Journal of Quantitative Spectroscopy & Radiative Transfer 99 (2006) 131–141

Journal of Quantitative Spectroscopy & Radiative Transfer

www.elsevier.com/locate/jqsrt

Onset of pseudo-thermal equilibrium within configurations and super-configurations

Michel Busquet*

ARTEP Inc., 2922 Excelsior Springs Court, Elicott City, MD 21042, USA

Accepted 26 April 2005

Abstract

Level populations within a configuration and configuration populations within super-configuration or within one ion are shown to follow a Boltzmann law at some effective temperature different from the actual electron temperature (as it would be when Griem criterion is valid). Origin of this pseudo-thermal equilibrium is discussed and basis of a model are presented.

Keywords: Non-local thermodynamic equilibrium; Populations kinetic; Collisional radiative models; Effective temperature; Super-configurations

1. Introduction

Non-local thermodynamical equilibrium (non-LTE) plasmas are found in physical regimes and the atomic populations of these plasmas can be evaluated with the collisional radiative models (CRM) [1]. However, for multi-electron atoms (with more than 3 electrons in open shells), there are too many levels for detail accounting, and averages over large sets of levels and configurations may be required [2]. The CRM will solve the populations of this "aggregated" sets of levels or configurations. Today CRMs will use super-configurations (SCs) [3], which are particular sets

*Corresponding author. Naval Research Laboratory, code 6730, 4555 Overlook Av., SW, Washington, DC 20375, USA.

E-mail address: busquet@this.nrl.navy.mil.

0022-4073/$ - see front matter
doi:10.1016/j.jqsrt.2005.05.010

including possibly hundreds of configurations. Average energies and averaged transition rates require hypotheses about the relative level populations within each SC. Statistical equilibrium, where populations are proportional to the statistical weight is often used for levels within one configurations, that is, for the population of level p within a configuration C, $N_p = N_C\omega_p/\sum_{q\in C}\omega_q$, where N_p and N_C are the populations of the level p and of the configuration C, respectively, and ω's are statistical weights. For levels or configurations of an SC, a common idea is to assume "partial LTE" in which populations, within this set only, are proportional to the Boltzmann factor, $N_p = N_{\mathrm{SC}}\omega_p \exp(-E_p/kT_{\mathrm{e}})/\xi$. Here the partition function ξ is a normalization factor equal to $\xi = \sum_{q\in \mathrm{SC}}\omega_q \exp(-E_q/kT_{\mathrm{e}})$ and N_{SC} is the total populations of the SC. Note that the Saha equation is recovered by subtracting from the energy level E_p an equivalent chemical potential $\mu = kT_{\mathrm{e}} \ln(A_{\mathrm{saha}}T_{\mathrm{e}}^{3/2}N_{\mathrm{e}}^{-1})$ times Q_p, where Q_p is the charge state of the level and $A_{\mathrm{saha}} = 6.04\times 10^{21}\,\mathrm{cm}^{-3}\,\mathrm{eV}^{-3/2}$. The next improvement is to assume a pseudo-LTE using an effective temperature T_{eff} in place of the actual electron temperature. Partial LTE and pseudo-LTE hypothesis are used in aggregated levels CRM, such as the mixed model [4] in an extended thermal band, or SCROLL [3] in SCs. We shall address both hypothesis in this paper.

The concept of effective temperature T_{eff} was introduced in 1960 by Griem [5] to describe with one parameter a complex non-LTE situation that can be broadly described as pseudo-LTE with a T_{eff} different from the actual electron temperature. In spectroscopy and optics it is also known as color temperature. Alternatively, Gabriel [6] used it to compare a transient plasma to a non-LTE stationary plasma. Busquet [7] proposed a compact model to derive an ionization temperature and compute a non-LTE equation of state and optical properties from LTE tables. Here our purpose is slightly different. First, using results [8,9] from CRMs, we demonstrate that level populations statistically follow a Boltzmann-like distribution at some effective temperature. The origin of this pseudo-LTE will be discussed. We present in Section 3 a refined version of the harmonic model (HM) [9] and we compare in Section 4 the predictions of this model to the effective temperatures derived by a linear regression of populations computed by our CRM.

In this paper, all atomic data, level energies and cross sections, are computed with the HULLAC [10] code either in its standard mode, or in the newly implemented "direct configuration average" mode [11]. For the analysis we shall use Boltzmann plots of reduced populations (i.e. populations divided by the statistical weight or the partition function) versus the total level energy (including all ionization potentials starting from the neutral atom). In these plots, Boltzmann-like distributions will appear as straight lines, with a slope being equal to $-1/T_{\mathrm{eff}}$. Only when T_{eff} is equal to the actual electron temperature T_{e} are levels in partial LTE. The origin and validity of partial LTE is discussed in Section 2.

2. Partial LTE, thermal band and Griem criterion

Partial LTE is obtained when collisional processes dictate the population of a restricted set SC of levels that, generally, will have small energy separations. This means that radiative transitions are either balanced (when the plasma is immersed in a black body radiation field at T_{e}) or are negligible. This leads to the Griem criterion [5] which says that radiative decay is 10 times less than collisional de-excitation for the pair of neighbor levels with the largest energy gap within the set SC. This criterion compare rates of "internal depopulating channels"; however, radiative decay to