Synthetic Spectra for Interstellar Molecules in LTE and non-LTE regimes

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Abstract

1 Introduction

Consider a mono-atomic or singly-charged chemical species in gaseous state with N energy levels defined as E_i with $i = 1 \dots N$ in ascending order. Pertaining to the temperature this chemical species exists at, each level will have certain occupation or population. These occupation numbers can change due to collisions between neighboring molecules and if the environment is sufficiently dense and temperatures are sufficiently high, this population distribution can be deemed as thermal and can be expressed as

$$\frac{N_j}{N_i} = e^{-(E_j - E_i)/k_B T} \tag{1}$$

Here, N_i (and N_j) represents the level occupation number density of state i (and j), k_B is the Boltzmann constant and T is the temperature of the gas. This thermal distribution is basis for the condition of *local thermodynamic equilibrium* or LTE. In other words, the mean free path of the (excited) molecules is much, much less than the scales at which the temperature varies in the medium.

Equation 1 can be modified to include the degeneracies of states through statistical weights, which results in

$$\frac{N_j}{N_i} = \frac{g_j}{g_i} e^{-(E_j - E_i)/k_B T} \tag{2}$$

where $g_i = 2l + 1$, l being the orbital angular momentum of electron in state i. And finally, we can obtain the fractional occupational numbers n_i using the partition function $Z(T)$ as

$$n_i = \frac{1}{Z(T)} g_i e^{-E_i/k_B T} \tag{3}$$

2 Radiative Transfer

2.1 The Escape Probability Scheme

2.2 Lambda Iteration and Accelerated Lambda Iteration