904–2440	0.029 [51]
O	$2p^4\ ^3P-2p^3 3s\ ^3S^0$	9.52	[45]	23	11–300	0.051 [51]
			[46]	15	10–340	
			[47]	20	11–100	
O	$2p^4\ ^3P-2p^3 3s'\ ^3D^0$	12.54	[47]	18	15–100	0.056 [52]
O	$2p^4\ ^3P-2p^3 3s''\ ^3P^0$	14.12	[47]	19	15–100	0.065 [51]
N	$2s^2 2p^3\ ^4S-2s^2 2p^2 3s\ ^4P$	10.332	[48]	3	30–50	0.266 [51]

cism of the use of the Van Regemorter approximation in the epoch of computers [5,18]. Nevertheless, the simplicity of the Van Regemorter formula makes it attractive for estimates, and it is reasonable to improve the accuracy of this formula by finding better approximations for the Gaunt factors for various classes of transitions.

In Sec. II we present rather accurate Gaunt factors for a broad class of transitions, namely, for allowed transitions between nl states in neutral atoms with the LS coupling. These transitions may be represented by the scheme

$$\gamma n l^m\ ^{2S+1}L \rightarrow \gamma n l^{m-1} n' l'\ ^{2S'+1}L' \tag{2}$$

with the selection rules [13]

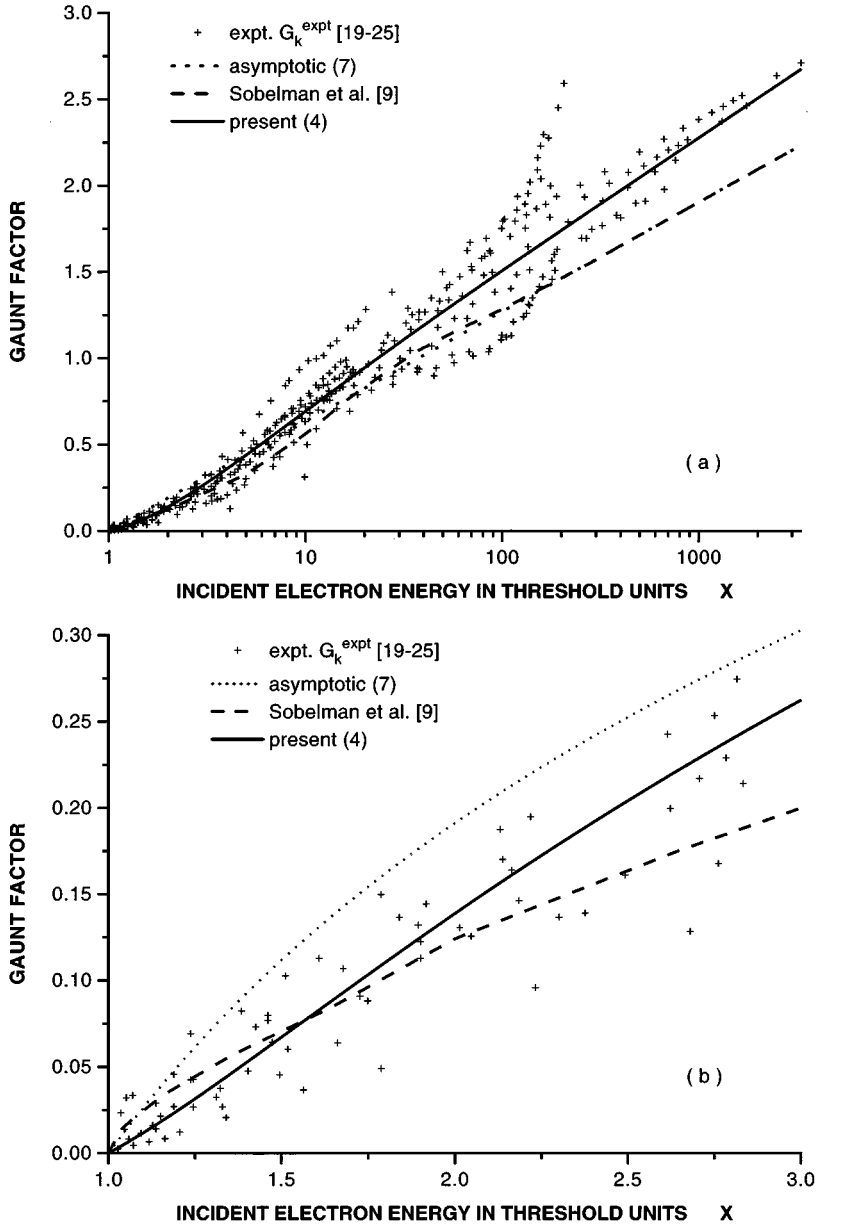


FIG. 1. (a). The Gaunt factor for allowed transitions with $\Delta n = 0$ in atoms with LS coupling. The values G_k^{expt} are inferred from experimental cross sections (listed in Table I) using the Van Regemorter formula. (b) Fragment of (a).

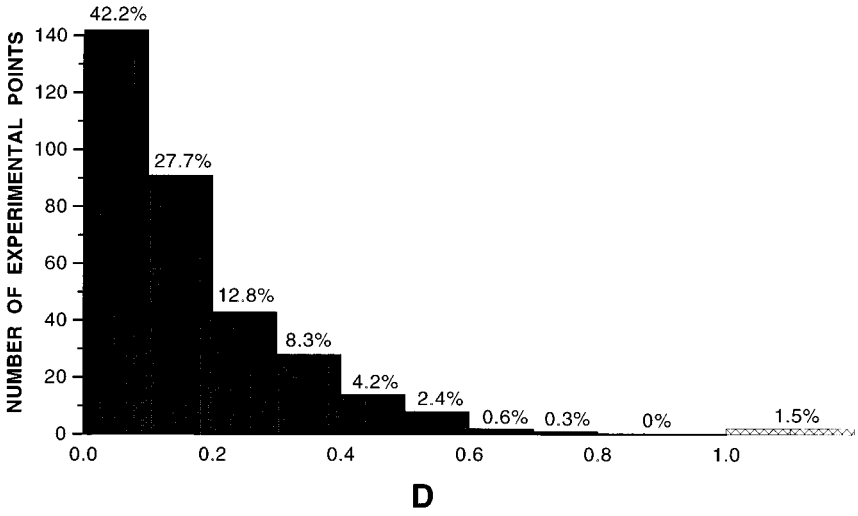


FIG. 2. Distribution of experimental values G_k^{expt} presented in Fig. 1(a) over their deviation from the Gaunt factor (4): numbers of G_k^{expt} per 10% intervals of deviation (5).

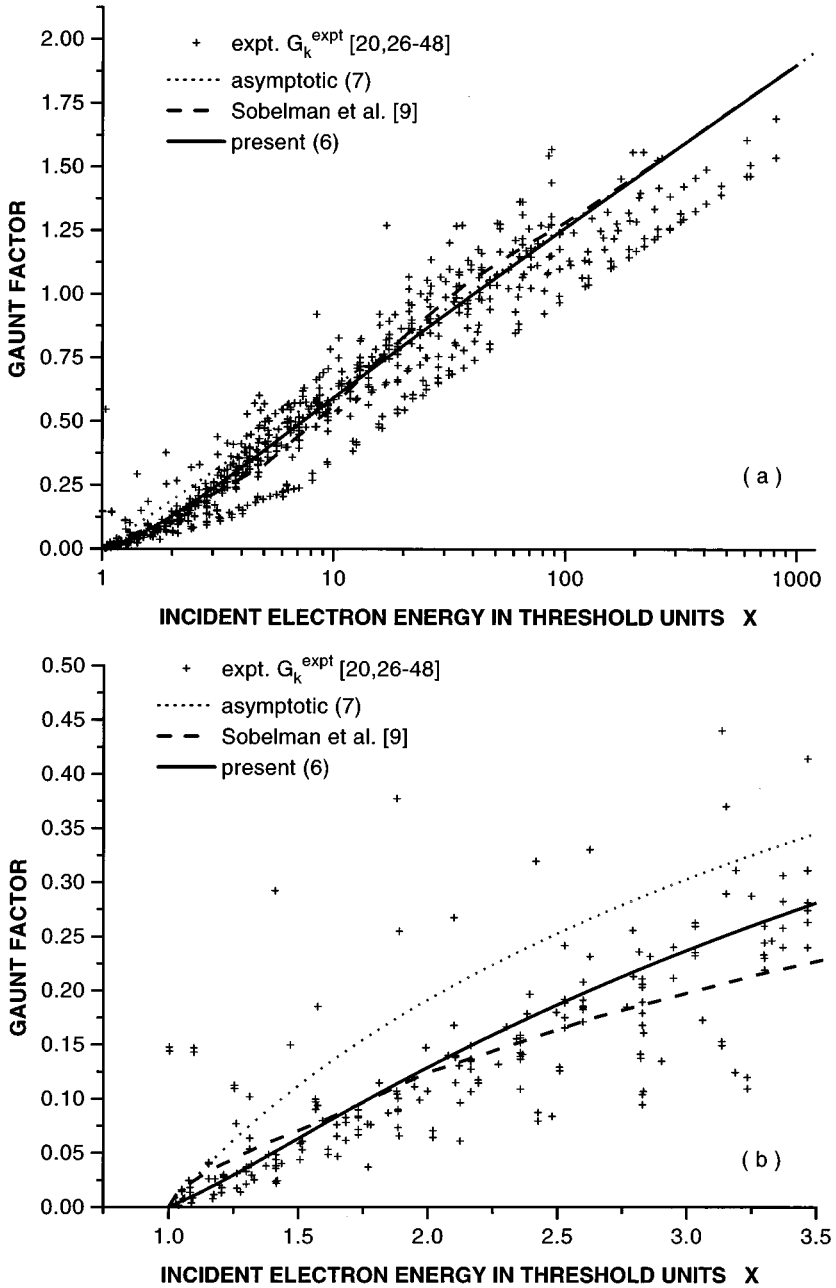


FIG. 3. (a) Gaunt factor for allowed transitions with $\Delta n>0$ in atoms with LS coupling. The values G_k^{expt} are inferred from experimental cross sections (listed in Table II) using the Van Regemorter formula. (b) Fragment of (a).

$$n' \geqslant n, \quad l' = l \pm 1, \quad S' = S,$$
$$L' - L = 0, \pm 1; \quad L + L' > 0, \tag{3}$$

where γ denotes all subshells that do not change their state in the collision. Our results relate to the case when the excitation occurs in the outer shell. The applicability of the obtained Gaunt factors to inner-shell excitation was not checked because of the lack of experimentally determined cross sections.

II. THE GAUNT FACTORS

Tables I and II present a list of experimentally studied electron-induced transitions that belong to the class considered here, namely, allowed transitions (2)–(3) in atoms. For convenience of further analysis, transitions with $\Delta n=0$ are listed separately from transitions with $\Delta n>0$. Various publications present from one to a hundred experimental points for each of the studied cross sections. In order to avoid a dominating influence of Ref. [19] in which in particular many points along x are given, we use at most 40 values for each cross section from any publication. When only part of the experimental points are taken, the points taken are either every second point or every third point along x. The number of accounted points is given in brackets in the fifth column of the tables.

Values of the Gaunt factor inferred from the experimentally studied cross sections $\sigma_{qq'}^{\mathrm{exc}}(x)$ for transitions with

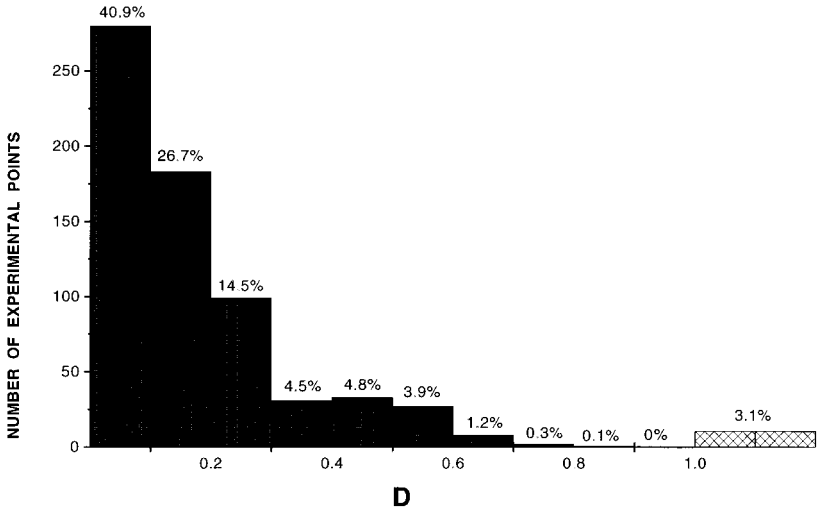
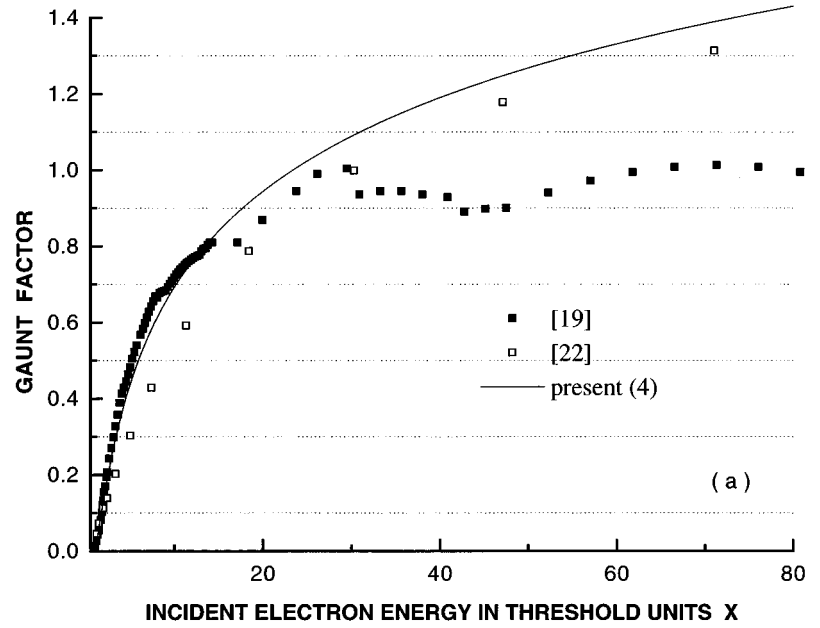


FIG. 4. Distribution of experimental values G_k^{expt} presented in Fig. 3(a) over their deviation from the Gaunt factor (6): numbers of G_k^{expt} per 10% intervals of deviation $D_k=|G_k^{\text{expt}}-G_>(x_k)|/G_>(x_k)$.



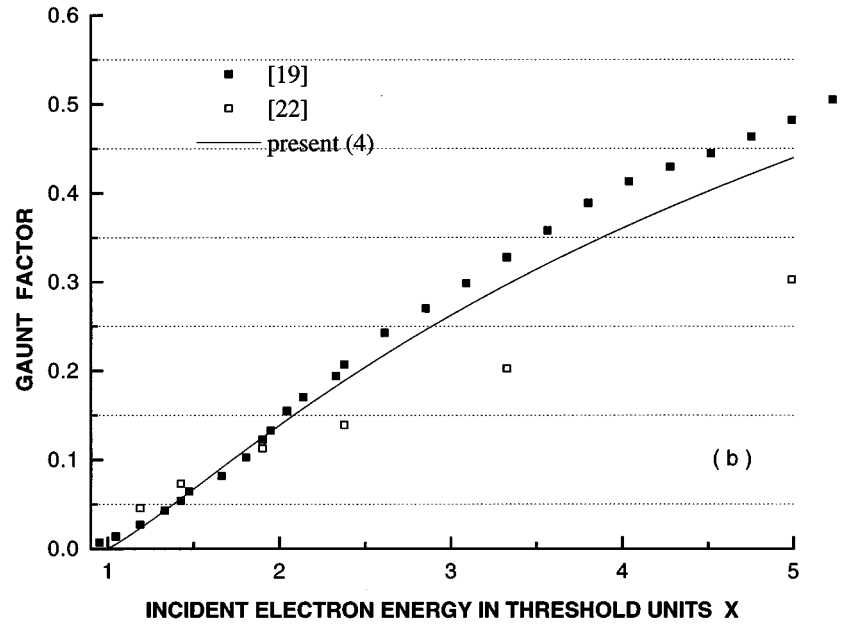


FIG. 5. (a) Gaunt factor for transition $3s-3p$ in Na. (b) Fragment of (a).

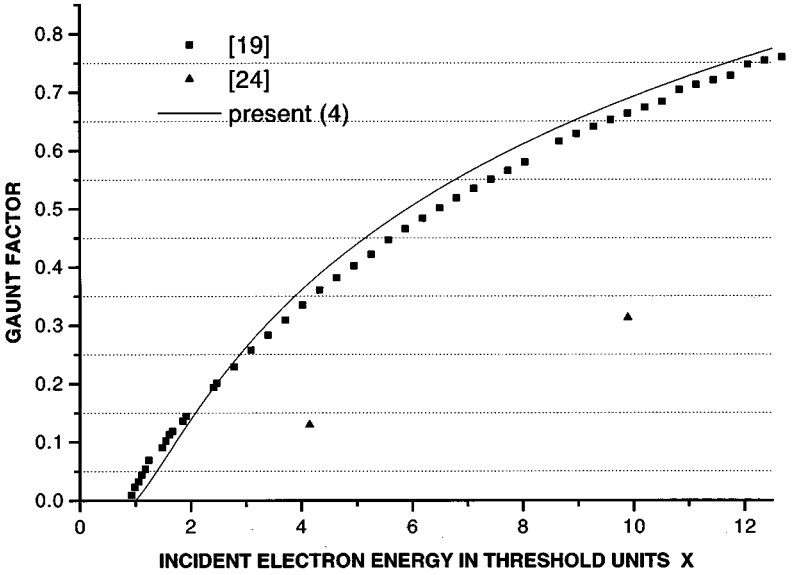


FIG. 6. Gaunt factor for transition $4s$-$4p$ in K.

$\Delta n=0$ are demonstrated in Fig. 1. These data may be fitted rather well by the expression

$$G_0(x)=(0.33-0.3x^{-1}+0.08x^{-2})\ \ \ln x \tag{4}$$

shown by the solid curve. The subscript 0 denotes the condition $\Delta n=0$. To illustrate the accuracy of the above expression, Fig. 2 presents a histogram of discrepancies D_k between experimental values $G_k^{\rm expt}$ and the semiempirical Gaunt factor $G_0(x_k)$. The discrepancy is defined as the ratio

$$D_k=\frac{|G_k^{\rm expt}-G_0(x_k)|}{G_0(x_k)}, \tag{5}$$

where k is the order number of the experimental point, and x_k is the value of x for this point. The histogram demonstrates the numbers of experimental points per 10% intervals of increasing D. One can see that for 95% of the experimental points the accuracy of the Gaunt factor (4) is better than $\pm 50\%$. For 82% of the points the accuracy is better than $\pm 30\%$.

Values of the Gaunt factor inferred from experimentally studied cross sections $\sigma_{qq'}^{\rm exc}(x)$ for transitions with $\Delta n>0$ are demonstrated in Fig. 3. These data may be fitted rather well by the expression

$$G_>(x)=(0.276-0.18x^{-1})\ \ \ln x \tag{6}$$

shown by the solid curve. The subscript $>$ denotes the condition $\Delta n>0$. When $x\to\infty$,

$$G_>(x)\approx\frac{\sqrt{3}}{2\pi}\ \ \ln x \tag{7}$$

and expression (1) becomes the Bethe formula [9]. For $x<10$, expression (6) provides a better fit to experimental data than the asymptotic expression (7) shown by the dotted line. The accuracy of the Gaunt factor (6) is demonstrated by the histogram in Fig. 4. For 82% of the experimental points the Gaunt factor is accurate to better than $\pm 30\%$. Two to three percent of the experimental points deviate from the Gaunt factors (4) and (6) by more than a factor of 2. Most of these points belong to the energy range $x\approx 1$ where the cross sections are small and measurements are less accurate.

It is worth mentioning that the deviation of the experimental data from the Gaunt factors (4) and (6) is not larger than the discrepancy between experimental results obtained by various research groups for the same studied transition. To illustrate this fact, Figs. 5–7, present experimental data obtained for three transitions: (i) 3s $\to 3p$ in Na, (ii) $4s\to$ 4p in K, and (iii) $1s^2\ {}^1S\to 1s4p\,{}^1P$ in He.

Two sets of experimental results are not included in our analysis: (i) results of Ref. [53] because they were shown to be inaccurate (see Ref. [48]) and (ii) results of Ref. [54] because of unreliable normalization using Ref. [53] and early theoretical results that do not fit later experimental data (see discussion in Ref. [48]).

III. DISCUSSION AND CONCLUSIONS

It is known that for positive atomic ions the Gaunt factors for transitions with $\Delta n=0$ are larger than the Gaunt factors for transitions with $\Delta n>0$ [10,15]. Here we demonstrate similar regularity for neutral atoms.

With the Gaunt factors (4) and (6), the Van Regemorter formula fits measured cross sections better than with the asymptotic Gaunt factor (7) and the semiempirical Gaunt factor given in Ref. [9]. This conclusion is based on the comparison with all available experimental cross sections for the allowed transitions $nl\to n'l'$ in atoms with the LS coupling: a total of 23 cross sections for 11 atoms with various electron configurations.

The inaccuracy of the Gaunt factors (4) and (6) and the inaccuracy of experimental data are about the same. The good fit may be treated as a proof of weak dependence of the Gaunt factor on electron configuration (for this class of transitions). Then the Gaunt factors (4) and (6) provide acceptable accuracy of the cross section for any electron-atom ex-

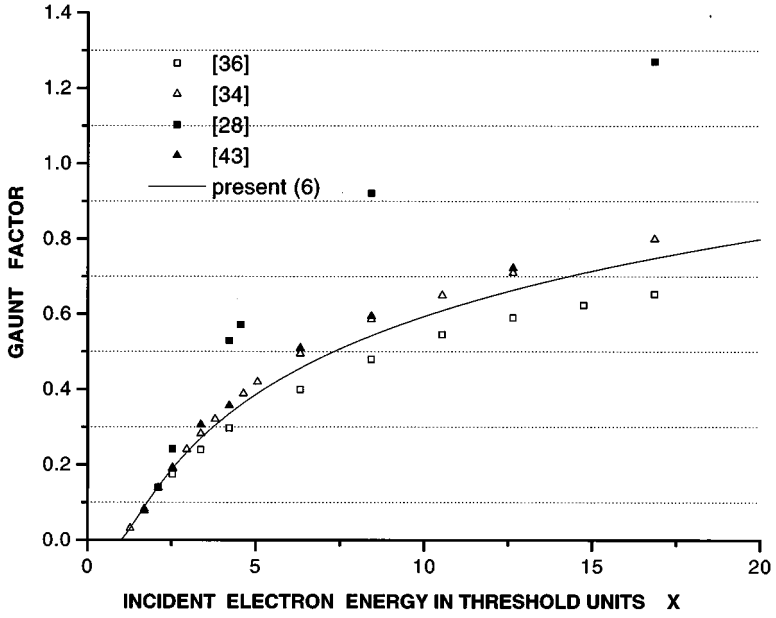


FIG. 7. Gaunt factor for transition $1s^2\ ^1S \rightarrow 1s4p\ ^1P$ in He.

citation (2),(3). This result is important for simulation of kinetic and transport processes in low-temperature non-LTE plasmas. However, all the transitions studied experimentally are from the states with $l=0$ or $l=1$; therefore, for transitions from $d,f,g,\ldots$, states we have no proof of independence of $G(x)$ on l.

Atoms of neon, argon, krypton, and xenon have a jlcoupling scheme. Effective Gaunt factors $G_k^{\rm expt}$ inferred from experimental cross sections [55–58] for these atoms are a few times less than our Gaunt factors (4) and (6), which are quite accurate for atoms with the LS coupling. This observation illustrates the dependence of the Gaunt factors on the coupling scheme.

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