Electron impact excitation cross sections for allowed transitions in atoms

V. Fisher, V. Bernshtam, H. Golten\textsuperscript{1}, and Y. Maron

Faculty of Physics, Weizmann Institute of Science, Rehovot 76100, Israel

\textsuperscript{1}Churchill College, Cambridge, UK

We present a semiempirical Gaunt factor for widely used Van Regemorter formula [Astrophys. J. 136, 906 (1962)] for the case of allowed transitions in atoms with the $LS$ coupling scheme. Cross sections calculated using this Gaunt factor agree with measured cross sections to within the experimental error.

I. INTRODUCTION

Interpretation of spectroscopic measurements and simulation of kinetic and transport processes in non-LTE plasmas require knowledge of many electron impact excitation cross sections for atoms and ions. In general, any excitation cross section may be calculated using one of 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 databases. However, published cross sections are not usually sufficient 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 situation, it is desirable to have easy-to-use formulae 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]

$$\sigma_{qq'}^{\text{exc}}(x) = \frac{8\pi}{\sqrt{3}} a_0^2 f_{qq'} \frac{Ry^2}{E_{qq'}} G_{qq'}(x),$$

(1)

which is derived for single-electron electric dipole transitions (in other words, for optically allowed transitions) [11]. Here $\sigma_{qq'}^{\text{exc}}(x)$ is the electron-induced excitation cross section from the lower state $q$ into the upper state $q'$, $x = \varepsilon/E_{qq'}$, $\varepsilon$ 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, $Ry$ 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 $\ell$, as is found for multiple ions [17] using high-accuracy theoretical results.

After the first publication by H. Van Regemorter in 1962 [8], there were a few attempts to infer reasonably accurate Gaunt factors for various classes of transitions including non-dipole 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 criticism 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 updating the Gaunt factor for various classes of transitions.

In section 2 we present rather accurate Gaunt factor for a broad and important class, namely, for allowed transitions between $n\ell$-states in atoms with $LS$ coupling. These transitions may be represented by the scheme

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

(2)

with selection rules [13]

$$n' \geq n, \quad \ell' = \ell \pm 1, \quad S' = S, \quad L' - L = 0, \pm 1 \quad \text{and} \quad L + L' > 0;$$

(3)

$\gamma$ denotes all subshells which do not change their state in the collision. Our results relate to the case when the excitation occurs in the outer shell. Applicability of the Gaunt factor obtained to excitation of inner-shell electrons is not checked because of no experimental data on the cross sections.
II. THE GAUNT FACTOR

Tables 1 and 2 present a list of experimentally studied electron-induced transitions which 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. To exclude any dominating influence of Ref. [19], we use not more than 40 values for each cross section from any publication. In the case, when only part of the experimental points are taken, the points taken are either every second point or every third point along \( x \) for the cross section of interest. 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 \( \sigma_{qq}^{\text{exc}}(x) \) for transitions with \( \Delta n = 0 \) are demonstrated in Figure 1. This data may be fitted rather well by the expression

\[
G_0(x) = (0.33 - 0.3x^{-1} + 0.08x^{-2}) \ln x
\]

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

\[
D_k = \frac{|G_{k}^{\text{exp}} - G_0(x_k)|}{G_0(x_k)},
\]

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 experimental points the accuracy of the Gaunt factor (4) is better than \( \pm 50\% \). This accuracy seems to be acceptable for any estimates. For 82% of the points the accuracy is better than \( \pm 30\% \).

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

\[
G_{>}(x) = (0.276 - 0.18x^{-1}) \ln x
\]

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

\[
G_{>}(x) \approx \frac{\sqrt{3}}{2\pi} \ln x
\]

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 Figure 4. For 82% of experimental points the Gaunt factor is accurate to better than \( \pm 30\% \).

From 2 to 3% of experimental points deviate from the Gaunt factor given by expressions (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 discrepancy between experimental results obtained by various research groups (for the same studied transition), is of a similar magnitude to the deviation of the experimental data from the Gaunt factor given by expressions (4) and (6). To illustrate this fact, figures 5, 6, and 7 present experimental data obtained for three transitions: (i) \( 3s \to 3p \) in Na, (ii) \( 4s \to 4p \) in K, (iii) \( 1s^2 1S \to 1s4p \, ^1P \) in He.

Some experimental results are not included in our analysis: results of Ref. [53] are not included because they were shown to be inaccurate (see Ref. [48]); results of Ref. [54] are not included because of unreliable normalization using Ref. [53] and early theoretical results which do not fit the experimental data (see discussion in [48]).

III. DISCUSSION AND CONCLUSIONS

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

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

Inaccuracy of the Gaunt factor (4), (6) and inaccuracy of experimental data are about the same. On one hand, 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 factor given by expressions (4) and (6) provides acceptable accuracy of the cross section for any electron-atom excitation (2),(3). This result is important for simulation of kinetic and transport processes in low-temperature non-LTE plasmas (such as ionospheric, gas-discharge, gas-laser, technological, or near-surface). On the other hand, all studied transitions are from the states with $\ell = 0$ or $\ell = 1$, therefore, for transitions from $d, f, g, \ldots$ states we have no proof of independence of $G(x)$ on $\ell$.

Atoms of Neon, Argon, Krypton, and Xenon have $j\ell$ coupling scheme. Effective Gaunt factor $G_{\text{exp}}^k$ inferred from experimental cross sections [55-58] for these atoms, is a few times less than our Gaunt factor (4),(6) which is quite accurate for atoms with $LS$ coupling. This observation illustrates a dependence of the Gaunt factor on the coupling scheme.

IV. ACKNOWLEDGMENTS

It is a pleasure to acknowledge fruitful discussions with Yuri Ralchenko. We are grateful to National Institute for Fusion Science (Nagoya, Japan) and H. Tawara for giving us an opportunity to use the NIFS atomic database. We are also grateful to the database of Opacity Project. This work was supported by the Israeli Academy of Science, Ministry of Science and Arts, and the Ministry of Absorption.

[1] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981)
[2] L. A. Vainshtein and V. P. Shevelko, *Structure and Features of Ions in Hot Plasmas* (Nauka, Moscow, 1986) in Russian.
[3] V. P. Shevelko and L. A. Vainshtein, *Atomic Physics for Hot Plasmas* (IPP, Bristol, 1993).
[4] A. K. Pradhan, Atomic data and nuclear data tables, 52, 227-317 (1992).
[5] D. Sampson and H. Zhang, Phys. Rev. A 45, 1556 (1992).
[6] *Atomic and Molecular Processes in R-matrix Approach*, edited by P. G. Burke and K. A. Berrington (IPP, Bristol, 1993).
[7] A few atomic codes are available via computer networks, see, e.g., URL http://plasma-gate.weizmann.ac.il/FSfAPP.html
[8] H. Van Regemorter, Astrophys. J. 136, 906 (1962).
[9] I. I. Sobelman, L. A. Vainshtein, and E. A. Yukov, *Excitation of atoms and Broadening of Spectral lines*, (Springer, 1981).
[10] D. H. Crandall. Ch. 4 in *Physics of Ion-ion and Electron-ion Collisions*, edited by F. Brouillard and J. W. Mc. Gowen (Plenum Press, New York, 1983).
[11] The Van Regemorter formula is derived from the Bethe formula [12,8,9] which is obtained for optically allowed transitions.
[12] H. A. Bethe, Ann. Phys., Lpz. 5 325 (1930).
[13] I. I. Sobelman, *Atomic Spectra and Radiative Transitions*, (Springer, 1979).
[14] R. Mewe, Astron. & Astrophys. 20, 215 (1972).
[15] S. M. Younger and W. L. Wieze, J. Quant. Spectrosc. Radial. Transfer 22, 161 (1979).
[16] D. H. Sampson and H. L. Zhang, Astroph. J. 335, 516-524, (1988).
[17] H. Golten, to be submitted for publication.
[18] This criticism is caused by a discrepancy of a factor of 10 in nearthreshold cross sections for some transitions $n, l, j \rightarrow n', \ell', j'$ in multiple ions [5]. Probably, to provide acceptable accuracy for multiple ions, the Gaunt factor has to depend on more parameters of transition (for example, on $\ell$ [17]) but we do not consider multiple ions in this paper.
[19] I. Zapesochnyi, E. Postoi and I. Aleksakhin, Sov. Phys. JETP 41, 865 (1976).
[20] Database of National Institute for Fusion Science (Nagoya, Japan).
[21] D. Leep and A. Gallgher, Phys. Rev. A 10, 1082 (1974).
[22] E. Enemark and A. Gallgher, Phys. Rev. A 6, 192 (1972).
[23] D. Leep and A. Gallgher, Phys. Rev. A 13, 148 (1976).
[24] W. Williams and S. Traymar, J. Phys. B 10, 1955 (1977).
[25] S. Chen and A. Gallgher, Phys. Rev. A 14, 593 (1976).
[26] R. Long, D. Cox and S. Smith, Journal of Research of the National Bureau of Standarts.-A. Physics and achemistry 72A, 521 (1968).
A. Mahan, A. Gallagher and S. Smith, Phys. Rev. A 13, 156 (1976).

J. de Jongh and J. Van Eck in *Electronic and Atomic Collision (Abstracts of Papers of the IXth International Conference on the Physics of Electronic and Atomic Collisions)*, 701 (1971).

J. de Jongh and J. Van Eck in *Electronic and Atomic Collision (Abstracts of Papers of the IXth International Conference on the Physics of Electronic and Atomic Collisions)*, 701 (1971).

R. Hall, G. Joyez, J. Mazeau, J. Reinhardt and C. Schermann, Le Journal de Physique 34, 827 (1973).

G. Joyez, A. Huetz, M. Landau, J. Mazeau and F. Pishou, in *Electronic and Atomic Collision (Abstracts of Papers of the IXth International Conference on the Physics of Electronic and Atomic Collisions)*, 827 (1975).

J. Jobe and R. Jonh, Phys. Rev. 164, 117 (1967).

J. K. Ballou, C. C. Lin and F. E. Fajen, Phys. Rev. A 8, 1797 (1973).

R. S. Schappe, M. B. Shulman, L. W. Anderson and C. C. Lin, Phys. Rev. A 50, 444 (1994).

I. P. Zapesochnyi and P. V. Felstan, Opt. and Spectrosk. (USSR) 20, 291 (1966).

**V. FIGURE CAPTIONS**

**Figure 1a.** The Gaunt factor for allowed transitions with $\Delta n = 0$ in atoms with $LS$ coupling. The values $G_{k}^{\exp}$ are inferred from experimental cross sections (listed in Table 1) using the Van Regemorter formula.

**Figure 1b.** Fragment of Figure 1a.

**Figure 2.** Distribution of experimental values $G_{k}^{\exp}$ presented in Figure 1a over their deviation from the Gaunt factor (4): numbers of experimental values of $G_{k}^{\exp}$ per 10% intervals of deviation (5).

**Figure 3a.** The Gaunt factor for allowed transitions with $\Delta n > 0$ in atoms with $LS$ coupling. The values $G_{k}^{\exp}$ are inferred from experimental cross sections (listed in Table 2) using the Van Regemorter formula.

**Figure 3b.** Fragment of Figure 3a.

**Figure 4.** Distribution of experimental values $G_{k}^{\exp}$ presented in Figure 3a over their deviation from the Gaunt factor (6): numbers of experimental values of $G_{k}^{\exp}$ per 10% intervals of deviation $D_k = (|G_{k}^{\exp} - G_{k}(x_k)|) / G_{k}(x_k)$.

**Figure 5a.** The Gaunt factor for transition $3s - 3p$ in Na.

**Figure 5b.** Fragment of Figure 5a.

**Figure 6.** The Gaunt factor for transition $4s - 4p$ in K.

**Figure 7.** The Gaunt factor for transition $1s^2 \, ^1S \rightarrow 1s4p \, ^1P$ in He.
VI. TABLE CAPTIONS

**Table 1.** Experimentally studied allowed outer-shell transitions with $\Delta n = 0$ in atoms with $LS$ coupling.

**Table 2.** Experimentally studied allowed outer-shell transitions with $\Delta n > 0$ in atoms with $LS$ coupling.
Figure 1a

- Experimental $G_k^{\text{exp}}$ [19-25]
- Asymptotic (7)
- Sobelman et al. [9]
- Present (4)
Figure 1b

- experimental $G_k^{\text{exp}}$ [19-25]
- asymptotic (7)
- Sobelman et al. [9]
- present (4)
Figure 2

NUMBER OF EXPERIMENTAL POINTS

D

0% 0% 0.3% 0.6% 2.4% 4.2% 8.3% 12.8% 27.7% 42.2% 0.6% 0.3% 0% 0% 1.8%
| ATOM | TRANSITION | ∆E (eV) | REFERENCES | NUMBER OF EXPERIMENTAL VALUES | PROJECTILE ELECTRON ENERGY RANGE (eV) | $f_{qq'}$ |
|------|------------|---------|------------|-------------------------------|----------------------------------|--------|
| H    | 1s -2p     | 10.199  | Long *et al.*[26] | 13                            | 1.1-19.91                        | 0.416  |
| H    | 1s -3p     | 12.088  | Mahan *et al.*[27] | 5                             | 2.9-50.6                         | 0.0791 |
| He   | 1s$^2$ 1S-1s2p 1P | 21.21  | de Jongh and Van Eck [28] Hall *et al.*[29] Shemanskiy *et al.*[30] Joez *et al.*[31] Dillon and Lassette [32] McConkey and Woolsey [33] Donaldson *et al.*[34] van Raan et al.*[41] Donaldson *et al.*[34] Van Raan et al.*[41] Bogdanova and Urgenson [42] Shemanskiy *et al.*[30] de Jongh and Van Eck [28] Showalter and Kay [40] Donaldson *et al.*[34] de Jongh and Van Eck [28] Showalter and Kay [40] Donaldson *et al.*[34] de Jongh and Van Eck [28] Moustafa et al.*[36] | 36 | 40-2000 | 0.276  |
| He   | 1s$^2$ 1S-1s3p 1P | 23.08  | Shemanskiy *et al.*[30] de Jongh and Van Eck [28] Showalter and Kay [40] Donaldson *et al.*[34] Van Raan et al.*[41] Bogdanova and Urgenson [42] McConkey and Woolsey [33] Westerveld et al.*[35] Moustafa et al.*[36] | 38 | 40-2000 | 0.0734 |
| He   | 1s$^2$ 1S-1s4p 1P | 23.74  | John *et al.*[43] Shemanskiy *et al.*[30] Showalter and Kay [40] Donaldson *et al.*[34] de Jongh and Van Eck [28] Moustafa et al.*[36] | 5 | 60-2400 | 0.0302 |
| 2p$^4$ 3P-2p$^3$3s 3S | 9.52 | Zipf E.C [44] | 23 | 11-300 | 0.051  |
| 2s$^2$2p$^3$ 4S-2s$^2$2p$^2$3s 4P | 10.332  | Stone E.and E.Zipf [45] Doering J.,et al.[47] | 3 | 30-50 | 0.266  |
| Element | Transition | Energy | Experimental Data | References |
|---------|------------|--------|-------------------|------------|
| He     | 1s^2 1S-1s5p 1P | 24.039 | Moustafa et al.[36] | 23 50-6000 0.0153 [52] |
|        |            |        | Showalter and Kay [41] | 1 2 |
| He     | 1s2s 1S-1s3p 1P | 2.474 | de Heer et al.[20] | 31 2.6-2000 0.1514 [49] |
| He     | 1s2s 1S-1s4p 1P | 3.124 | de Heer et al.[20] | 31 3.283-2525 0.0507 [52] |
| He     | 1s2s 3S-1s3p 3P | 3.19  | de Heer et al.[20] | 31 3.2-2000 0.0645 [49] |
|        |            |        | Rall et al.[44] | 4 4.5-16 |
| He     | 1s2s 3S-1s4p 3P | 3.89  | de Heer et al.[20] | 31 3.904-2440 0.029 [51] |
| O      | 2p^4 3P-2p^33S 3S | 9.52  | Zipf [45] | 23 11-300 0.051 [51] |
|        |            |        | Stone and Zipf [46] | 15 |
|        |            |        | Wang and McConkey [47] | 20 11 - 100 |
| O      | 2p^4 3P-2p^3 3s^3D | 12.54 | Wang and McConkey [47] | 18 15 - 100 0.056 [52] |
| O      | 2p^4 3P-2p^3 3s^3P | 14.12 | Wang and McConkey [47] | 19 15 - 100 0.065 [1] |
| N      | 2s^22p^3 4S- 2s2p23s 4P | 10.332 | Doering et al.[48] | 3 30-50 0.266 [51] |
Figure 3a

- Experimental $G_k^{\text{exp}}$ [20,26-48]
- Asymptotic (7)
- Sobelman et al. [9]
- Present (6)
Figure 3b

- Experimental $G_k^{\text{exp}}$ [20,26-48]
- Asymptotic (7)
- Sobelman et al. [9]
- Present (6)
Figure 5a

GAUNT FACTOR vs INCIDENT ELECTRON ENERGY IN THRESHOLD UNITS (X)

[19]
[22]

present (4)
Figure 5b

Graph showing the relationship between Gaunt factor and incident electron energy in threshold units (X). Data from [19] and [22] are plotted, with the present (4) data shown by a line. The x-axis represents incident electron energy in threshold units, while the y-axis represents the Gaunt factor.
Figure 6

Incident electron energy in threshold units (X)

Gaunt factor

[19]

[24]

present (4)
Figure 7

GAUNT FACTOR

[36]

[34]

[28]

[43]

present (6)

INCIDENT ELECTRON ENERGY IN THRESHOLD UNITS (X)
| ATOM | TRANSITION | ΔE (eV) | REFERENCES | NUMBER OF EXPERIMENTAL VALUES | PROJECTILE ELECTRON ENERGY RANGE (eV) | f qq' |
|------|------------|---------|------------|-------------------------------|----------------------------------------|------|
| He   | 1s2s 1S - 1s2p 3P | 1.144 | de Heer et al.[20] | 35 | 1.3 - 2000 | 0.539 [49] |
|      | 1s2s 1S - 1s2p 1P | 0.602 | de Heer et al.[20] | 37 | 0.7 - 2000 | 0.38 [49] |
| Li   | 2s 2S - 2p 3P | 1.845 | Leep and Gallagher [21] Zapesochnyi et al.[19] | 94 (33) | 2 - 300 |
| Na   | 3s 2S - 3p 3P | 2.104 | Enemark and Gallagher [22] Zapesochnyi et al.[19] | 95 (35) | 2 - 300 |
| Mg   | 3s 1S - 3s3p 1P | 4.346 | Leep and Gallagher [23] | 26 | 4.6 - 1400 | 1.9 [49] |
| K    | 4s 2S - 4p 3P | 1.617 | Williams and Traymar [24] Zapesochnyi et al.[19] | 96 (32) | 1.5 - 300 |
| Rb   | 5s 2S - 5p 3P | 1.589 | Zapesochnyi et al.[19] | 94 (32) | 1.5 - 300 | 0.99 [49] |
| Cs   | 6s 2S - 6p 3P | 1.455 | Zapesochnyi et al.[19] | 100 (34) | 1.5 - 300 | 1.07 [49] |
| Ba   | 6s 2S - 6s6p 3P | 2.239 | Chen and Gallagher [25] | 29 | 2.3 - 1500 | 1.6 [49] |