Collapsing of Atomic Energy Levels: A Primer on Atomic Models

In this memo, we describe the collapsing (or bundling) of atomic energy levels: why it is important, how it is done, and what are the ramifications. In doing this, we provide some background on *atomic models*, and how they relate to the *ATBASE atomic database*.

Atomic Models, the ATBASE Atomic Physics Database, and AtomicModelBuilder

An *atomic model* is a set of energy levels and the associated collisional and radiative transition data that are used by a particular applications code for a specific calculation. In general, different calculations can utilize different atomic data models. For instance, some calculations may require a very detailed Ar L-shell model, some may need only an approximate treatment of the Ar L-shell, while others may completely neglect any effects of Ar L-shell lines. A plasma applications code, such as *SPECT3D*, *PrismSPECT*, or *HELIOS-CR*, reads in the atomic data model, and computes the emission and absorption properties of the plasma by first computing atomic level populations. Once the populations are obtained, the frequency-dependent emissivity and opacity are computed (see, *e.g.*, Mihalas, *Stellar Atmospheres*, 1978), and the emergent spectrum can be computed by solution of the radiative transfer equation. A primary function of the plasma applications code is first to determine the atomic level populations (which also defines the distribution of charge states). This is typically accomplished by solving a coupled set of atomic rate equations. Once the atomic level populations are obtained, the frequency-dependent radiative properties of the plasma can be computed.

The *ATBASE atomic database* is a reasonably comprehensive collection of energy levels, and associated radiative and collisional data. (In reality, no existing atomic databases are truly comprehensive, due to the complexity of nature.) The ATBASE 4.0 atomic database includes energy levels and transition data for all charge states of all elements up through Z = 36 (Kr). These transition data include: oscillator strengths, photoionization cross sections, autoionization rates, radiative recombination rate coefficients, electron capture coefficients, dielectronic recombination rate coefficients, electron impact excitation and ionization rate coefficients and cross sections.

How much detail should be included in the atomic data model of a given application? How should the energy level splitting be modeled? How can the data in the atomic database be assembled into atomic data models suitable for a wide variety of diverse applications?

Because of the need to provide researchers the ability to set up, or tailor, atomic models for their particular need, we have developed a tool, *AtomicModelBuilder*, that gives users control over how to set up atomic models (*e.g.*, which levels to include, and details of energy level splitting).

Figure 1 illustrates why modeling of energy level splitting is important. It shows a Grotrian diagram for O III (top) and an example of energy level splitting for two electronic configurations of O III (bottom). The $1s^2 2s^2 2p^2$ configuration splits into ^1S, ^1D, and ^3P states when L-S term splitting is considered. The ^3P state further splits into $^3P_2$, $^3P_1$, and $^3P_0$ states due to fine-structure splitting. Thus, in modeling the $1s^2 2s^2 2p^2$ and $1s^2 2s^2 2p^1 3s^1$ configurations and the transitions between them, one can choose to model them as just 2 levels (and therefore only one transition), or 5 levels (L-S term split), or 9 levels (fine-structure splitting) with a correspondingly larger number of transitions in each model. Depending on the application, one may wish to treat ground states and low-lying excited states (say, up to $n = 3$) with fine-structure splitting, intermediate levels (perhaps $n = 4$ and 5) with L-S term splitting, and higher levels ($n \geq 6$) with configuration averaging or even a hydrogenic approximation (*i.e.*, 6s, 6p, 6d, etc., grouped together into a single level). Alternatively, it may only be necessary to model all levels of a given ion using configuration-averaged levels. It depends on the application.

This type of "grouping," or "bundling," of atomic levels can greatly reduce both the computational and memory requirements of an applications code. As an example of the complexity of the problem, atomic data models for a solar composition plasma with ~ 8 – 10 elements, with fine-structure splitting up through just $n = 4$ will easily exceed 10^4 energy levels and 10^7 transitions. This issue is particularly important for applications that model plasmas with a spatial distribution of temperatures and densities; even more so for multidimensional spatial distributions. Including photoionization and photoexcitation effects presents even greater challenges. Thus, deciding on the appropriate atomic model depends on what, or how much, data can practically be utilized in the applications code, and what are the research goals of the user.

AtomicModelBuilder is a tool that allows researchers to control the level of detail in atomic data used for ionization dynamics and/or spectral calculations. Figure 2 shows a screenshot from the main window of the *AtomicModelBuilder*. A list of ions is shown at the left. A list of levels contained in the ATBASE database is shown at the right. Levels are selected (or deselected) simply by checking (or unchecking) the box adjacent to the energy level.

Figure 3 shows a screenshot from the window used to set up how the energy levels are collapsed (or bundled). This can be done independently for the *populations* portion of a calculation or the *spectral* portion of a calculation. Additional details of how to perform these operations is provided in the on-line users guide for *AtomicModelBuilder*.

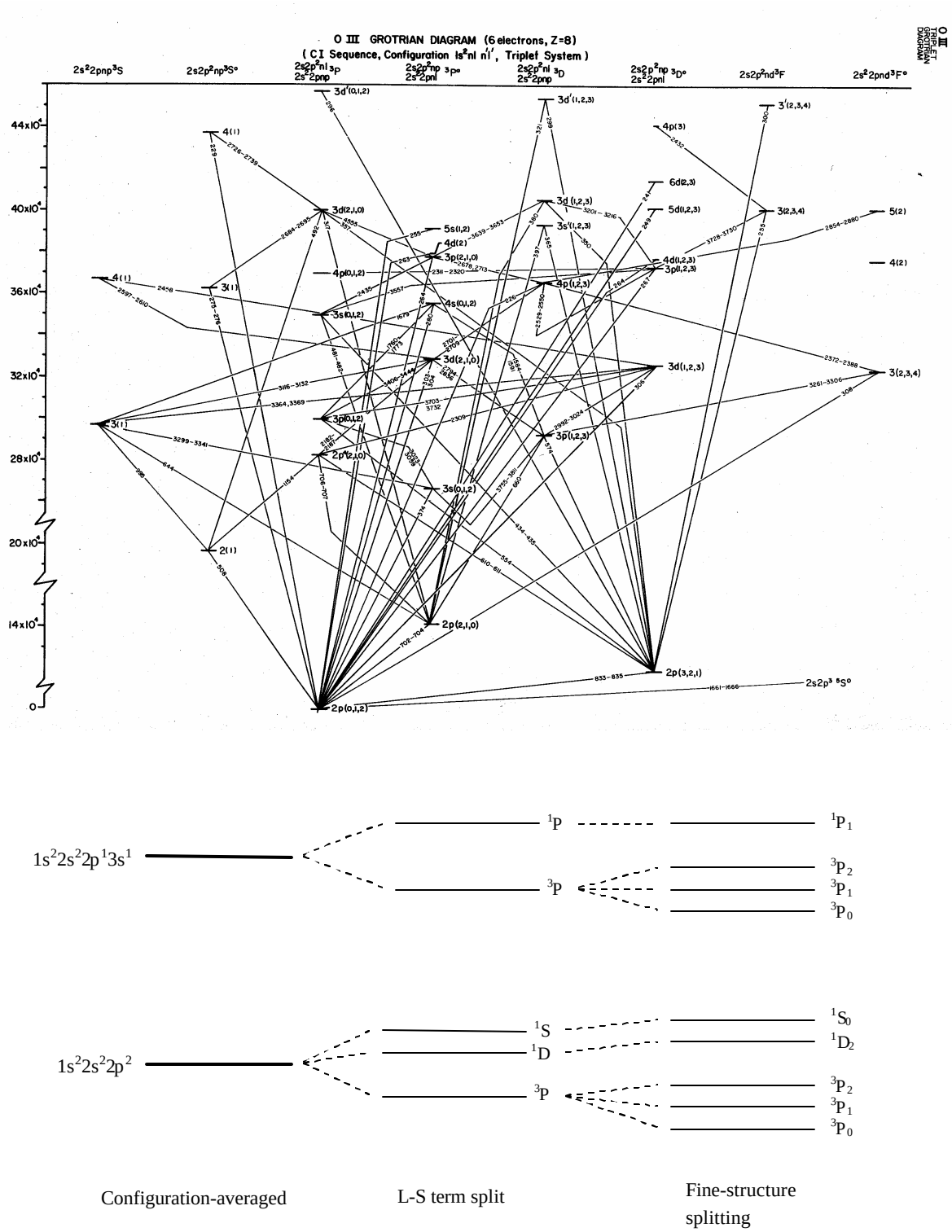

Figure 1. (Top) Grotrian diagram for the triplet system of OIII (Bashkin & Stoner 1975). Labels on the solid lines refer to the transition wavelengths. (Bottom) Schematic illustration for two levels of O III showing the energy level splitting for a configuration-averaged model, an L-S term split model, and a fine-structure splitting model. (Note that the 3s excited state was chosen for this illustration because of its relative simplicity.)

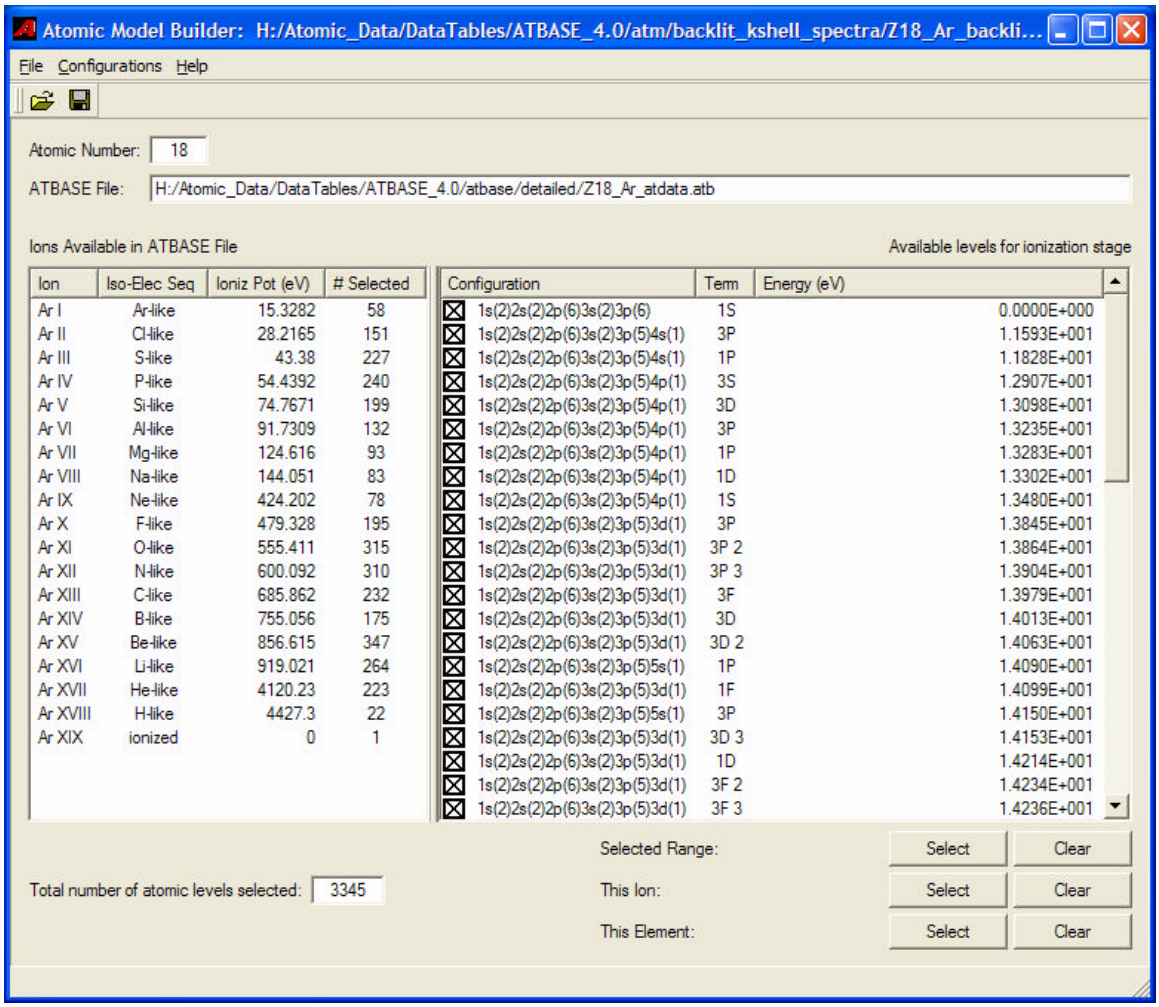

Figure 2. Illustration from *AtomicModelBuilder* main window.

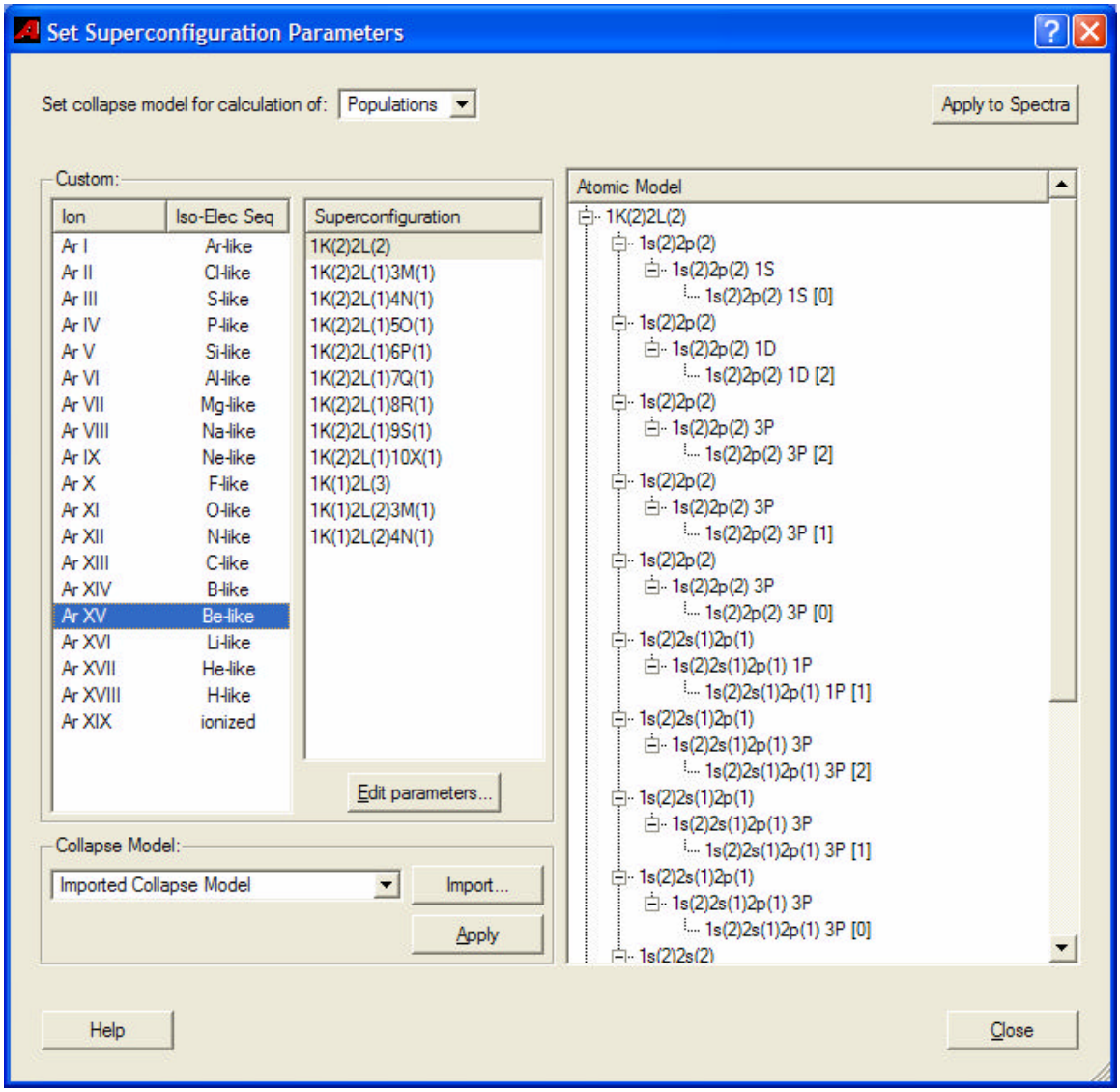

Figure 3. Illustration from *AtomicModelBuilder* window that is used to set up parameters for energy level collapsing (or bundling).