§9. Near-LTE Linear Response Calculations with a Collisional-radiative Model for He-like Al Ions

More, R. (Lawrence Livermore National Laboratory), and Kato, T.

We investigate atomic kinetics from the viewpoint of nonequilibrium thermodynamics [1]. Steady-state emission is calculated for aluminum ions immersed in a specified radiation field having fixed deviations from a Planck spectrum. We modify an existing CR (collisional-radiative) model [2] for near-LTE conditions and compute the response to changes in line brightness temperature. The calculated net emission is represented as a NLTE (non-local thermodynamic equilibrium) response matrix.We obtain a symmetric response matrix and find the response is linear over a surprisingly large range.

Non-equilibrium thermodynamics predicts that a near-equilibrium steady state of any system is constrained by rigorous general requirements of energy conservation, by the principle of minimum entropy production and by Onsager relations which require that the linear response matrix should be symmetric. This symmetry can be a powerful consistency test for a NLTE atomic model.

The calculations describe He-like aluminum. Maxwellian free electrons have a fixed density $n_e = 10^{20}$ cm^{-3} and temperature $T_e = 150$ eV. The CR model [2] includes 65 He-like levels up to n=22, with n,l,S-splitting up to n = 4. We modify this model by adding stimulated emission and absorption for all line transitions.

The radiation is described by n_ν, the number of photons per mode. In equilibrium, n_ν is $n_\nu{}^0 = [\exp(h\nu/kT_e) - 1]^{-1}$. Non-LTE is caused by any difference $\delta n_\nu = n_\nu - n_\nu{}^0$.

A series of NLTE calculations is performed to construct the response matrix. For each calculation $n_{\nu'}$ is altered for one specific line ν'; other lines still couple to the black-body spectrum. For any line ν, in NLTE there is a net radiated power,

$$P_{ij} = h\nu\ [A_{ij}\, N_i\, (n_\nu + 1) - A_{ji}\, N_j\, n_\nu]$$

P_{ij} can be positive (*emission*) or negative (*absorption*). P_{ij} is zero in LTE, and is proportional to $\delta n_{\nu'}$ for small perturbations. The response matrix is

$$RL_{\nu,\nu'} = [P_{ij}][\partial n_{\nu'}{}^0/\partial T]/[\delta n_{\nu'}]$$

$RL_{\nu,\nu'}$ is the net emission from line ν induced by a variation $\delta n_{\nu'}$ imposed on the line ν'.

Table I identifies 4 transitions in the singlet spectrum, and gives the 4x4 linear-response matrix for small perturbations $\delta n/n = \pm 1\%$. The response matrix is accurately symmetric.

Calculations with larger perturbations show a large range of linear response.

Similar results are obtained for the same density-temperature conditions from the NLTE screened-hydrogenic average-atom model.[1]

Table I. Some He-like aluminum transitions, and linear response coefficients (Watts/eV-atom).

transition 1 : $1s^2\ {}^1S$ - $1s2p\ {}^1P$ 1.600 keV
transition 2 : $1s^2\ {}^1S$ - $1s3p\ {}^1P$ 1.870 keV
transition 3 : $1s2s\ {}^1S$ - $1s3p\ {}^1P$ 0.276 keV
transition 4 : $1s2p\ {}^1P$ - $1s3s\ {}^1S$ 0.268 keV

	1	2	3	4
1	$-5.234\ 10^{-10}$	$3.564\ 10^{-10}$	$-9.317\ 10^{-12}$	$-1.662\ 10^{-12}$
2	$3.564\ 10^{-10}$	$-6.221\ 10^{-10}$	$1.068\ 10^{-11}$	$1.590\ 10^{-12}$
3	$-9.317\ 10^{-12}$	$1.068\ 10^{-11}$	$-2.344\ 10^{-12}$	$1.178\ 10^{-14}$
4	$-1.662\ 10^{-12}$	$1.590\ 10^{-12}$	$1.177\ 10^{-14}$	$-3.601\ 10^{-13}$

References

1.) More, R., and Kato, T., submitted to Physical Review Letters.

2.) Fujimoto, T., and Kato, T., unpublished report IPPJ-647; Fujimoto, T., and Kato, T., Phys. Rev. A35, 3024 (1987).