T-4
Atomic & Optical Theory

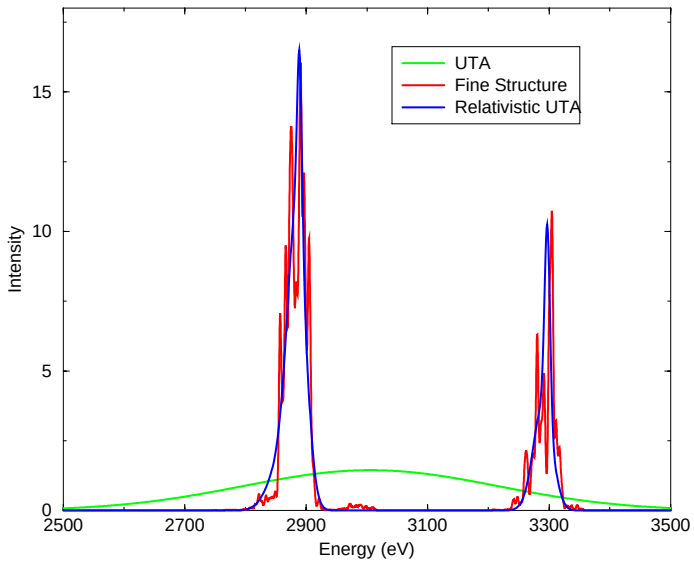
Representation of Atomic Spectral Transition Arrays by Simple, Accurate Methods

David P. Kilcrease and Joseph Abdallah, Jr. (T-4) and Christopher J. Fontes (XCI)

When an electron in an atom undergoes a transition and releases a photon, it gives rise to a spectral line. If the atom has many electrons bound to it, the number of possible lines that can be produced can be enormous. When it becomes necessary to calculate the spectra of many different transitions in atoms in different ionization stages, the computational resources required can become prohibitive. However, it is possible to represent the overall features of groups of these spectral lines (transition arrays) by the calculation of their statistical moments (such as the mean and standard deviation). Theoretical methods have been developed that allow the calculation of these moments from first principles without the necessity of calculating each individual line in the array. These methods allow many complicated problems in atomic spectroscopy to be solved quickly with a minimum of computer resources. They also allow very large calculations to be performed that would be impossible if it were necessary to calculate each of the many spectral lines that make up a transition array. Here we show three levels of approximation to the emission spectra for a 3p to 4d transition in nickel-like gold. This case illustrates some of the difficulties of these calculations. Gold is a heavy element and can exhibit strong relativistic spin-orbit splitting. As a reference case, we have shown the full fine structure calculation from the Dirac equation that leads to approximately 1500 separate lines. The simplest approximation is that of the Unresolved Transition Array (UTA) theory. It reproduces the correct average transition energy and standard deviation but does not give a good approximation to the more complete fine structure calculations. A much more accurate approximation is given by the Relativistic UTA theory. This reproduces the large splitting in the transition array and gives the overall shape of the grouping of lines seen in the fine structure calculation. The relativistic UTA approximation is therefore essential for the calculation of the spectra of heavy relativistic atoms.

These methods allow many complicated problems in atomic spectroscopy to be solved quickly with a minimum of computer resources.

Representations of Nickel-like Gold Transitions



dpk@lanl.gov