Treatment of rotational excitation/deexcitation used in the EEDF package

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Let us note that there is an important specific feature of the EEDF package [1] in application to H_2, N_2, O_2 and CO molecules. It is associated with the correct description of energy exchanges between electrons and molecular rotations. In the limit of the thermal rotational distribution function, summation of multiple energy exchange processes between electrons and molecular rotations was performed resulting in a compact expression for the respective collision integral term [2, 3]. Recently similar expression was derived in paper [4]. Let us describe this expression in more detail.

Electron energy distribution function in 2-term approximation for steady state and uniform plasma satisfies the following equation [5]:

$$\frac{1}{3}\left(\frac{E}{N}\right)^2 \frac{d}{du}\left(\frac{u}{Q_m(u)}\frac{df(u)}{du}\right) + St(f) = 0, \tag{1}$$

where E is the electric field strength, N is the gas density, u is the electron energy, $f(u)$ is the EEDF, Q_m is the momentum transfer cross section and $St(f)$ is the collision integral. Distribution function is normalized as

$$\int_0^\infty \sqrt{u} f(u) du = 1 . \tag{2}$$

The part of the collision integral related to excitation and de-excitation of rotational levels by electron impact is written as [2-4]:

$$St_{rot}(f) = B\frac{d}{du}\left(\sigma_R(u)u\left(f(u) + \frac{kT}{e}\frac{df(u)}{du}\right)\right), \tag{3}$$

where T is the gas temperature, k is the Boltzmann constant, e is the electron charge, B is the rotational constant and σ_R is the effective cross section.

Nitrogen

The expression for the effective cross section σ_R for N_2 molecules is as follows [3]

$$\sigma_R(u) = 6\sigma_{02}(u) + 20\sigma_{04}(u), \tag{4}$$

where σ_{02} and σ_{04} are the cross sections for the transitions j=0 -> j=2 and j=0 -> j=4 (j is the number of the rotational level), respectively. Cross section data were taken from papers [6, 7]. Effective cross section σ_R for nitrogen was verified in refs. [8, 9] by comparison of the calculated rate of fast gas heating in glow discharge (in N_2, N_2-He and N_2-He-CO_2 mixtures) with the experimental data.

Oxygen

The expression for the effective cross section σ_R for O_2 molecules is as follows [10]

$$\sigma_R(u) = 10\sigma_{13}(u) + 12\sigma_{15}(u), \tag{5}$$

where σ_{13} and σ_{15} are the cross sections for the transitions j=1 -> j=3 and j=1 -> j=5, respectively. Cross section data were taken from paper [6].

Hydrogen.

The effective cross section σ_R derived for H_2 molecules is written as [11]

$$\sigma_R(u) = 6\sigma_{02}(u), \tag{6}$$

cross section data were taken from papers [12].

Carbon monoxide.

A procedure for determination of the effective cross section σ_R for CO is described in [13].

[1] Napartovich A. P., Dyatko N. A., Kochetov I. V. and Sukharev A. G. EEDF: The software package for calculations of Electron Energy Distribution Function. http://fr.lxcat.net/download/EEDF/

[2] N. V. Karlov, Yu. B. Konev, I. V. Kochetov, V. G. Pevgov, *Preprint FIAN №91*, 1976 (in Russian)

[3] N. A. Dyatko, I. V. Kochetov, A. P. Napartovich, *J. Phys. D: Appl. Phys.*, **26**, 418-423, 1993

[4] M. A. Ridenti, L. L. Alves, V. Guerra and J. Amorim, 2015, Plasma Sources Sci. Technol. **24** 035002

[5] I. P. Shkarofsky, T. W. Johnston, M. P. Bachynski, The particle kinetics of plasma, Addison-Wesley publishing company, 1966

[6] Yu. D. Oksyuk, *Zh. Eksp. Teor. Fiz*., **49**, 1263-1273, 1965

[7] M. A. Morrison, N. F. Lane, *Phys. Rev.,* **16**, 975, 1977

[8] I. V. Kochetov, V. G. Naumov, V. G. Pevgov, V. M. Shashkov, *Sov. J. Quantum Electron*. **6**, 847, 1979

[9] A. P. Napartovich, I. V. Kochetov, *Plasma Sources Sci. Technol.,* **20**, 025001 (9pp), 2011

[10] R. Sh. Islamov, I. V. Kochetov, V. G. Pevgov, *Preprint FIAN №169*, 1977 (in Russian)

[11] V.E. Galtsev, A. V. Demyanov, , I. V. Kochetov, V. G. Pevgov, V.F. Sharkov, Preprint IAE-3156, 1979 (in Russian).

[12]. D. K. Gibson, *Aust. J. Phys*., 1970, **v.23**, 683-96.

[13] Dyatko, N. A., Kochetov, I. V., Kurnosov, A. K., Napartovich, A. P., *Plasma Physics Reports*, 1995, **21**, p.172.