Chapter 1
Balancing Detail and Completeness in Collisional-Radiative Models

Stephanie B. Hansen

Abstract Collisional-radiative models based on highly detailed atomic structure (e.g. fine-structure levels) tend to demonstrate very good agreement with highly resolved experimental data. Such models typically predict X-ray line positions with high accuracy and can faithfully reproduce the intensities of lines from metastable and dielectronic states. Models based on less detailed structure (e.g. configurations) necessarily have lower fidelity at the spectroscopic level. Their key advantage lies in the completeness of their state structure: highly averaged models can capture the population flux through high-n and multiply excited states critical for accurate predictions of charge state distributions. For complex multi-electron ions, highly detailed models with extensive structure become intractable. This Chapter explores the tension between detail, completeness, and tractability in collisional-radiative modeling.

1.1 Introduction

Two principal design elements of a collisional-radiative model are the states to be included and the rates that couple them. This chapter focuses on the first design element: the selection of electronic orbitals or states that form the basis of the atomic model. Because state-space design is a critical determinant of the accuracy and applicability of a given model, this Chapter will cover considerations related to the extent of the modeled state space, its degree of detail, and the generation of atomic data. Chapter 3 focuses on the second design element: the spontaneous, collisional, and radiative rates that connect the set of electronic states.

In a collisional-radiative model, "state" (and sometimes "level") is used to denote a particular member of the population vector X that satisfies the rate equation $dX/dt = \mathbf{A}\mathrm{X}$, with $\mathbf{A}$ the rate matrix. For the screened hydrogenic models (SHM) discussed in Chap. 3, the basic states are Layzer complexes of the form

S.B. Hansen (✉)
Sandia National Laboratories, Albuquerque, NM, USA
e-mail: sbhanse@sandia.gov

Yu. Ralchenko (ed.), *Modern Methods in Collisional-Radiative Modeling of Plasmas*, Springer Series on Atomic, Optical, and Plasma Physics 90, DOI 10.1007/978-3-319-27514-7_1

$(n_1)^{N_1}(n_2)^{N_2}\ldots(n_{max})^{N_{max}}$, where n_m are the principal quantum numbers of n-shell orbitals and N_m are their *populations*. The total number of bound electrons in an ion with charge $Z - N$ is $N = \sum N_m$ for each Layzer complex. These complexes are sometimes called non-relativistic superconfigurations (SCs). This notation offers a useful and compact representation of the extent of a model's state space and can be used to describe even non-hydrogenic models: for example, the state space of more detailed models based on relativistic unresolved transition arrays (UTAs) or fine structure terms can be compactly described using this n-shell notation *as long as each Layzer complex is completely filled by the more detailed states*. Even models that are less detailed than the SHM, such as models that combine several high-n orbitals into a single state, can be described by a variation of this notation with n_m replaced by a range of n.

The ideal state space of a collisional-radiative model is one that is both strictly complete and fully detailed. Strict completeness for an N-electron ion means that all permutations of N electrons in all possible n-shell orbitals are explicitly included in the state space. "Full detail" is a less rigorous concept: for the purposes of this Chapter, fully detailed means that all of the superconfigurations included in the model are split into states with sufficient detail to meet the intended application of the model. For example, the radiative power losses from high-temperature plasmas with negligible emission from $\Delta n = 0$ transitions can be well described by an SHM model, while high-resolution spectroscopic measurements often require a state space based on fine-structure terms, and collisional-radiative calculations in the presence of strong fields or anisotropic electron distributions might demand further splitting of the state space into magnetic sublevels.

In practice—and even in principle, for isolated ions with unbounded n—strictly complete and fully detailed models are computationally intractable. Collisional-radiative models thus fall into a class of computational science where the exact solution can be theoretically but not computationally determined. Balancing the requirements of state-space completeness and degree of state detail is an essential part of the art of collisional-radiative modeling, and this Chapter offers some guidelines for constructing reliable, tractable, and useful collisional-radiative models for a variety of applications.

1.2 State-Space Completeness

State-space completeness is a critically important feature of a reliable collisional-radiative model, but can be difficult or even impossible to achieve. In a completely isolated ion, the maximum principle quantum number is unbounded. Thus, a strictly complete model based on Layzer complexes is not achievable for even one-electron ions. Even effective completeness, by which we mean convergence in the charge state distribution with increasingly extensive structure, is not possible for isolated ions at finite temperature because level populations do not converge with increasing n.

To illustrate this point, consider a one-electron (H-like) ion with nuclear charge Z and SHM state energies defined in reference to the binding energy of the $1s$ electron: the $(n)^1$ superconfigurations have energies $E_n = RyZ^2(1 - 1/n^2)$ and statistical weights $g_n = 2n^2$. In the simplest case of local thermodynamic equilibrium (LTE) at a finite temperature T, the populations of the of the $(n)^1$ superconfigurations follow Boltzmann statistics: $X_n = g_n \exp[-E_n/T]$. For low temperatures, the exponential term ensures that X_1 holds the majority of the population among the low-n states. However, because the E_n and therefore the exponential term asymptote to constant values, while g_n increases with n, there is for each finite temperature some n such that $X_n > X_1$, above which the high-n populations will dominate. Thus the solution to even the simplest (LTE) treatment of the simplest (one-electron) ion is divergent.

In real physical systems, the influence of neighboring particles truncates the high-n state space, lowering the ionization potential by roughly ΔI (eV) $\sim 8 \times (Z^* + 1)^{2/3}(N_e/10^{22})^{1/3}$ in the ion sphere approximation [1], with N_e the electron density in e/cm^3 and Z^* the ion charge. This ionization potential depression (IPD)—also called pressure ionization or continuum lowering—destroys high-n orbitals with binding energies less than ΔI. As a very rough rule of thumb, states with $n < 2(Z^* + 1)^{1/2}/(N_e/10^{22})^{2/15}$ must be included for strict completeness. For plasmas at near-solid densities, the state-space restriction due to pressure ionization can be significant: at $N_e = 10^{22}$ e/cm^3 one must include only states up to $n_{max} = 10$ for hydrogen-like ions with $Z = 30$ and up to $n_{max} = 3$ for $Z = 1$. By contrast, strict completeness requires $n_{max} > 100$ for mid-to high-Z hydrogen-like ions in low-density astrophysical or tokamak plasmas.

For multi-electron ions, strict completeness becomes even more difficult to achieve due to the large number of possible permutations of N electrons into n shells. Even using a relatively undetailed state structure like the superconfigurations of the SHM, the explosion of statistical weight for high-n, multiply excited states very quickly reaches the memory capacity of modern computing facilities. Figure 1.1 illustrates the growth of statistical weight, which is roughly equivalent to the number of highly detailed states, for models with $n_{max} = 8$ and either single or single and limited double excitation. Collisional-radiative models with 10^6 states require TB of computing memory to store the rate matrix, and solving the rate matrix for systems at this scale approaches intractability. Balancing the demands of completeness and tractability thus requires a thoughtful approach to state-space design.

Two general approaches to resolving the tension between completeness and tractability have proven successful. The first approach uses information about the intended model application to generate a fixed state space that does not introduce too much inaccuracy: this is effective completeness by design. For example: hot plasmas at moderate densities driven by collisions with thermal electrons can be reliably modeled using a fairly restricted set of singly and doubly excited states; plasmas driven by intense, high-energy radiation fields require "hollow-ion" states with multiple inner-shell holes, and modeling the emission and relaxation from charge exchange requires multiply excited high-n states. Limiting the anticipated plasma conditions can be very effective in restricting the states that must be modeled especially since closed-shell ions have smaller statistical weights (see Fig. 1.1) and can dominate

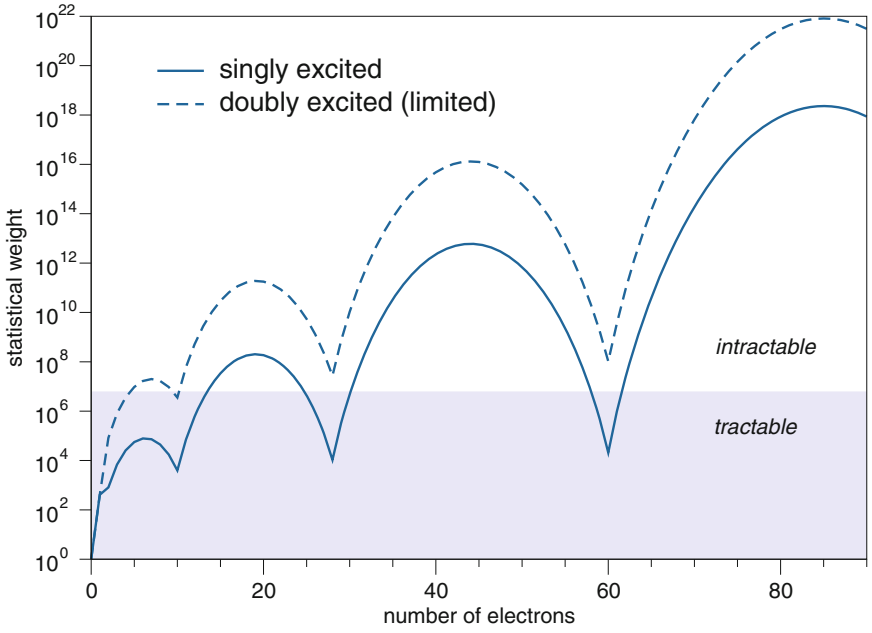

Fig. 1.1 Statistical weight per ion increases dramatically with the number of bound electrons. The statistical weight is an upper limit for the number of states in a highly detailed model; highly averaged models can have many fewer states encompassing the same statistical weight. The state space illustrated by the *solid line* includes all states formed by single excitation (including all inner-shell excitation) to $n_{max} = 8$. The *dashed line* also includes double excitation to $n_{max} = 8$ from the valence and first inner shells. Computational tractability for highly detailed models is roughly indicated by the *shaded region*. Less detailed models can cover the same configuration space with many fewer state: a superconfiguration model would require only about 100 states per ion for these configurations

the charge state distribution over fairly wide ranges of temperature due to their relatively large ionization potentials. The second approach is to design a model with a dynamic state space that can adapt to different applications: this is explicitly enforced effective completeness. This can be done either by generating states on an as-needed basis within the population solver itself (as in the Monte Carlo approach taken in [2] and discussed further below) or by a methodical stepwise increase in the state space that solves the rate matrix and tests for convergence at each step. While this second approach produces more generally reliable models, it does not guarantee tractability.

State-space completeness impacts the accuracy of collisional-radiative calculations in two ways: First, the enormous statistical weights of high-n and multiply excited states can hold a great deal of population, as illustrated by the one-electron example above. The population in such states can directly and significantly affect the charge state distribution (CSD) and the emission or absorption signatures from the plasma. This aspect of completeness is particularly critical for plasma at high density

or under intense external irradiation, where excitation rates are of the same order as spontaneous radiative decay rates and high-lying electronic configurations can maintain near-LTE occupations. It is also critical for ions undergoing charge exchange, where electrons are preferentially (and multiply) captured into high-n orbitals. In high-density plasma, pressure ionization helps to restrict the state space, however in that case, the particular treatment of IPD becomes a critical consideration, which is by no means resolved [3]. And in low-density photoionized or recombining plasmas, there is no such grace.

The second critical aspect of high-n multiply excited states is their role as dielectronic recombination channels, which can have a major influence on the CSD even for low-density plasmas without significant radiation fields. In this "coronal limit," spontaneous radiative and Auger decay rates are much more rapid than collisional rates and the vast majority of population resides in the ground states of the ions. But even here, the charge state distribution is highly sensitive to the treatment and completeness of the high-n multiply excited states, because these states provide the channels for the critical dielectronic recombination process. The sensitivity of CR calculations to dielectronic recombination is illustrated in Fig. 1.2, which gives the results of a test case from a NLTE code comparison workshop [4]. When dielectronic capture and Auger decay processes are excluded, there is very good agreement among a wide

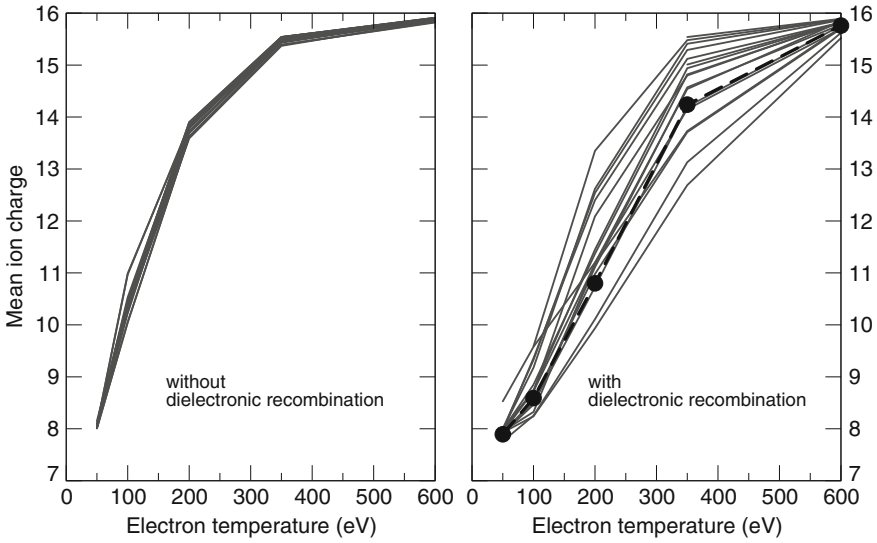

Fig. 1.2 The average ion charge predicted by a variety of collisional-radiative models is highly sensitive to the completeness of dielectronic recombination channels. The plot on the *left* shows good agreement between a wide variety of models with very different degrees of detail and completeness for a coronal argon plasma ($N_e = 10^{12}$ e/cm^3) when dielectronic processes are excluded. The plot on the *right* shows the significant disagreement that results from including dielectronic processes in models with diverse detail and completeness. The heavy *dashed line* is from an effectively complete coronal model that uses a tabulated dielectronic recombination rate [5]

range of models—but this agreement all but vanishes when DR is included, largely due to the idiosyncratically incomplete state structure in the individual models.

Models with insufficient state-space completeness tend to overpredict ionization. In the low-density coronal limit, incomplete excitation-autoionization (EA) and dielectronic recombination (DR) channels lead to inaccurate rates between charge states. This is illustrated in Fig. 1.2: excluding both EA and DR processes entirely, as is done in the left-hand plot, results in a significant overestimation of the average ion charge. On the right-hand plot, most of the models have limited completeness and thus predict a higher charge state than the effectively complete coronal model shown by the dashed line; the few models that predict lower charge states are screened hydrogenic models that use approximate rates and may exclude $\Delta n = 0$ EA and DR channels. Models can achieve effective completeness in the coronal regime by treating high-n doubly excited states implicitly, using pre-calculated EA and DR rates summed to convergence in n (e.g. [5]) rather than tracking dielectronic capture and Auger decay through high-n states explicitly included in the population vector. This implicit approximation breaks down at moderate densities, where pressure ionization invalidates the n-summed dielectronic recombination rate and collisions open new DR channels by moving significant population into excited states. Incomplete models also tend to overpredict ionization in the high-density LTE limit, where three-body recombination dominates over dielectronic recombination and excitation rates support near-statistical populations of highly excited states. The reason for this can be seen by again considering the simple one-electron ion, where high-n states can hold significant population due to their high statistical weights. Excluding these high-n states forces population into the continuum and artificially increases the calculated charge state.

1.3 Degree of State Detail

We have seen that the completeness of modeled state space influences the first-order accuracy of the charge state distribution (CSD) in collisional-radiative models, affecting gross predictions like the equation of state, radiative power loss (RPL), and the spectral location of emission features. This Section will show that the detail with which the modeled states are treated influences the finer features of the CSD and spectra. The effects of state detail on emission and absorption spectra are particularly important because detailed spectroscopic data is a primary touchstone between collisional-radiative models and the atomic systems they represent. Plasma diagnostics based on comparisons of model predictions with high-resolution spectroscopic data necessarily require that the model treat both the electronic states and the rates that govern their populations with fairly high fidelity.

To illustrate the importance of detailed state structure on modeled spectra, consider the lowest two superconfigurations of a two-electron (He-like) argon ion: $(1)^2$ and $(1)^1(2)^1$. This superconfiguration includes three configurations: $1s^2$, $1s2s$, and $1s2p$,

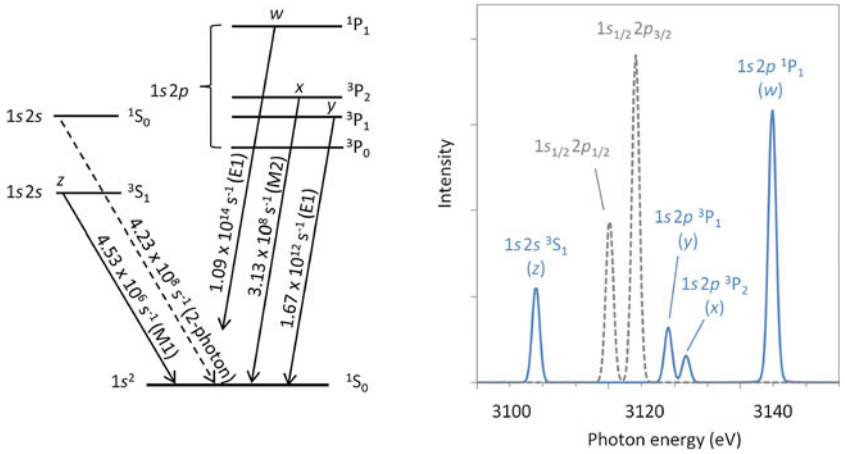

Fig. 1.3 On the *left* is a level diagram of the fine structure states in the $1s^2$, $1s2s$, and $1s2p$ configurations of He-like argon. Transition rates are given for electric dipole (*E1*), magnetic dipole (*M1*), magnetic quadrupole (*M2*), and two-photon decay rates [6]. On the *right* are calculated He-like emission spectra at coronal conditions ($T_e = 1$ keV, $N_e = 10^{12}$ e/cm^3) from both a fine-structure model (*solid*), which captures the character of the metastable emission, and from a configuration-averaged model (*dashed*), which produces only a rough representation of the emission

whose seven fine-structure levels are illustrated in Fig. 1.3. The intercombination line (denoted y) arises from a transition from $1s2p\ ^3P_1$ to $1s^2\ ^1S_0$ with a radiative decay rate about 100 times smaller than the decay rate of the $1s2p\ ^1P_1$ to $1s^2\ ^1S_0$ resonance line (w). Other dipole-forbidden lines (x and z) have even smaller decay rates. Yet despite the orders-of-magnitude differences in their radiative decay rates, all four lines are observed with significant intensities in measured emission spectra from low-density plasmas such as tokamaks. This is because emission line intensities depend on the product of upper-level populations and radiative decay rates, and since the upper levels of the x, y, and z transitions are metastable, they can accumulate significant populations in low-density plasmas.

In a low-density plasma, any electron that finds itself in an excited state will undergo radiative (or Auger) stabilization. As this stabilization proceeds via either direct decay to ground or cascading decay into lower excited states, population can accumulate in long-lived, low-lying excited states. These metastable states do not autoionize and have only small radiative decay rates to the ground state. Absent significant collisional depopulation, these states will collect population that can be many times larger than the population of nearby resonance states with stronger decay channels, leading to comparable line intensities. Figure 1.3 illustrates the emission spectrum from He-like argon in a low-density plasma, where all of the metastable states are populated at sufficient levels to produce strong emission.

As electron densities increase, collisional processes depopulate the metastable states, resulting in a disappearance of the associated lines until they reach their statistical limits, where upper level populations follow Boltzmann distributions and

the relative intensities of the lines are proportional to the statistical weights of the upper levels and the radiative decay rates of the transitions. This density dependence makes emission signatures from He-like and other closed-shell ions powerful plasma diagnostics. While the exact density dependence of the line intensities depends on the details of the collisional and radiative rates that govern the populations, intercombination-to-resonance line ratios tend to be sensitive to densities around $N_e \sim 5 \times 10^9 \Delta E^{7/2}$ cm^{-3}, with ΔE the transition energy in eV.

High populations in metastable states can also contribute to a process called ladder ionization, which becomes important when the electron temperature is too small to support significant collisional ionization from the ground state but large enough to support ionization from excited states that lie much closer to the continuum limit. The collisional ionization flux and charge state distribution therefore depend on the degree of state detail. In addition, some mid-shell ions support excitation-autoionization processes for states formed by single excitation from inner subshells (e.g. the $1s^2 2s 2p^6 nl$ states in F-like iron are autoionizing for $n > 6$). Models that average over subshells do not generally capture the resultant $\Delta n = 0$ excitation-autoionization and dielectronic recombination channels (cf. Fig. 1.2). Thus, models with insufficient detail tend to underpredict ionization around closed shells. Usually, however, this is a smaller effect than the overpredicition of ionization one finds in models with insufficient completeness. And because models with more complete high-n structure will more accurately represent the cascades that populate metastable states, completeness remains important even for simple few-electron ions in low-density plasmas.

While the degree of detail in the state structure can have a significant impact on population dynamics and line intensities, it plays an even more critical role in the accuracy of line positions. Transition energies between n-shells of even complex ions can be grossly obtained to within about 10 % by very simple screened hydrogenic estimates, which account for shell energies and screening. Transition energies between nl or nlj orbitals can be determined within about 1 % using relatively straightforward Hartree- or Dirac-Fock methods, which account for spin-orbit coupling and relativistic effects. However, high-resolution spectrometers can measure line positions to parts per million, and reliable line identification generally requires multiconfiguration calculations that include extensive configuration interaction effects, which influence both transition energies and rates. The poor performance of models with even modest averaging (by relativistic configuration) is illustrated by the dashed-line spectrum in Fig. 1.3, which shows transitions from a Dirac-Fock structure calculation [7] in comparison to the emission predicted by a fine-structure calculation based on atomic data from the Flexible Atomic Code [8]. Not only does the less detailed calculation fail to capture line emission from metastable states at low densities, but its predictions for transition energies are significantly less accurate.

Like completeness, the degree of state detail plays a significant role in model accuracy at all densities. The importance of detailed state structure is most obvious at low densities, where metastable effects are large, collisional broadening is

small, and emission lines can be measured with high precision from long-lived and well-characterized plasmas. At higher densities, collisions move level populations towards LTE, broaden emission lines through collisional and Stark effects, and increase the population in high-n and highly excited states. This population transfer shifts emission from distinct single-line resonance transitions to complex satellite features that can be reasonably well described by unresolved transition arrays (UTAs) [9] or other statistical treatments [10]. But as population moves into these exotic states, the precise treatment of the pressure ionization that truncates the state space begins to play a determining role in model predictions, and the degree of state detail determines how accurate that treatment will be. In aluminum at T = 100 eV and solid density, for example (cf. [3]), the $n = 3$ M-shell is significantly perturbed by free electrons and neighboring ions. But a $3s$ orbital has a much different shape and character than a $3d$ orbital and is affected differently by the dense plasma environment. Such differences cannot be resolved by models that do not account for subshell splitting.

1.4 Application-Driven Approaches to Balancing Detail and Completeness

The tension between state-space completeness and the degree of state detail arises because computational resources are finite. In the present computational environment, collisional-radiative calculations with $\sim 10^3$ states can be done quickly and routinely, and $\sim 10^6$ states can be calculated with heroic effort. To illustrate this tension between completeness and detail, consider a three-electron Li-like ion with n_{max} = 10—a relatively simple and restricted system. The number of fine-structure levels scales roughly with statistical weights, which grow factorially as $g_n!/[N!(g_n\text{-}N)!]$ for each $(n)^N$ complex. A strictly complete fine-structure representation of even this simple three-electron system has more than 10^6 states and is approaching intractability. A highly averaged SHM model, which grows roughly as $(n + N - 1)!/[N!(n\text{-}1)!]$, is strictly complete with only a few hundred states for the same ion. An effectively complete coronal fine-structure model limited to only the ground and singly excited configurations (reliable only at coronal densities) also has only a few hundred states.

Restricting the state space and reducing the degree of state detail can both increase computational efficiencies in collisional radiative models by orders of magnitude, and both are viable strategies for designing tractable CR models. But each concession, each departure from the ideal, has implications for the model's accuracy and range of applicability. The sections below describe the advantages and limitations of approaches to collisional-radiative modeling that have been developed in response to the tension among state-space completeness, the degree of state detail, and computational tractability.

1.4.1 Coronal Fine-Structure Models

In low-density plasmas like those found in tokamaks ($N_e \sim 10^{14}$ e/cm^3), electron beam ion traps (EBITs, $N_e \sim 10^{12}$ e/cm^3), and stellar coronae ($N_e \sim 10^{10}$ e/cm^3), collisional rates are dwarfed by radiative decay rates and the overwhelming majority of population resides in ground states. High-resolution emission spectroscopy of these plasmas produces sharp, well-defined lines that can only be matched by highly detailed and accurate atomic structure calculations. Bright emission lines from metastable states in these plasmas require extensive modeling of collisional, radiative, and cascade processes among the singly excited states. Distinct dielectronic recombination satellite lines formed by radiative stabilization of autoionizing states following dielectronic capture are present but tend not to dominate the emission spectra.

These observations have driven extensive development of highly detailed fine-structure collisional-radiative models. Since only ground states have significant population, most emission can be adequately described by including only states formed by single excitation from the ground configuration. Including a modest number of doubly excited states with $\Delta n = 1$ or 2 above the valence shell is generally sufficient to account for observed DR satellite emission, and completeness in the DR channels can be ensured by implicit inclusion of doubly excited high-n states through DR rate tables (e.g. [5]).

These coronal CR models can produce very good agreement with high-precision data from low-density plasmas and are used to diagnose temperatures, densities, and velocities (through Doppler shifts of well-resolved lines). They can generally handle non-thermal electron velocity distributions and modest external radiation flux. But as electron densities increase past $\sim 10^{17}$ e/cm^3 or photon fluxes brighten towards $T_{rad} \sim T_e$, increasing excitation rates can move significant population into excited configurations, invalidating tabulated ground-state DR rates and opening up population channels into multiply excited states that are not generally included in these models. At high densities, these models tend to be significantly overioinized and produce spectra with profound deficits in both emission and absorption.

1.4.2 General Models for Moderate-Density Plasmas

Laboratory plasmas generated by high-power lasers or high-current discharges through solid, foam, or gas targets produce emission spectra with distinct emission lines and satellite complexes that cannot, in general, be completely described by coronal-style models. At densities of 10^{18}–10^{22} e/cm^3, the emission from these plasmas can be measurably influenced by collisional and Stark broadening, and the charge state distribution is governed by a complex interplay of all of the collisional and spontaneous processes that inform the rate matrix. Excited-state populations are high enough to require explicit treatment of dielectronic capture and multiple excitation,

opening up new configuration space that presents a computational challenge for detailed models. Highly averaged general models like the SHM that can more easily handle this required completeness are challenged by the continuing presence of metastable states and produce only rough agreement with high-precision spectroscopic measurements. The tension between model completeness and detail is thus profound in this moderate-density plasma regime, and many different approaches have been taken.

Some models start with an extensive database of fine-structure states and rates calculated using sophisticated multi-configuration atomic structure codes and perform a brute-force averaging of the fine-structure states and rates in order to obtain a tractable collisional-radiative rate matrix (e.g. [11]). After the CR solution is obtained, the fine structure states can be populated according to Boltzmann statistics and used to generate spectra with accurate line positions. Such models typically limit the principal quantum number to $n_{max} \sim 6$ and the number of allowed excitations to two or three—and these excitation are allowed only from near-valence shells. These restrictions help keep the atomic structure and rate calculations tractable, and the CSD and RPL predictions from these models tend to be of very high quality. At low densities, the CSDs from these models will not be quite as accurate as those from coronal models, since they lack both the complete implicit DR channels and ladder ionization from metastable states. At high densities, the models must incorporate ad-hoc continuum lowering effects and, since they exclude extensive multiply excited state structure, may lack the completeness to provide highly accurate charge state distributions and spectra. Finally, although the line positions from these models are as accurate as their underlying atomic data, the intensities of lines arising from states that are not statistically populated (e.g. by cascades into metastable sates or strong dielectronic capture) can be highly inaccurate and would not be suitable for density diagnostics based on line ratios.

Other models start with a database of either relativistic or semi-relativistic configuration-averaged states (e.g. [12]), which can be calculated much more efficiently and permit an extension of the state space to a higher n (typically $n_{max} \sim 8$) and more extensive excitation (for example, multiple excitations from the valence shell or excitation from inner shells). These extensions in state-space completeness improve the performance of these models at both high and low densities, and such models typically produce high-quality CSDs and RPLs over a very wide range of plasma conditions. However, their spectra can be only roughly compared with experimental data, as we have illustrated in Fig. 1.3. While the spectra could not be used for density diagnostics based on metastable line intensities, they can certainly be used to assess temperature based on the observed charge states. This class of model is discussed further in Chap. 2.

A third class of generally applicable model is based on the screened hydrogenic approach described in Chap. 3 (e.g. FLYCHK [13, 14] and DCA [15]). These models can calculate level structure and rates for arbitrary superconfigurations as needed for the calculation at hand; they do not require pre-existing atomic structure or rate databases. They tend to be orders of magnitude faster than either of the model types

described above, while being also significantly more complete. They tend to provide good-quality CSDs over a wide range of densities but only fair estimates for RPLs, since $\Delta n = 0$ emission for $nl - nl'$ transitions within the superconfigurations has to be added with an ad-hoc representation of the subshell populations. Since the spectra produced from the n-shell state structure of these models bears little resemblance to all but the simplest experimental data, those SHM models that produce spectra generally use external atomic structure data that includes subshell splitting, impose statistical or Boltzmann internal distribution functions to populate subshells within the screened hydrogenic SCs, and are used only for rough estimates of emission or absorption spectra. Although these models are not particularly reliable for plasma diagnostics, they are extremely useful as aids to experimental design, are fast enough to be used inline in radiation-hydrodynamic calculations (see Chap. 4), and are accurate enough to help define the required state space for or bootstrap calculations with more detailed CR models.

A fourth class of general CR model is based on hybrid- structure states. These models attempt to use the highest degree of detail necessary for the desired application, but implement that detail as selectively as possible in order to maintain tractability. One such hybrid-structure model [16] starts with a relatively complete set of highly averaged states and then splits these states on successive iterations of the collisional-radiative solver until convergence is reached in the CSD and RPL. Another model [17] couples a limited fine-structure database of "coronal" states to a more extensive set of configuration-averaged and SHM states. The coronal states ensure good agreement with experimental line positions and intensities at low densities, the configuration-average states provide a reasonable treatment of satellite emission from high-n and multiply excited states, and completeness is ensured by the superconfigurations, which are determined by a bootstrap SHM calculation that dynamically extends the state space until the CSD and RPL converge. A third example of the hybrid-structure approach augments the spectrum from a configuration-average calculation with selected strong fine-structure transitions [18].

These hybrid-structure models can efficiently produce both accurate spectra and reliable CSDs and RPLs. But they are more difficult to design and implement than models with uniform state structure because they require combining data structures that can have a quite disparate properties. Fine-structure states typically have relatively small statistical weights, are well represented by a degenerate element in the population matrix without internal energy structure, and include extensive configuration interaction (CI) that ensures high accuracy in line positions. By contrast, configuration-averaged states are typically calculated with only limited CI and can have much larger statistical weights with implicit internal energy structure. Often, the internal partition function of configuration-averaged states is well-represented by simple Boltzmann statistics (low-lying metastable states are a significant exception; these must be treated individually in the rate matrix). Finally, superconfiguration states average over even spin-orbit effects, excluding CI entirely, and can have enormous statistical weights. Worse still, superconfigurations can have significant implicit internal structure, with energy splitting similar to the ionization potential

for complex many-electron ions. Combining such disparate state structures without enforcing consistency among them can lead to unphysical results. For example, satellite emission from configuration-averaged levels that do not include extensive CI can easily fall on the wrong side of fine structure lines that do [19]. And assuming statistical populations within extensively averaged states at low densities, where population is highly concentrated in the low-lying implicit levels, can lead to gross inaccuracies in state populations [20].

1.4.3 Self-consistent Field Models for Dense Plasma

Plasmas near solid density ($N_e > 10^{23}$ e/cm^3) tend to emit and absorb radiation in a broad quasi-continuum, with density-broadened lines and strong satellite features that can be reasonably well described by unresolved transition arrays. Pressure ionization of high-n states plays a major role in determining the state space, as the populated valence wavefunctions are distorted by interactions with free electrons and neighboring ions. Precise measurements are difficult to make in the high-energy-density regime due to the short lifetimes and high gradients of laboratory experiments and the opaque material surrounding astrophysical sources that reach these extreme conditions. Thus model development in this regime is often driven by theoretical constraints rather than experimental data. Theoretical validation is enabled by the highly collisional environment that drives populations towards LTE.

One example of models that perform well at the high density extreme are ion sphere models, which solve for the wavefunctions of nl or nlj orbitals in a self-consistent field surrounding a fictitious average atom. The average atom is allowed to have non-integer shell occupations and can respond to dense plasma environments in a physically consistent way. Because continuum lowering is natively included and the average atom is fully described by a small set (tens) of fractionally populated orbitals, strict completeness is easy to achieve with these highly averaged models. They thus provide a rigorous standard for more detailed models in the dense plasma regime, at least in LTE. Fractional shell populations X_n can be computed from detailed models by $X_n = \sum_i X_i N_n$, with X_i the fractional population of the state i and N_n the n-shell occupation in that state, and directly compared with the average-atom shell populations. Any deficit in the detailed model X_n indicates incompleteness in its state structure. However, average atom models tend to produce very poor spectra, since specific configurations are required to produce distinct transitions. And moving average-atom models comfortably into the non-LTE collisional-radiative regime is difficult [21], since they lack the basic structure of distinct doubly excited states through which the critical dielectronic recombination process occurs.

While the average-atom approach has significant drawbacks, the self-consistent field approach itself provides a strong foundation for collisional-radiative modeling in the high-density regime. A highly successful class of models uses expansions of average-atom wavefunctions to form configurations with integer occupations that

are amenable to standard collisional-radiative modeling treatments. Unlike models based on isolated-ion data, which impose ad hoc external treatments to account for continuum lowering and pressure ionization effects, these self-consistent field models include density effects in a native and self-consistent way. The two major drawbacks to most models of this type are the general lack of extensive configuration interaction and the computational overhead required to generate the state space and rate coefficients from scratch for each specific set of plasma conditions. However, the ability to generate new states can facilitate novel approaches to CR modeling: one appealing approach starts with a state space consisting of a single configuration, then computes final states and rate-based probabilities for all one- and two-electron processes out of that configuration. A Monte Carlo algorithm takes a random walk through the state space, constructing the state space and state populations simultaneously and requiring much less memory than a fixed-state-space model of equivalent size [2]. Another approach uses expansions of average atom orbitals to determine the required state space for particular conditions and then refines the atomic structure to produce reliable emission and absorption data [22].

1.5 Conclusions

Balancing the competing requirements of state detail, state-space completeness, and computational tractability is a key challenge in collisional-radiative modeling. An ideal general model that includes both the highly detailed state structure required for accurate spectroscopic predictions and the strictly complete state space required for accurate charge state distributions would be utterly intractable for all but the simplest ions. Designing a reliable and tractable collisional-radiative model requires understanding the consequences of each departure from the ideal and must be informed by the model's intended application. A model intended for inline use in radiative hydrodynamics codes, where speed and validity over a wide range of conditions are essential, will have a very different character than a model intended for spectroscopic analysis of high-resolution data, where highly accurate state structure and populations are required. This Chapter has explored the impact of limiting state-space completeness and detail on model reliability and has described a variety of model design approaches for diverse applications.

Acknowledgments Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. This work was supported by the U.S. Department of Energy, Office of Science Early Career Research Program, Office of Fusion Energy Sciences under FWP-14-017426.

References

1. D.A. Libermann, J.R. Albritton, J. Quant. Spectr. Rad. Transfer **51**, 197 (1994)
2. B.G. Wilson, J.R. Albritton, D.A. Libermann, preprint UCRL-JC-104252 (1990)
3. O. Ciricosta, S.M. Vinko, H.-K. Chung, B.-I. Cho, C.R.D. Brown, T. Burian, J. Chalupsky, K. Engelhorn, R.W. Falcone, C. Graves, V. Hajkova, A. Higginbotham, L. Juha, J. Krzywinski, H.J. Lee, M. Messerschmidt, C.D. Murphy, Y. Ping, D.S. Rackstraw, A. Scherz, W. Schlotter, S. Toleikis, J.J. Turner, L. Vysin, T. Wang, B. Wu, U. Zastrau, D. Zhu, R.W. Lee, P. Heimann, B. Nagler, J.S. Wark, Phys. Rev. Lett. **109**, 065002 (2012)
4. H.-K. Chung, C. Bowen, C.J. Fontes, S.B. Hansen, Y. Ralchenko, High En. Dens. Phys. **9**, 645 (2013)
5. P. Mazzotta, G. Mazzitelli, S. Colafrancesco, N. Vittorio, Astron. Astrophys. Suppl. Series **133**, 403 (1998)
6. A. Derevianko, W.R. Johnson, Phys. Rev. A **56**, 1288 (1997)
7. D.A. Liberman, J.R. Albritton, B.G. Wilson, W.E. Alley, Phys. Rev. A **50**, 171 (1994)
8. M.F. Gu, Astrophys. J. **582**, 1241 (2003)
9. A. Bar-Shalom, J. Oreg, W.H. Goldstein, Phys. Rev. A **40**, 3183 (1989)
10. C.A. Iglesias, High En. Dens. Phys. **8**, 253 (2012)
11. S. Mazevet, J. Abdallah Jr., J. Phys. B **39**, 3419 (2006)
12. C.J. Fontes, H.L. Zhang, J. Abdallah Jr., R.E.H. Clark, D.P. Kilcrease, J. Colgan, R.T. Cunningham, P. Hakel, N.H. Magee, M.E. Sherrill, J. Phys. B, (in press) (2015)
13. H.-K. Chung, M.H. Chen, W.L. Morgan, Y. Ralchenko, R.W. Lee, High En. Dens. Phys. **1**, 3 (2005)
14. H.-K. Chung, M.H. Chen, R.W. Lee, High En. Dens. Phys. **3**, 57 (2007)
15. H.A. Scott, S.B. Hansen, High En. Dens. Phys. **6**, 39 (2010)
16. O. Peyrusse, J. Phys. B **33**, 4303 (2000)
17. S.B. Hansen, J. Bauche, C. Bauche-Arnoult, M.F. Gu, High En. Dens. Phys. **3**, 109 (2007)
18. Q. Porcherot, J.-C. Pain, F. Gilleron, T. Blenski, High En. Dens. Phys. **7**, 234 (2011)
19. S.B. Hansen, Can. J. Phys. **89**, 633 (2011)
20. S.B. Hansen, J. Bauche, C. Bauche-Arnoult, High En. Dens. Phys. **7**, 27 (2011)
21. G. Faussurier, C. Blancard, E. Berthier, Phys. Rev. E **63**, 026401 (2001)
22. M. Jeffery, L.M. Upcraft, J.W.O. Harris, D.J. Hoarty, High En. Dens. Phys. **9**, 642 (2011)

http://www.springer.com/978-3-319-27512-3

Modern Methods in Collisional-Radiative Modeling of Plasmas

Ralchenko, Y. (Ed.)
2016, X, 212 p. 76 illus., 52 illus. in color., Hardcover
ISBN: 978-3-319-27512-3