How Do Type Ia Supernova Nebular Spectra Depend on Explosion Properties? Insights from Systematic Non-LTE Modeling

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Abstract

We present a radiative transfer code to model the nebular phase spectra of supernovae (SNe) in non-LTE (NLTE). We apply it to a systematic study of SNe Ia using parameterized 1D models and show how nebular spectral features depend on key physical parameters, such as the time since explosion, total ejecta mass, kinetic energy, radial density profile, and the masses of $^{56}$Ni, intermediate-mass elements, and stable iron-group elements. We also quantify the impact of uncertainties in atomic data inputs. We find the following. (1) The main features of SN Ia nebular spectra are relatively insensitive to most physical parameters. Degeneracy among parameters precludes a unique determination of the ejecta properties from spectral fitting. In particular, features can be equally well fit with generic Chandrasekhar mass ($M_{\text{Ch}}$), sub-$M_{\text{Ch}}$, and super-$M_{\text{Ch}}$ models. (2) A sizable ($\gtrsim 0.1 M_\odot$) central region of stable iron-group elements, often claimed as evidence for $M_{\text{Ch}}$ models, is not essential to fit the optical spectra and may produce an unusual flat-top [Co III] profile. (3) The strength of [S III] emission near 9500 Å can provide a useful diagnostic of explosion nucleosynthesis. (4) Substantial amounts ($\gtrsim 0.1 M_\odot$) of unburned C/O mixed throughout the ejecta produce [O III] emission not seen in observations. (5) Shifts in the wavelength of line peaks can arise from line-blending effects. (6) The steepness of the ejecta density profile affects the line shapes, offering a constraint on explosion models. (7) Uncertainties in atomic data limit the ability to infer physical parameters.

Key words: line: formation – radiation mechanisms: nonthermal – radiative transfer – supernovae: general

1. Introduction

Spectra taken of supernovae (SNe) at late times (in the nebular phase, $\gtrsim 100$ days after explosion) probe the central regions of the ejecta and thus contain a wealth of information about the explosion, such as nucleosynthetic yields, compositional mixing, and geometry. The quantity and breadth of nebular spectra have grown rapidly in recent years owing to international observational efforts. However, further modeling is needed to develop a systematic understanding of how nebular spectra depend on explosion parameters and how atomic data inputs affect spectral modeling.

Nebular spectra can be used to study the uncertain progenitors of Type Ia SNe (SNe Ia; Sollerman et al. 2004; Maeda et al. 2010b; Mazzali et al. 2011, 2015; Mazzali & Hachinger 2012). While SNe Ia are thought to be the result of the explosion of carbon–oxygen white dwarfs (C/O WDs) in a binary system (Hoyle & Fowler 1960), their progenitor systems and explosion mechanisms are still unknown. Despite the success of the empirical width–luminosity relation (Phillips 1993) to calibrate luminosities of SNe Ia, systematic variation due to intrinsic SN Ia diversity is an ongoing challenge for precision cosmology (Howell 2011).

Several candidates for the progenitors of “normal” SNe Ia have been proposed (see Branch et al. 1993; Wang & Han 2012; Maoz et al. 2014, and references therein). In the single-degenerate $M_{\text{Ch}}$ model, the WD gains mass from a nondegenerate binary companion (Whelan & Iben 1973) and ignited carbon burning when the mass approaches $M_{\text{Ch}} \approx 1.4 M_\odot$. In the double-detonation model, a layer of helium gas from a binary companion detonates above the primary C/O WD, causing the WD to detonate at a mass $\leq M_{\text{Ch}}$ (Livne 1990; Woosley & Weaver 1994; Fink et al. 2007; Guillochon et al. 2010; Shen & Bildsten 2014). In the double-degenerate model, two WDs coalesce or collide and may detonate violently on impact or subsequent to the merger (Iben & Tutukov 1984; Webbink 1984; Benz et al. 1989; Raskin et al. 2009; Rosswog et al. 2009; Pakmor et al. 2012; Kushnir et al. 2013; Moll et al. 2014; Kashyap et al. 2015). It may be that SNe Ia come from, if not all, of these progenitor channels. A main goal of spectral modeling is to help understand the origin of different events.

Nebular spectra reveal emission throughout the entire ejecta and so are a valuable probe of density and compositional structure. If the ejecta mass, kinetic energy, and or compositional yields can be determined, these can differentiate explosion scenarios. For example, it is thought that $M_{\text{Ch}}$ models produce more stable iron-group elements (IGEs) (such as $^{58}$Ni and $^{54}$Fe) than sub-$M_{\text{Ch}}$ mass models, due to burning at higher central densities (Iwamoto et al. 1999). Nebular line profiles are also sensitive to global asymmetries and therefore offer a way to study the imprints of the explosion mechanism on ejecta geometry.

Initial work by Axelrod (1980) enabled a number of codes used to model the nebular spectra of SNe (Ruiz-Lapuente & Lucy 1992; Liu et al. 1997; Kozma & Fransson 1998a, 1998b). Updated codes use improved atomic data and incorporate more sophisticated radiative transport and nonthermal deposition physics (Sollerman et al. 2000, 2004; Mazzali et al. 2001, 2007a; Kozma et al. 2005; Maeda et al. 2006; Maurer et al. 2010; Dessart & Hillier 2011; Jerkstrand et al. 2011; Li et al. 2012). Despite the publication of numerous 3D hydrodynamic simulations of SNe Ia (e.g., Hillebrandt et al. 2013), few such explosion models have been analyzed in the nebular phase (but see Kozma et al. 2005). Furthermore, previous nebular modeling work has focused on interpreting events individually.
The aim of this work is to systematically study how variations in explosion properties, density and abundance structure, and atomic data inputs affect the spectra of SNe Ia at late times. To that end, we present a new non-LTE (NLTE) code to model the nebular spectra of SNe. In Section 2, we present our method of calculating level populations, nonthermal deposition, temperature and ionization balance, and nebular spectra. In Section 3, we use a fiducial model to describe the physics of nebular spectral formation in SNe Ia. We then vary the parameters of the model to probe the sensitivity of the spectra to ejecta mass, composition, and kinetic energy (Sections 4.1–4.6), as well as density profile (Section 4.7) and atomic data inputs (Section 4.8).

2. Methods

We have developed a new 3D radiative transfer tool to model nebular spectra of SNe. Given an initial ejecta model, the code calculates the emissivity of each atomic transition by solving for the temperature, ionization state, and NLTE atomic level populations, including nonthermal effects from radioactive decay products, and generates spectra by integrating the radiative transfer equation in a moving medium.

2.1. Basic Assumptions

The underlying SN ejecta model is specified by the mass density and elemental abundances in each zone on a 3D Cartesian grid. We assume that the ejecta are in homologous expansion (i.e., velocity proportional to radius), which is appropriate for SNe Ia at a few seconds to days after explosion (e.g., Röpke 2005). The structure of a homologous model at one epoch can be easily scaled to any other time, taking into account compositional changes due to radioactive decay. The models in this paper study SNe Ia out to 400 days and include the following species: C, O, Si, S, Ca, Fe, Co, and Ni (see Appendix A for a description of atomic data sources).

Our calculations assume stationarity—i.e., that the gas temperature and level populations reach equilibrium on a timescale short compared to the ejecta expansion timescale. This assumption is reasonable except at rather late times (≥500 days), when thermal and ionization freeze-out may become important (Fransson & Kozma 1993; Kozma & Fransson 1998a; Sollerman et al. 2004; Fransson & Jerkstrand 2015).

Our transport solver assumes that the ejecta are optically thin to radiation. For many SNe, this is true in the optical and infrared regions at times ≥100 days. However, at blue and ultraviolet wavelengths (≤4000 Å), the ejecta may remain opaque to iron-group lines for hundreds of days (Friesen et al. 2017). This limits the reliability of our nebular models at short wavelengths and may affect the calculated ionization fractions (e.g., Sollerman et al. 2004), issues that will be addressed in the future by incorporating a more general transport solver.

2.2. Non-LTE Level Populations

To calculate spectral emission from the SN nebula, one has to determine the level populations of each ion in the gas. Since LTE is a poor approximation at these epochs, we solve for each species the set of NLTE equations expressing statistical equilibrium

\[ \mathbf{M} \mathbf{n} = 0, \]

where \( \mathbf{n} \) is a vector of level populations for the species and the matrix \( \mathbf{M} \) encodes the transition rates between the various levels and ionization states (see, e.g., Li & McCray 1993). To the set of equations must be added the constraint of number conservation.

A generalized form for the statistical equilibrium rate equations is

\[ n_i \left( R_{ij} + \sum_{j=1}^{n_{\text{species}}} \sum_{k=1}^{n_i} E_{kj} \right) = \sum_{k=1}^{n_i} n_k E_{ki} + n_{i+1,\text{g}} n_e \alpha_i, \]

where \( n_i \) is the level population of the \( i \)th level of the ion with \( i \)th ionization state, \( n_e \) is the electron density, \( R_{ij} \) is the total ionization rate from the \( i \)th to the \( j \)th ionization state (including photoionization, collisional ionization, and nonthermal ionization), and \( \alpha_i \) (\( T \)) is the total recombination coefficient from ionization state \( j \)'s ground state to the \( i \)th level (including radiative, dielectronic, and three-body recombination). \( E \) are bound–bound rate coefficients between levels \( i \) and \( j \), including spontaneous emission, stimulated absorption/emission, and collisional excitation/de-excitation.

The microphysics relevant to the nebular phase calculation is encoded into the transition matrix of Equation (1). For the SN Ia problem, we treat collisional (“electron-impact”) bound–bound and bound–free processes, radiative and dielectronic recombination, and nonthermal deposition of \(^{56}\text{Co}\) energy into heating, excitation, and ionization channels. Following Nahar & Pradhan (1997), we assume that all collisional ionization rates are ground-state rates and that radiative recombinations come from the ground state. Details of the implementation of these processes are given in Appendix C.

2.3. Nonthermal Effects

Energy deposition due to the radioactive decay chain \(^{56}\text{Ni} \rightarrow ^{56}\text{Co} \rightarrow ^{56}\text{Fe}\) is the dominant energy source for SNe Ia in the nebular phase (Colgate & McKee 1969; Kuchner et al. 1994). Since \(^{56}\text{Ni}\) decays on a timescale of \( \tau_{\text{SN}} = 7.7 \) days, its contribution to heating is minor by nebular times, while \(^{56}\text{Co}\) decay (\( \tau_{\text{SN}} = 111.3 \) days) is generally the most important source of radioactive energy. Other radioactive isotopes with half-lives in the nebular range (e.g., \(^{22}\text{Na}\), \(^{35}\text{S}\), \(^{45}\text{Ca}\), \(^{46}\text{Sc}\), \(^{49}\text{V}\), \(^{54}\text{Mn}\), \(^{53}\text{Fe}\), \(^{57}\text{Co}\), \(^{58}\text{Co}\), \(^{63}\text{Zn}\), and \(^{68}\text{Ge}\)) are usually not produced in enough abundance to significantly contribute to heating at the epochs we consider here (Iwamoto et al. 1999; Seitenzahl et al. 2013) and are not included in the present calculations.

We determine the radioactive energy deposition rate in each zone using a 3D Monte Carlo radiation transport scheme (Kasen et al. 2006) that samples gamma-ray wavelengths from the radioactive decay lines and treats energy losses due to Compton scattering and photoionization. Positrons from \(^{56}\text{Co}\) decay are assumed to be trapped locally, in accordance with
recent observations of SNe Ia at late times (Leloudas et al. 2009; Kerzendorf et al. 2014; but see Dimitriadis et al. 2017).

The gamma rays from $^{56}$Co decay produce high-energy electrons ($E_0 \sim 1$ MeV) that interact with the ejecta through heating (Coulomb interactions), ionization, and excitation. These interactions affect the temperature and ionization state of the gas. The rates of excitation and ionization, respectively, by nonthermal electrons/positrons are given by

$$R_{\text{ex}} = \frac{\epsilon_{\text{rad}} \eta_{ij}}{\Delta E_{ij} n_l},$$

$$R_{\text{ion}} = \frac{\epsilon_{\text{rad}} \eta_{ik}}{I_k n_k},$$

where the transition from level $i$ to level $j$ (with $j > i$) has energy $\Delta E_{ij}$, $n_l$ is the level population of the atomic level, $I_k$ is the ionization potential of the ion indexed by $k$ having number density $n_k$, $\epsilon_{\text{rad}}$ is the reactive energy deposition rate per unit volume, and $\eta_{ij}$ and $\eta_{ik}$ refer to the nonthermal excitation and ionization deposition fractions, respectively, described in Appendix B.

### 2.4. Temperature and Ionization Balance

We use an iterative nonlinear solver to determine the free electron density and temperature in each zone. The electron density is constrained by the charge conservation condition that all free electrons come from ionization, i.e.,

$$n_e = \sum_{k,i} n_{k,i},$$

where $n_{k,i}$ represents the population of the $i$th ionization stage of the $k$th species ($i = 0$ is neutral). Given that the nonthermal deposition fractions ($\eta_{ij}$ and $\eta_{ik}$ in Equations (3)–(4)) are level population dependent, we recalculate them during each iterative step until convergence is reached.

The temperature of each zone is calculated from the balance of heating from radioactive decay and cooling due to line emission. The line emissivity (units erg s$^{-1}$ cm$^{-3}$) from a transition between the $i$th and $j$th levels of an ion ($E_j > E_i$) is

$$\dot{\nu}_j(T) = h\nu_A n_j,$$

where $\nu_j$ is the photon frequency of the transition, $A_j$ is the spontaneous radiative decay rate (Einstein A coefficient), and $n_j$ is the population of the $j$th level of the ion. The temperature sensitivity of $\dot{\nu}_j$ arises primarily from the temperature-dependent collisional excitation rates, which are important in setting the populations $n_j$ for low-lying states.

The total emissivity per unit volume is then a sum over all line transitions, which, in equilibrium, is equal to the energy deposition by radioactivity

$$\sum_{ij} \dot{\nu}_j = \dot{\nu}_{\text{rad}},$$

where $\{i, j\}$ runs over all transitions. Note that Equation (7) represents a balance of all emission and deposition processes, not just the thermal processes.

We use an iterative Brent–Dekker method to solve the nonlinear Equations (5) and (7) for the temperature and electron density in each zone. For each iteration, we solve the NLTE rate equations to determine the ionization/excitation state and emissivity. The values of $T$ and $n_e$ are then adjusted and the procedure iterated until thermal and ionization equilibrium is reached. A single zone typically converges within 200–400 iterative steps to reach an accuracy of 0.1% in temperature.

### 2.5. Spectrum Calculation

Once the line emissivities (Equation (6)) are known for all transitions in a converged model, we can integrate the emission for any arbitrary geometry to determine the nebular spectrum of the SN. Assuming homologous expansion ($r = vt$) and choosing the direction to the observer to be the z-axis, the nonrelativistic Doppler effect along the line of sight is

$$\lambda_{\text{obs}} = \lambda_j \left(1 - \frac{z}{ct}\right),$$

where $\lambda_{\text{obs}}$ is the observed wavelength of a line transition with rest-frame wavelength $\lambda_j$. Equation (8) allows us to associate the observed flux at wavelength $\lambda_{\text{obs}}$ with the line emission integrated over a specific plane (perpendicular to the z-axis) sliced through the ejecta. For isolated transitions, this mapping can be used to constrain the geometrical distribution of material along the line of sight (see, e.g., Shivvers et al. 2013). Since the bulk of the emission typically comes from ejecta with velocities $\lesssim 10,000$ km s$^{-1}$, using the nonrelativistic Doppler shift leads to errors in $z$-mapping of only $\lesssim 3\%$.

Assuming that the ejecta are optically thin, the observed specific intensity can be expressed as the integral

$$L_\lambda(\lambda) d\lambda = \left[\sum_{i,j} \int_{\omega} \dot{\nu}_j(x, y, z) dxdy\right] d\lambda,$$

where the sum $\{i, j\}$ runs over all possible transitions and the integration is over the $x$–$y$ plane at location $z = ct (\lambda_j - \lambda)/\lambda_j$. The spectral flux observed at Earth is simply $F_\lambda = L_\lambda/(4\pi D^2)$, where $D$ is the distance to the source.

### 2.6. Physical Processes Neglected

Dust formation might be possible in SNe Ia at late times, but not necessarily in significant amounts (Nozawa et al. 2011). Further, observations of the nearby SN 2011fe show no evidence for dust formation at 930 days past maximum (Kerzendorf et al. 2014). We therefore neglect dust formation and plan on implementing it for future work.

While implementing photoionization and stimulated radiative processes in our code, we neglect them for the work published in this paper under the assumption that there is negligible continuum radiation field.

Charge transfer (CT) is expected to occur in SNe between neutral atoms and ions (Swartz 1994). While CT might affect ionization fractions of SNe Ia at later times, we tested CT between ions of Fe and found that their effect on the nebular spectrum at 200–400 days is negligible. This is because the nebula is primarily ionized gas, and therefore the rate of ionization/recombination due to CT is subdominant. Since CT preferentially ionizes neutral atoms (as Coulomb repulsion suppresses ion–ion interactions), we expect that neutral atoms like O I and Fe I should not contribute much to nebular emission. We plan to add a detailed CT treatment to the code in the near future in order to quantify this effect.
2.7. Code Verification

We ran a number of tests to verify the code. We tested the NLTE level population solver in the limit that collisional processes dominate and the limit that the radiation field is the Planck function, both resulting in the expected LTE level populations. We also tested the ionization solution in the collisional ionization equilibrium (CIE) regime and found good agreement with previous results (e.g., Sutherland & Dopita 1993). We further compared total CIE cooling functions for individual ions to published results from the Cloudy code (Gnat & Ferland 2012). Given disparities in the atomic data inputs, exact agreement of the cooling functions is not expected, but we found reasonably similar values and temperature dependences in the regimes of interest. The radiation transport calculation of synthetic spectra was verified by comparing single line profiles to analytic solutions.

3. Modeling Type Ia Nebular Spectra

To study the nebular spectra of SNe Ia, we construct spherically symmetric models in which the ejecta properties (e.g., total mass, energy, and abundances) are free parameters. We first describe the general properties of spectrum formation in a “fiducial” model that resembles the ejecta structure expected for normal SNe Ia. In Section 4 we carry out a parameter survey that demonstrates how the nebular spectra depend on explosion properties.

3.1. Ejecta Modeling

We model the ejecta with a broken power-law density profile that is shallow in the core and steep in the outer layers (Chevalier & Soker 1989; Kasen 2010):

\[
\rho(v) = \begin{cases} 
\rho_0 \left( \frac{v}{v_1} \right)^{-\delta} & v \leq v_1 \\
\rho_0 \left( \frac{v}{v_1} \right)^{-n} & v > v_1 
\end{cases},
\]

where \(\rho_0\) can be interpreted as the central density of a perfectly flat core profile (\(\delta = 0\)) and \(v_1\) is the transition velocity marking the interface of the two regions. Integration gives (assuming \(\delta < 3 \text{ and } n > 3\))

\[
\rho_0 = \frac{M_{ej}}{4\pi (v_1 t_{ex})^3} \left[ \frac{1}{3 - \delta} + \frac{1}{n - 3} \right]^{-1},
\]

\[
E_K = \frac{1}{2} M_{ej} v_1^2 \left[ \frac{1}{5 - \delta} + \frac{1}{n - 5} \left[ \frac{1}{3 - \delta} + \frac{1}{n - 3} \right]^{-1} \right],
\]

where \(M_{ej}\) is the total ejecta mass, \(E_K\) is the ejecta kinetic energy, and \(t_{ex}\) is the time since explosion. The radial density profile is thus completely set by the choice of \(M_{ej}, E_K, \) and the exponents \(\delta, n.\) In our calculations, we cut off the model at a radius that encompasses 99% of the total ejecta.

We find that the values \(\delta = 0, \ n = 10\) give reasonable fits to the nebular spectra of SNe Ia and so use these values for our fiducial model. In this case, the characteristic velocity and density scales are

\[
v_1 = 10,943 E_{51}^{1/2} M_{1}^{-1/2} \ \text{km s}^{-1},
\]

\[
\rho_0 = 4.90 \times 10^{-17} E_{51}^{-3/2} M_{1}^{5/2} t_{200}^{-3} \ \text{g cm}^{-3},
\]

where \(M_1 = M_{ej}/M_\odot\), \(E_{51}\) is the kinetic energy in units of \(10^{51}\) erg, and \(t_{200}\) is the time since explosion scaled to 200 days. We explore using different power-law exponents, as well as an exponential density profile, in Section 4.7.

The compositional structure of the ejecta models is assumed to be stratified into three distinct zones (Woosley et al. 2007). The center of the ejecta is assumed to consist of stable IGEs of mass \(M_{IGE}\). The stable IGEs are assumed to be composed of a ratio, \(R_{stb}\), of \(^{56}\text{Fe} / ^{56}\text{Ni}\). Surrounding the stable IGE region is a zone consisting (initially) mostly of \(^{56}\text{Ni}\) of mass \(M_{56Ni}\). We include a small amount of stable IGEs in this region with mass abundance \(X_{stb}\) and the same isotopic ratio \(R_{stb}\). Above the \(^{56}\text{Ni}\) is an outer layer of intermediate-mass elements (IMEs) of mass \(M_{IME}\). We compose the IME layer of 70% \(^{28}\text{Si}\), 29% \(^{32}\text{S}\), and 1% \(^{40}\text{Ca}\), roughly consistent with the nucleosynthetic results in the SN Ia explosion models of Plewa (2007) and Seitenzahl et al. (2013). We study the presence of unburned C/O mixed into the nickel zone and IME layer in Section 4.6. The parameters describing the masses of the elements are constrained to add to the total ejecta mass.

The total radioactive energy deposition rate (and hence bolometric luminosity) of a model depends not only on \(M_{56Ni}\) but also on the efficiency of the trapping of radioactive decay products. Since the ejecta are largely transparent to gamma rays at nebular phases, the gamma-ray trapping fraction is \(f_{\gamma,c} = 1 - e^{-\gamma_c} \approx \tau_c\), where \(\tau_c\) is the mean optical depth to gamma rays. Taking a typical gamma-ray opacity \(\kappa_{\gamma} \approx 0.03 \text{ cm}^2 \text{ g}^{-1}\) (Swartz et al. 1995) and integrating the radial optical depth from the center \((r = 0)\) gives an estimate

\[
f_{\gamma,c} \approx 0.025 E_{51}^{-1} M_1^2 t_{200}^{-2} \]

Equation (15) presumably overestimates the gamma-ray trapping fraction (since \(\tau_c\) is evaluated at \(r = 0\)), but the scaling of \(f_{\gamma,c}\) with \(M_0, E_K, \) and \(r\) will be useful for interpreting how the radioactive deposition rate depends on physical parameters.

3.2. Fiducial Model

To describe the basic features of nebular spectrum formation, we present first a fiducial model with parameters (given in Table 1) typical of standard SN Ia explosion models, i.e., \(M_{ej}\) near the Chandrasekhar mass and \(M_{56Ni} = 0.6 M_\odot\). The fiducial model has a transition velocity of 10,131 km s\(^{-1}\), while the
interface between the nickel zone and IME layer is near 8800 km s⁻¹.

Figure 1 shows our calculation of the synthetic nebular spectrum of the fiducial model at 200 days after explosion. We compare to the observed spectrum of the well-studied nearby SN Ia SN 2011fe (Nugent et al. 2011; Shappee et al. 2013; Mazzali et al. 2015). The model spectrum reproduces most of the prominent features.

Figure 2 shows a breakdown of the contribution from various ions to the fiducial model spectrum. The strongest features are due to forbidden transitions of Fe II and Fe III that are collisionally excited in the nickel zone. Emission due to IME lines is also visible at redder wavelengths. Most of the important individual line transitions are listed in Table 2.

The spectrum in the nebular phase forms primarily from the collisional excitation of ions by thermal electrons, followed by spontaneous de-excitation via the emission of a line photon. Given the relatively low ejecta temperatures, electrons can only excite low-lying atomic levels, among which radiative transitions are typically electron dipole forbidden (see Table 2). Nevertheless, the rate of collisional de-excitations is generally so small in the low-density nebula that essentially every collisional excitation eventually leads to radiative emission through a forbidden line.

The temperature of the ejecta is determined by the balance of radioactive heating and cooling by line emission. Figure 3 shows the radioactive heating rate and temperature for the fiducial model. The interior ejecta density profile is flat in this model, and so the ejecta temperature is nearly constant at T ≈ 9000 K in the inner layers. Above the radioactive nickel zone, the temperature drops, due to the declining heating rate, but increases again in the very low density outermost layers, due to the inability of the ejecta to cool efficiently.

The important emission lines appearing in the nebular spectra depend on the composition and ionization state of the ejecta. In SNe Ia, ionization is primarily caused by the nonthermal electrons produced by radioactive decay (the collisional ionization rate from thermal electrons is subdominant), which is balanced by radiative recombination. Figure 3 shows the radial dependence of the ionization fractions of iron for the fiducial model. Though Fe IV and Fe V are the most abundant ions, they lack low-lying levels that are able to be excited by the thermal electrons. Thus, the most prominent lines are due to Fe III and Fe II.

As a comparison, we also run a model with the same parameters as the fiducial model but with an exponential density profile similar to the commonly used W7 model (Nomoto et al. 1984; Thielemann et al. 1986). Specifically, we use \( \rho_0 e^{-r/v}\), where \( \rho_0 \) and \( v \) are set by total ejecta mass, kinetic energy, and time since explosion. We show the calculated ejecta properties in Figure 4. Higher central density in this model results in higher gamma-ray deposition overall. In general, the degree of ionization increases as the density declines at higher velocities, reflecting the reduced rate of radiative recombination. For the same reason, the overall ionization state of iron is lower in the W7-like model, due to
higher overall densities. See Section 4.7 for synthetic spectra of this model and a systematic study of density profiles.

As a more comprehensive description of SN Ia nebular spectra, we discuss the features appearing in each key wavelength region seen in Figure 1:

- **3500–4500 Å**: This region contains emission from \([\text{S II}]\) and \([\text{Fe II}]\) transitions. Similar to other studies (e.g., Mazzali et al. 2015; Friesen et al. 2017), our model fails to reproduce all of the observed features, which could be a result of ions missing in the model, uncertainties or incompleteness of the atomic line data, or the neglect of optical depth effects that may produce a pseudo-continuum at the bluest wavelengths. There is some evidence that \([\text{Fe II}]\) emission at 4400 Å contributes to this feature in SN 2011fe (Friesen et al. 2017).

- **4500–5500 Å**: This region is dominated by emission from \([\text{Fe III}]\), which produces prominent features at 4658 and 5270 Å. The latter feature also includes a significant contribution from \([\text{Fe II}]\) \(\lambda 5159\); therefore, the ratio of these two lines is a diagnostic of the ionization state of the gas. The small emission line appearing between the two strong lines is due to \([\text{Fe III}]\) \(\lambda 5011\) and can be washed out if the ejecta velocities are too high.

- **5500–7000 Å**: The feature in this region is a blend of multiple \([\text{Fe II}]\) lines and a broad \([\text{Ca II}]\) line. In addition, \([\text{Ni II}]\) emission can contribute if sufficient stable \(^{58}\text{Ni}\) is present in the gas, but for our fiducial model \([\text{Ni II}]\) does not dominate this feature.

- **7000–7700 Å**: The feature in this region is a blend of multiple \([\text{Fe II}]\) lines and a broad \([\text{Ca II}]\) line. In addition, \([\text{Ni II}]\) emission can contribute if sufficient stable \(^{58}\text{Ni}\) is present in the gas, but for our fiducial model \([\text{Ni II}]\) does not dominate this feature.

**4. Systematic Parameter Study**

We present the following systematic study probing the sensitivity of synthetic nebular spectra to model parameters and
4.1. Time since Explosion

Figure 5 shows the nebular spectrum of the fiducial model at times between 200 and 400 days after explosion. As the SN evolves in time, ejecta densities decline and radioactive isotopes decay. The bolometric luminosity drops with time owing to the declining radioactive heating and a decreasing gamma-ray trapping fraction. The relative strength of prominent Fe lines does not evolve significantly, indicating that the Fe $\text{III}/\text{Fe II}$ ionization ratio remains fairly constant over time. However, as gamma-ray trapping becomes inefficient at late times, the relative strength of IME features to IGE features decreases.

The biggest change in the spectral features over time is the strength of the [Co $\text{III}$] emission at 5888 Å, which decreases as $^{58}\text{Co}$ decays to $^{56}\text{Fe}$. This behavior has been seen in observations (Childress et al. 2015) and exploited to derive explosion properties such as $^{56}\text{Ni}$ mass and total ejecta mass. In addition, the declining gamma-ray deposition in the IME layer results in lowered relative strength of IME features.

4.2. Explosion Kinetic Energy

The amount of kinetic energy ($E_K$) imparted to the ejecta by an SN explosion depends on the nucleosynthetic yields and initial binding energy (Woosley et al. 2007). The typical energy of SNe Ia is around a Bethe ($1\text{B} = 10^{51}\text{erg}$). Various theoretical models have predicted kinetic energies in the range of 0.87–1.6 B (Gamezo et al. 2005; Golombek & Niemeyer 2005; Plewa 2007; Röpke et al. 2007; Röpke & Niemeyer 2007; Jordan et al. 2008, 2012; Bravo et al. 2009).

Figure 6 shows synthetic spectra of the fiducial model with $E_K$ varied between 1 and 2 B. The lower $E_K$ models are more efficient at trapping radioactive energy (due to the higher ejecta density, Equation (14)) and so have higher bolometric luminosities.

Changing $E_K$ has a modest effect on the shape of the spectral features. An increase of $E_K$ from 1 to 1.4 B increases the velocity scale by only 18%, which results in a subtle increase in the line widths (as these widths are also set in part by line blending). A larger change of $E_K$ by a factor of 2 (from 1 to 2 B) does have noticeable effects, causing the Fe $\text{III}/\text{Fe II}$ complex to be so blended that the small central emission near 5000 Å becomes indistinguishable. Observations of this small feature may therefore be a useful diagnostic of the velocity of the nickel zone in SNe Ia.

4.3. Total Ejecta Mass

Theoretical models of SNe Ia predict an ejected mass in the range of 0.8–2.0 $M_\odot$, depending on the progenitor scenario. Approximate light-curve modeling studies have suggested that observed SNe Ia could span this entire range (Stritzinger et al. 2006; Scalzo et al. 2010, 2014a, 2014b).

Figure 7 shows synthetic spectra of the fiducial model with $M_{ej}$ varied between 1 and 2 $M_\odot$. For a fixed kinetic energy, a higher $M_{ej}$ results in higher ejecta densities and lower velocities. As a result, higher-$M_{ej}$ models have greater gamma-ray trapping, a brighter bolometric luminosity, and less Doppler-broadened spectral features. This effect of $M_{ej}$ is therefore somewhat degenerate with that of kinetic energy.

The relative features in the synthetic spectra of Figure 7 show only subtle variations with $M_{ej}$. For our super-$M_{ch}$ case with $M_{ch} = 2.0 M_\odot$, the IME features become visibly stronger as a result of the higher total IME mass. The Fe $\text{III}/\text{Fe II}$ line ratio also decreases due to the increased rate of recombination at higher densities.

While we have studied the effect of varying ejecta mass alone in Figure 7, this parameter is likely correlated with kinetic energy and $^{56}\text{Ni}$ mass (Woosley et al. 2007); for example, a super-$M_{ch}$ explosion is likely to produce more $^{56}\text{Ni}$ and higher kinetic energy. We therefore ran three additional models in which we fixed the ratios $M_{56\text{Ni}}/M_{ej} = 1/2$ and $E_{bol}/M_{ej} = 1.2/1.4$. Based on the above discussion of gamma-ray trapping (Section 3.1), we expect luminosity to approximately scale as $L_{bol} \approx M_{ej}^2$ if these ratios are held constant.

Figure 8 shows synthetic spectra of these scaled models with total ejecta masses of 1.0, 1.4, and 2.0 $M_\odot$. We find that the spectral features are remarkably unchanged despite a substantial variation in the masses. The only major difference is the bolometric luminosity. This indicates that, in a generic sense, the nebular spectra of SNe Ia are consistent with non-$M_{ch}$ models, provided that $E_K$ and $M_{56\text{Ni}}$ scale accordingly.

4.4. Radioactive Nickel Mass

A number of observational studies and theoretical models indicate that the $^{56}\text{Ni}$ masses of normal SNe Ia range from 0.3 to 1.2 $M_\odot$ (Gamezo et al. 2005; Mazzali et al. 2007b; Plewa 2007; Röpke & Niemeyer 2007; Röpke et al. 2007; Jordan et al. 2008, 2012; Bravo et al. 2009; Raskin et al. 2009; Rosswog et al. 2009; Seitenzahl et al. 2011, 2013), with a typical value near 0.6 $M_\odot$ (Branch & Khokhlov 1995).

Figure 9 shows synthetic spectra of the fiducial model with $M_{56\text{Ni}}$ varied between 0.4 and 0.8 $M_\odot$. Naturally, the bolometric luminosity increases proportionally with $M_{56\text{Ni}}$. The line ratios in these spectra are relatively insensitive to $M_{56\text{Ni}}$, with the exception being greater blending around the [Fe $\text{III}$] λ5011 feature in higher $^{56}\text{Ni}$ mass models due to the larger size of the $^{56}\text{Ni}$ core. The decrease in IME emission in higher-$M_{56\text{Ni}}$ models is due to the lower total mass of IMEs in these models by construction (since $M_{56\text{Ni}} + M_{IME}$ is held fixed).

4.5. Neutron-rich IGEs

Stable IGEs are produced in SN Ia ejecta in two distinct ways. The trace presence of neutron-rich isotopes (in particular $^{22}\text{Ne}$) due to the metallicity of the progenitor WD and pre-explosion carbon simmering leads to the production of up to $\approx 25\%$ by mass of neutronized IGEs (in particular $^{56}\text{Fe}$ and $^{58}\text{Ni}$) throughout the nickel core (Timmes et al. 2003; Piro & Bildsten 2008; Martínez-Rodríguez et al. 2016). In addition, electron capture occurring in nuclear burning at high central densities can lead to the production of $\approx 0.05–0.4 M_\odot$ of neutronized IGEs (Nomoto et al. 1984; Thielemann et al. 1986; Seitenzahl et al. 2011, 2013). The latter effect only occurs in white dwarfs with $M_{ej} \gtrsim M_{ch}$ (due to their higher central densities) and is also influenced by the timing of a possible deflagration-to-detonation transition (Seitenzahl et al. 2013). 1D $M_{ch}$ models often predict stable IGEs to be produced at the core (Nomoto et al. 1984; Mazzali et al. 2007b), while...
Table 3
List of Models Included in the Physical Parameter Study

| Model | $v_i$ (km s$^{-1}$) | $n_e$ ($10^{17}$ cm$^{-3}$) | $M_{\text{Fe II}}$ ($M_\odot$) | $M_{\text{Ni II}}$ ($M_\odot$) | $L_{\text{bol}}$ ($10^{40}$ erg s$^{-1}$) | $L_{4665}/L_{5272}$ |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Fiducial | 10,131 | 8.65 | 0.75 | 0.016, 0.016 | 7.96 | 2.30 |
| $t_{\text{ex}} = 250$ days | 10,131 | 4.43 | 0.75 | 0.016, 0.016 | 3.93 | 2.45 |
| $t_{\text{ex}} = 200$ days | 10,131 | 2.56 | 0.75 | 0.016, 0.016 | 2.11 | 2.53 |
| $t_{\text{ex}} = 350$ days | 10,131 | 1.61 | 0.75 | 0.016, 0.016 | 1.19 | 2.54 |
| $t_{\text{ex}} = 400$ days | 10,131 | 1.08 | 0.75 | 0.016, 0.016 | 0.70 | 2.48 |
| $M_3 = 1.0 M_\odot$ | 12,000 | 3.73 | 0.36 | 0.016, 0.016 | 5.27 | 2.75 |
| $M_3 = 1.1 M_\odot$ | 11,442 | 4.73 | 0.46 | 0.016, 0.016 | 5.82 | 2.65 |
| $M_3 = 1.2 M_\odot$ | 10,954 | 5.88 | 0.54 | 0.016, 0.016 | 6.58 | 2.53 |
| $M_3 = 1.3 M_\odot$ | 10,525 | 7.19 | 0.65 | 0.016, 0.016 | 7.18 | 2.41 |
| $M_3 = 2.0 M_\odot$ | 8485 | 21.10 | 1.33 | 0.016, 0.016 | 13.91 | 1.86 |
| $E_K = 1.0$B | 9258 | 11.37 | 0.75 | 0.016, 0.016 | 8.90 | 2.15 |
| $E_K = 1.1$B | 9710 | 9.86 | 0.75 | 0.016, 0.016 | 8.33 | 2.23 |
| $E_K = 1.3$B | 10,556 | 7.67 | 0.75 | 0.016, 0.016 | 7.57 | 2.37 |
| $E_K = 1.4$B | 10,954 | 6.86 | 0.75 | 0.016, 0.016 | 7.22 | 2.44 |
| $E_K = 1.5$B | 11,339 | 6.19 | 0.75 | 0.016, 0.016 | 6.96 | 2.50 |
| $E_K = 2.0$B | 13,093 | 4.02 | 0.75 | 0.016, 0.016 | 5.79 | 2.73 |
| $M_{\text{Ni II}} = 0.4 M_\odot$ | 10,131 | 8.65 | 0.96 | 0.011, 0.011 | 5.49 | 2.25 |
| $M_{\text{Ni II}} = 0.5 M_\odot$ | 10,131 | 8.65 | 0.85 | 0.013, 0.013 | 6.77 | 2.28 |
| $M_{\text{Ni II}} = 0.7 M_\odot$ | 10,131 | 8.65 | 0.64 | 0.019, 0.019 | 9.22 | 2.32 |
| $M_{\text{Ni II}} = 0.8 M_\odot$ | 10,131 | 8.65 | 0.55 | 0.021, 0.021 | 10.21 | 2.33 |
| $M_{\text{Fe II}} = 0.05 M_\odot$ | 10,131 | 8.65 | 0.71 | 0.040, 0.040 | 7.75 | 2.28 |
| $M_{\text{Fe II}} = 0.10 M_\odot$ | 10,131 | 8.65 | 0.64 | 0.066, 0.066 | 7.81 | 2.25 |
| $M_{\text{Fe II}} = 0.15 M_\odot$ | 10,131 | 8.65 | 0.59 | 0.093, 0.093 | 7.64 | 2.21 |
| $M_{\text{Fe II}} = 0.20 M_\odot$ | 10,131 | 8.65 | 0.54 | 0.116, 0.116 | 7.55 | 2.17 |
| $M_{\text{Fe II}} = 1.0$ scaled | 10,240 | 6.15 | 0.46 | 0.013, 0.013 | 5.35 | 2.49 |
| $M_{\text{Fe II}} = 1.4$ scaled | 10,240 | 8.65 | 0.64 | 0.019, 0.019 | 9.21 | 2.32 |
| $M_{\text{Fe II}} = 2.0$ scaled | 10,240 | 12.40 | 0.91 | 0.027, 0.027 | 16.88 | 2.17 |
| $M_{\text{CO}} = 0.05 M_\odot$ | 10,131 | 8.65 | 0.70 | 0.016, 0.016 | 7.85 | 2.25 |
| $M_{\text{CO}} = 0.10 M_\odot$ | 10,131 | 8.65 | 0.64 | 0.017, 0.017 | 8.04 | 2.20 |
| $M_{\text{CO}} = 0.15 M_\odot$ | 10,131 | 8.65 | 0.59 | 0.018, 0.018 | 7.90 | 2.15 |
| $M_{\text{CO}} = 0.20 M_\odot$ | 10,131 | 8.65 | 0.55 | 0.019, 0.019 | 7.82 | 2.09 |
| $M_{\text{CO}} = 0.40 M_\odot$ | 10,131 | 8.65 | 0.53 | 0.023, 0.023 | 7.76 | 1.86 |
| $\delta = 0.5, n = 10^8$ | 10,528 | 66.89 | 0.75 | 0.016, 0.016 | 8.21 | 2.17 |
| $\delta = 1.0, n = 10^9$ | 11,098 | 486.5 | 0.75 | 0.016, 0.016 | 8.95 | 1.88 |
| Exponential | N/A | 106.6 | 0.75 | 0.016, 0.016 | 12.56 | 1.63 |

Notes. The parameter varied from the fiducial value in each model is shown in the model description, and some derived values are shown. $v_i$ is the transition velocity of the density profile determined by power-law exponents $\delta$ and $n$. $n_e$ is the central density. The column for $M_{\text{Fe II,bol}}$ is the sum of neutron-rich core material and stable isotopes mixed into the nickel zone, reported $^{54}$Fe and $^{58}$Ni masses separately. $L_{\text{bol}}$ is the total luminosity over all wavelengths. $L_{4665}/L_{5272}$ is the ratio of luminosities at 4665 and 5272 Å, the wavelengths at which the prominent [Fe II] and [Fe III]/[Fe II] features peak, respectively.

* In these models, we keep the following ratios fixed: $M_{\text{Ni II}}/M_3 = 1/2$ and $E_K/M_3 = 1.2/1.4$. See Section 4.3 for further details.

+ These refer to the power-law exponents in Equation (10). A higher value of $\delta$ produces a steeper density profile.

+ This refers to the exponential density profile explained in Section 4.7.

+ $Q_\text{fe}$ is the collisional (electron-impact) ionization cross section for the ground state of ion $k$.

+ $\sigma_{ij}$ is the thermal collisional (electron-impact) excitation rate for a transition $ij$. 

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multidimensional simulations indicate that buoyancy should mix IGEs throughout the $^{56}$Ni region (Gamezo et al. 2005; Kasen et al. 2009; Seitenzahl et al. 2011). As a result, nebular spectral indicators of stable IGEs would be valuable for inferring the progenitor scenario.

Figure 10 shows synthetic spectra of the fiducial model varying $M_{\text{sh}}$, the mass of a neutron-rich core, between 0.05 and 0.20 $M_\odot$. The stable IGEs are assumed to be an equal mix of $^{54}$Fe and $^{58}$Ni. As expected, the [Ni II] $\lambda$7378 feature becomes apparent with a stable core mass of 0.05 $M_\odot$, which corresponds to 0.025 $M_\odot$ of $^{56}$Ni. [Fe II] $\lambda$7388 emission can also produce a peak near these wavelengths, in some cases dominating the feature, suggesting that [Ni II] may not even be needed to fit this peak (see Section 4.7).

Higher stable core mass also increases the relative fraction of Fe II compared to Fe III, which is a result of lowered nonthermal ionization in the nonradioactive core region. Another noteworthy product of a stable core is the flat-topped profile of the [Co III] $\lambda$5888 feature, produced by the absence of cobalt in the core region. The lower flux in IME features is due to the lower mass of IMEs in higher-$M_{\text{sh}}$ models by construction.

A comparison between two $M_{\text{sh}}$ models and the fiducial model with a W7-like exponential density profile is shown in Figure 11. In the $M_{\text{sh}} = 0.2 M_\odot$ model we find an apparent blueshift of the [Ni II] $\lambda$7378 peak by $\approx 1500$ km s$^{-1}$ due to the relative blending of this line with [Fe II] $\lambda$7155. The feature is also sensitive to [Ca II] emission, which is stronger in the low-$M_{\text{sh}}$ model. The [Fe II] $\lambda$7453 feature redward of [Ni II] $\lambda 7378$ may also dominate in some models, resulting in an apparent redshift of the composite peak (see also Section 4.7). In the exponential model, both peaks are redshifted owing to line blending, which may lead to misinterpretation as ejecta asymmetry.

Maeda et al. (2010a) find shifts in the $\lambda 7378$ peak of up to 3000 km s$^{-1}$, which they interpret as indications of ejecta asymmetry. Our models suggest that this geometrical interpretation is complicated by line blending. Isolating the [Ni II] emission in this feature can be attempted (Maeda et al. 2010b) but is subject to model-dependent uncertainties.

Surprisingly, the mixing of stable nickel through the nickel zone (i.e., varying the parameter $X_{\text{sh}}$ between 0.05 and 0.20) does not produce a visible effect on the synthetic spectrum, even for $^{58}$Ni masses comparable to those in the core stable IGE region of Figure 10. This confirms the findings of Maeda et al. (2010b). This is due to the high level of ionization of Ni in the nickel zone, which suppresses [Ni II] emission. For the same reason, the ratio of $^{56}$Fe to $^{58}$Ni ($R_{\text{sh}}$) in the nickel zone also had no visible effect on the synthetic spectra in the range (0.5–1.5) that we tested. We predict that up to 0.1 $M_\odot$ of stable nickel can be hidden in the ejecta of an SN Ia model with fiducial parameters as a result of this ionization effect.

4.6. Mass of Carbon/Oxygen in Ejecta

Observational studies have estimated that about 30% of SNe Ia show carbon in their early-time spectra (Maoz et al. 2014, and references therein). The nearby SN 2011fe also showed both carbon and oxygen in very early observations (Nugent et al. 2011; Mazzali et al. 2014), and hydrodynamical simulations have predicted various amounts of unburned C/O material mixed throughout the ejecta (Röpke 2005; Pakmor et al. 2012; Seitenzahl et al. 2013; Moll et al. 2014). 3D nebular modeling by Kozma et al. (2005) showed clear [O I] features for a pure deflagration model of Röpke (2005), which contained 0.6 $M_\odot$ of unburned C/O material. There have also been detections of possible [O I] emission in subluminous SNe Ia (Kromer et al. 2013; Taubenberger et al. 2013).

Figure 12 shows synthetic spectra of the fiducial model with C/O mass varied between 0.1 and 0.4 $M_\odot$. We keep a fixed carbon–oxygen ratio of 1:9 and mix C/O into both the nickel zone and IME layer with the same mass fraction, consistent with the expected nucleosynthetic yields of delayed detonation explosions (Seitenzahl et al. 2013).

We find a strong contribution of [O III] at 5007 Å, as well as a weak contribution of [O I] $\lambda 6300/\lambda 6364$ and a blend of [O II] features at 7320 Å. The high ionization state of oxygen prevents the [O I] emission seen in Kozma et al. (2005) from contributing significantly, but we expect that [O I] would become stronger if oxygen were more concentrated in the higher-density central regions, or if the mass of $^{56}$Ni (and hence radioactive deposition) were lower. In addition, our 1D models assume microscopic mixing of the C/O with IGEs; multidimensional models may find that clumps of oxygen isolated...
from $^{56}$Co have lower ionization. C/O within the IME layer does not produce a significant nebular feature.

### 4.7. Sensitivity to Density Profile

The choice of the ejecta density profile is a critical input into nebular modeling. A broken power law with a relatively flat interior was found to approximate the density structure in some 2D delayed detonation models (Kasen 2010), while a steeper exponential profile more closely fits the structure of the commonly used 1D W7 model (Nomoto et al. 1984; Thielemann et al. 1986). For the case of SN 2003hv, Mazzali et al. (2011) found that a core of lowered density provided a better fit to observed nebular spectra than a W7-like density profile. Here, we attempt to illuminate the effect of steepening our interior power-law density profiles. We also consider an exponential profile of the form $\rho = \rho_0 e^{-v/\nu_c}$, where $\rho_0$ and $\nu_c$ can be determined from $M_{\text{ej}}$, $E_K$, and $t_{\text{ex}}$.

Figure 13 shows synthetic spectra of the fiducial model with varied density profiles. Steeper profiles, which concentrate more mass at low velocities, produce stronger and narrower spectral profiles. In particular, an exponential profile helps resolve the individual peaks in the feature around 7300 Å. Figure 11 shows the nebular emission of the exponential model around 7300 Å decomposed into contributions from individual ions. The bluer peak is dominated by [Fe II] $\lambda$7155, while the redder peak is dominated by [Fe II] $\lambda$7388 and [Fe II] $\lambda$7453, with some contribution from [Ni II] $\lambda$7378. [Ca II] $\lambda$7291 adds an offset to the feature. These are consistent with the findings of Ashall et al. (2016) from their W7-like models for SN 1986G. Therefore, [Fe II] can account for the emission in the redder peak if stable Ni is absent, and it could potentially redshift that peak if stable Ni is present. In either case, we find that isolation of [Ni II] $\lambda$7378 emission would be difficult.

Higher gamma-ray trapping due to higher central densities produces higher bolometric luminosities in steeper density profiles. Furthermore, steeper density profiles lead to lower central temperatures, as cooling becomes more efficient at higher densities. Therefore, the ionization state is lower, which changes the main Fe II/Fe III line ratio.

When comparing to the nebular spectrum of SN 2011Fe, we find that a broken power law with a flat interior profile ($\delta = 0$) best reproduces the shape of the features and the main iron line ratios, whereas an exponential density produces lines that are too centrally peaked and overestimates the Fe II/Fe III ratio (indicated by high flux in the [Fe II] feature at 5159 Å). While there is some degeneracy with other parameters, such as kinetic energy, nebular models may be able constrain the interior ejecta density, which should be useful in testing explosion models.

### 4.8. Sensitivity to Atomic Data Uncertainties

One important factor for the modeling of nebular spectra is the extensive atomic data inputs. Uncertainties in published atomic data, discrepancies between different sources for the same data, and the need for crude approximations where data are lacking impact the model predictions. Here we attempt to quantify some of the uncertainties by systematically changing the values of three of the most important and uncertain atomic data—the collisional ionization cross sections ($Q_i$), the thermal collisional excitation rates ($C_{ij}$), and the radiative recombination rates ($\alpha_i$).

We show the impact of systematically varying atomic data in Figures 14–15. To explore the effect of the collisional ionization cross sections (Figure 14), we carried out calculations in which (a) all ionization cross sections were increased by a factor of 2, (b) all ionization cross sections were decreased by a factor of 2, (c) the cross section of Fe II was decreased by a factor of 2 and that of Fe III was increased by a factor of 2, and (d) the cross section of Fe II was increased by a factor of 2 and that of Fe III was decreased by a factor of 2. These variations in $Q_i$ affect the ionization ratio of Fe III/Fe II and can modify the Fe III/Fe II line ratio by up to $\pm 25\%$. There are also indirect effects, since changes to the atomic data of one element can alter the calculated gas temperature and so result in changes in the emission from other species.

To explore the effect of the thermal collisional excitation rates (Figure 15), we carried out calculations in which all $\sigma_{ij}$ were increased or decreased by a factor of 2. These variations in $\sigma_{ij}$ affect the strength of emission features and can modify the Fe III/Fe II line ratio by up to $\pm 10\%$.

We show in Figure 16 the fiducial model calculated using recombination rates from two different databases. Our calculations throughout have used recombination rates from the CHIANTI database, but more recent data for Fe I–V are available from the Nahar OSU Radiative Atomic Database.
(NORAD; Nahar 1996, 1997; Nahar et al. 1997, 1998). With the latter data set, we have access to state-specific recombination rates, which we neglected in the above treatment. We also neglected CT in the above analyses, which becomes important for a nickel zone with low ionization state (as is the case with NORAD recombination rates). We therefore include CT in Fe I–IV with data from Krstic et al. (1997).

While there is reasonable agreement between the synthetic spectra, the strength of emission features does depend on the atomic data set. In particular, the Fe III/Fe II line ratio shows a higher Fe II population when NORAD recombination rates are used, due to higher total recombination rates for Fe I–III in the NORAD data set, leading to a ~30% decrease in Fe III/Fe II line ratio. Similar variations are seen in most other spectral features.

5. Discussion and Conclusion

We have presented a new tool for calculating nebular spectra of SNe and applied it to a systematic parameter study of SNe Ia. We summarize some of our main results as follows:

Robustness and Degeneracy of Spectral Features: On the whole, we found that the features in SN Ia nebular spectra were remarkably insensitive when physical parameters were changed within the range expected for white dwarf explosions. Individually changing the ejected mass, $^{56}$Ni mass, or kinetic energy by 50% produced only minor changes in the relative strength of features (although the bolometric luminosity was affected owing to changes in gamma-ray trapping). Varying parameters by a larger factor of ≈2 began to show noticeable spectral changes.

In addition, we found degeneracies in the effect of different physical parameters. An increase in the total ejecta mass, for example, could be mostly offset by a corresponding increase in kinetic energy so as to keep the overall density and velocity scale roughly fixed. As a result, quite different sets of physical parameters may be able to fit the same nebular spectrum.

Progenitor Mass: Though some previous studies have favored Chandrasekhar mass models in explaining SN Ia nebular spectra, our model survey demonstrates that observed nebular spectra are equally well fit by generic sub-Chandrasekhar mass, Chandrasekhar mass, and super-Chandrasekhar mass models. The spectral features remained essentially unchanged when the total mass, $^{56}$Ni mass, and kinetic energy were scaled up or down in unison (Figure 8). Nebular spectra therefore do not alone constrain the overall mass scale of SNe Ia and instead are more diagnostic of the relative abundance yields and the density profile.

Stable IGEs: Previous studies have fit the nebular spectra of SNe Ia with models having a ~0.1–0.2 $M_\odot$ sphere of stable IGEs at the ejecta center. The presence of such an IGE “core” would favor a Chandrasekhar mass model (where electron capture occurs during high-density deflagration burning), while disfavoring double-detonation and violent merger models.

A stable IGE “core” has been claimed necessary to explain the Fe III/Fe II line ratio in observed spectra (Maeda et al. 2010b; Mazzali et al. 2015). We show that this line ratio also depends on other explosion parameters, such as the density profile and kinetic energy, and is sensitive to the atomic data inputs. We present models that well fit the SN 2011fe iron line ratio without invoking any stable IGE “core.”

Our models that did include a large ($\geq 0.1 M_\odot$) stable IGE “core” produced a flat-topped [Co III] feature near 5900 Å. Such a flat-top [Co III] profile is not seen in the nebular spectra of SN 2011fe (Mazzali et al. 2015), indicating that at least some radioactive cobalt exists at the lowest ejecta velocities. Höflich et al. (2004) and Motohara et al. (2006) observe relatively flat-topped profiles of the 1.64 $\mu$m [Fe II] feature in SN 2003du and SN 2003hv, respectively, which they take as evidence that SNe Ia have a stable IGE “core” lacking any radioactive heating. The lack of an obvious flat-topped optical [Co III] feature in SN 2011fe appears to provide evidence to the contrary.

Another diagnostic of stable IGE is the feature at ~7300 Å usually attributed to [Ni II]. Similar to Mazzali et al. (2015), we find that a small amount (~0.01 $M_\odot$) of central $^{58}$Ni is sufficient to reproduce a peak at 7300 Å. However, we note that in some models the $^{58}$Ni $\lambda\lambda 7388$ and 7453 lines can alone account for this peak, while in general [Fe II] $\lambda\lambda 7155$ and [Ca II] $\lambda\lambda 7291$ emission also shape the overall line profile. The steepness of the inner ejecta density profile also affects how narrow and resolved the separate line peaks of the $\lambda 7300$ feature are. We find that additional $^{58}$Ni mixed throughout the lower-density layers of the radioactive $^{56}$Ni zone may be too
ionized to produce significant [Ni II] \( \lambda 7378 \) emission. As a result, we consider it difficult to derive a precise \(^{56}\)Ni mass constraint from analysis of the \( \lambda 7300 \) feature.

In sum, our parameter study does not provide strong evidence that SNe Ia possess a substantial stable IGE “core,” nor do we see a robust way of accurately inferring the total stable IGE mass from nebular spectrum analysis. We therefore do not consider the nebular spectra of SNe Ia as providing particularly strong support for the Chandrasekhar mass model over other progenitor scenarios. However, our study did not focus on infrared features (Höflich et al. 2004; Motohara et al. 2006; Gerardy et al. 2007; Telesco et al. 2015) or the effects of positron transport (Penney & Höflich 2014). Further study of stable IGE signatures using specific multidimensional explosion models is warranted.

**IME indicators:** While the nebular spectra of SNe Ia are dominated by iron lines, we emphasize that some features provide constraints on IME abundances. In particular, the feature at 7300 Å is sensitive to [Ca II] emission at 7291 Å, while the feature at 9500 Å is dominated by [S III] emission. We showed that the relative strength of the [S III] \( \lambda 9500 \) feature to the [Fe III] \( \lambda 4664 \) feature tracked the relative abundance of IGE to IME (see Figure 9). Analysis of this line ratio may thus provide valuable constraints on the nucleosynthetic yields and hence progenitors of SNe Ia. Our successful fit to the calcium and sulfur features in SN 2011fe suggests that the total IME yields may be as high as \( \approx 0.75 \, M_\odot \). However, we note that material at high velocities does not contribute significantly to nebular emission, so it is not possible to constrain all of the IME mass using nebular modeling.

**Line Shifts and Ejecta Geometry:** Shifts in the wavelength of nebular line peaks are seen in many SNe Ia (Black et al. 2016) and have been used to deduce asymmetries of, e.g., IGEs (Maeda et al. 2010b). Though we have only considered spherically symmetric models in this paper, we nevertheless see shifts in the location of emission peaks due to line blending. For example, the feature around 7300 Å is a blend of [Ni II], [Fe II], and [Ca II] lines. Depending on the ejecta compositional structure and time evolution of line strengths, the location of the composite peak can vary by 1500 km s\(^{-1}\) in different models. This highlights the difficulty in using the \( \lambda 7300 \) feature shift to derive reliable kinematic measures of asymmetry (though see Maeda et al. [2010b] for attempts to separate components in the blend). Our models do not show a strong, progressive redshift evolution in the main IGE features as a function of time. This supports the claim of Black et al. (2016) that these shifts are due to permitted line emission that may help shape the spectrum even at times \( \gtrsim 200 \) days after explosion.

**Carbon/Oxygen Mixing:** We find that C/O material mixed into a nickel zone is highly ionized. For large enough C/O masses (\( \gtrsim 0.1 \, M_\odot \)) this produces a visible [O III] feature at 5007 Å, which is not seen in SN 2011fe. This disfavors models leaving significant amounts of oxygen mixed throughout the ejecta. To produce a narrow [O I] feature like that seen by Taubenberger et al. (2013) in the subluminous SN 2010lp would presumably require the C/O to be located in a dense central region with less nonthermal ionization from radioactivity. C/O in the outermost ejecta layers (within or above the IME zone) does not experience significant radioactive heating and has no impact on the nebular spectra.

**Density Profile:** We have shown that ejecta having a steep interior density profile produce narrower and more central peaked nebular emission features. In fact, the line widths depended more on the density profile than on the kinetic energy, since the former sets the degree of central concentration of mass. Comparing to the spectra of SN 2011fe, we find that a flat density profile (power-law index \( \delta = 0–1 \)) best reproduces the observed spectral profiles. This suggests that nebular spectra may be able to test the density structures predicted by detailed SN Ia explosion models.

**Atomic Data:** Though it is well known that synthetic nebular spectra are affected by uncertainty and incompleteness in the input atomic data, the level of error has not been well quantified. We showed here that factor of 2 errors in some of the key atomic data inputs can result in changes in spectral features at the \( \approx 25\% \) level. This level of variation is similar to the level we found when varying the physical ejecta parameters. Given the uncertainties, we advise against over-interpreting model fits to extract quantitative mass estimates from individual observed SNe Ia. The trends seen among a sample of nebular spectra, however, are likely less affected by the atomic data limitations.
E is the mean energy \( EE \)) = iron-group features. The declining IME mass (a result of keeping \( M_{ej} \) fixed while increasing \( M_{\odot} \)) results in declining IME emission.

**Figure 9.** Same as Figure 5, but for the \( M_{\odot} \) parameter study. Higher nickel mass models have larger nickel cores and so produce slightly wider and more blended iron-group features.

**Limitations:** While the spectral models presented here included a broad range of the most important and complex atomic processes, other physical effects may be relevant and should be addressed in future work. While the ejecta are mostly optically thin at optical wavelengths, there is evidence that some lines are nevertheless optically thick, especially in the ultraviolet (Friesen et al. 2017). Furthermore, dust/molecule absorption and emission may be important at some phases. At very late times, the freezing out of ionization requires that the problem be treated time-dependently (Kozma & Fransson 1998a; Jerkstrand et al. 2015). The collection of a reliable and complete atomic data set has been and remains a substantial challenge for all nebular phase modeling efforts.

Finally, while this paper was restricted to 1D parameterized models, the asphericity found in more realistic explosion models, and inferred from polarization observation of SNe, is expected to affect the nebular spectra. Our NLTE nebular spectrum code is 3D, and future work on SNe Ia and other types of SNe will aim to explore the predictions of 3D hydrodynamical models that have complex abundance distributions, clumping on multiple scales, and global ejecta asymmetries.

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**Appendix A**

**Atomic Data**

We use the atomic data compilation of the CMFGEN code (Hillier & Miller 1998; Li et al. 2012) for radiative transition probabilities (Einstein \( A \)-coefficients), effective collisional strengths \( \Upsilon_{ij} \) (see Appendix C.1 for treatment of missing data), and photoionization cross sections. We take ground-state ionization energies from NIST (Kramida et al. 2016). For thermal collisional ionization rates, we use the results of Voronov (1997). For collisional ionization cross sections, we use Mattioli et al. (2007) and references therein. Radiative and dielectronic recombination rates are taken from the CHIANTI database v.8 (Dere et al. 1997; Del Zanna et al. 2015).

**Appendix B**

**Nonthermal Deposition Fractions**

Radioactive decay of \( ^{56}\text{Co} \) atoms produces a population of high-energy, nonthermal electrons that deposit their energy into the ejecta. The electrons either heat, ionize, or excite the gas, and the fraction of energy going into these three channels has been shown to be insensitive to the initial energy of the electrons (Kozma & Fransson 1992; Li et al. 2012). Due to the similar asymptotic behavior of collisional cross sections and plasma loss function (see below), our treatment is also independent of initial energy of nonthermal electrons. Following the Continuous Slowing Down Approximation formulation of Xu & McCray (1991), we can write the fraction of deposition into heating \( (\eta_h) \), ionization \( (\eta_i) \), and excitation \( (\eta_e) \) as follows:

\[
\eta_h = \frac{L_v(E_0) + f \sum_k x_k I_k Q_k(E_0)}{A},
\]

\[
\eta_i = \frac{x_i I_i Q_i(E_0)}{A},
\]

where \( E_0 \) is the injection energy of electrons, \( L_v \) is the Coulomb loss function (see below), \( k \) labels an ion and its ionization potential \( I_k \), ionization fraction \( x_k = n_k/n \), and collisional ionization cross section \( Q_k(E) \), and \( f \sim 0.3 \) is the mean energy of a secondary electron, and

\[
\eta_e = \frac{x_i E_{ij} \sigma_{ij}(E_0)}{A},
\]

where \( ij \) labels a transition with energy \( E_{ij} = E_j - E_i > 0 \), the fractional level population of the lower-energy state is \( x_i = n_i/n \), and the collisional excitation cross section is \( \sigma_{ij} \), and

\[
A = L_v(E_0) + (1 + f) \sum_k x_k I_k Q_k(E_0) + \sum_{ij} x_i E_{ij} \sigma_{ij}(E_0)
\]

is the normalization constant. The Coulomb loss function (Schunk & Hays 1971; Xu & McCray 1991) for high-energy
electrons is

$$p_{\text{z}} = \frac{n_e}{n} e \ln \left( \frac{4E}{\xi_e} \right).$$  \hspace{1cm} (20)$$

where $E$ is the electron energy, $e$ is the electron charge, $x_e = n_e/n$ is the electron fraction, and $\xi_e = 2/\omega_p$ for plasma frequency given by

$$\omega_p(n_e) = \sqrt{\frac{4\pi n_e e^2}{m_e}} = 56414.6 \sqrt{\frac{n_e}{\text{cm}^3}} \text{ s}^{-1}. \hspace{1cm} (21)$$

For collisional ionization cross sections, we use the approximate form (Younger 1981)

$$Q_i(E) = \frac{1}{uI^2} \left[ A \left( 1 - \frac{1}{u} \right) + B \left( 1 - \frac{1}{u} \right)^2 \right]$$

$$+ C \ln(u) + D \frac{\ln(u)}{u} \text{ cm}^2,$$  \hspace{1cm} (22)

where $u = E/I$, $I$ is the ionization potential, and $A$, $B$, $C$, and $D$ are fitting coefficients. We use the fitting coefficients published by Arnaud & Rothenflug (1985), taking into consideration updates by Arnaud & Raymond (1992) and Mattioli et al. (2007). While more recent calculations are available, Dere (2007) points out that the discrepancies between new and old ionization rates are minor except for Ni V–Xi, which are not important for this work. Coefficients are unavailable for Co II–IV, so we use Fe II–IV cross sections instead and plan to update these data when they become available in the future.

For collisional excitation cross sections of allowed transitions by nonthermal electrons, we use the approximation of van Regemorter (1962),

$$\sigma_{ij} = \frac{8\pi}{\sqrt{3}} \frac{1}{k_i^2} \frac{I_{i1}}{f_{j1}} \bar{g} \pi a_0^2,$$  \hspace{1cm} (23)

where $I_{i1}$ is the ionization potential of hydrogen, $k_i^2$ is the initial electron energy scaled to 13.60 eV, $f_{j1}$ is the oscillator strength, $a_0$ is the Bohr radius, and $\bar{g}$ is given by a quadratic fit to the results of van Regemorter (1962),

$$\bar{g} \sim -0.0065 \left( \frac{E}{\Delta E_{ij}} \right)^2 + 0.228 \left( \frac{E}{\Delta E_{ij}} \right) - 0.07, \hspace{1cm} (24)$$

with an imposed high-energy limit of

$$\bar{g} = \frac{\sqrt{3}}{2\pi} \ln \left( \frac{E}{\Delta E_{ij}} \right), E/\Delta E_{ij} > 36 \hspace{1cm} (25)$$

for all ions, and a low-energy limit for positive ions

$$\bar{g} = 0.2, E/\Delta E_{ij} < \sqrt{2}. \hspace{1cm} (26)$$
Figure 12. Same as Figure 5, but for the $M_{CO}$ parameter study in which we mix C/O into both nickel zone and IME layer (with a 1:9 carbon-to-oxygen ratio). Note the emergence of the [O III] $\lambda$5007 feature with increasing C/O mass.

Figure 13. Fiducial model with varying density profiles. $\delta$ refers to the exponent of the inner region in which $\rho \propto r^{-\delta}$, and the exponential model has a density $\rho \propto e^{-r/v_e}$ with a characteristic e-folding velocity $v_e(M_{ej}, E_K)$. Steeper density profiles concentrate more mass toward the center and have narrower features, higher bolometric luminosities, and lower ionization states (as indicated by the ratio of fluxes at 4665 and 5272 Å).

Figure 14. Fiducial model in which collisional ionization cross section values were scaled by the same factor. Uncertainties at the factor of 2 level in the cross sections produce $\approx 25\%$ changes in the spectral features.

Figure 15. Fiducial model in which collisional excitation rates for all transitions of all species were scaled by the same factor.

Figure 16. Fiducial model with two different sets of recombination rates for Fe I–V.
Forbidden transitions must be treated separately. We use the following form for the collision cross sections:

$$\sigma_{ij} = \frac{1}{g_i g_j} \Omega_{ij} g \pi a_0^2,$$  

where $g_i$ is the statistical weight and $\Omega_{ij}$ is the collision strength given by Equation (31).

### Appendix C

#### Implementation of Atomic Processes

##### C.1. Collisional Excitation and De-excitation

To determine collisional excitation and de-excitation rates relevant for the thermal pool of electrons, we assume that electrons adhere to a Maxwell–Boltzmann distribution. The subsequent “effective” or “Maxwellian-averaged” collision strength can be calculated for each transition using

$$\Upsilon_{ij} = \int_0^\infty \Omega_{ij} e^{-\epsilon_j/kT} d(\epsilon_j/kT),$$  

where $\Omega_{ij}$ is the collision cross section for an electron to excite the $i$-$j$ transition and $T$ is the electron temperature. These collision strengths can be found in the literature and data tables.

The subsequent rates of collisional excitation and de-excitation, respectively, are

$$C_{ei}(T) = \frac{8.63 \times 10^{-6}}{g_i \sqrt{T}} e^{-E_{ij}/kT} \Upsilon_{ij} n_e \text{ s}^{-1},$$  

$$C_{di}(T) = \frac{8 \pi e^2}{g_i} \frac{E_{ij}}{kT} C_{ei},$$

where $E_{ij}$ is the energy difference between the two levels and $j > i$.

In cases where atomic data for $\Upsilon$ are unavailable, one can use the dipole approximation (van Regemorter 1962; Jefferies 1968), which gives results for neutral atoms and positive ions, respectively, as

$$C_{ei}(T) = \begin{cases} 
2.16f_j n_e \left[ \frac{E_{ij}}{kT} \right]^{-1/2} T^{-3/2} e^{-E_{ij}/kT} \text{ s}^{-1}, \text{ (neutral atoms)} \\
3.9f_j n_e \left[ \frac{E_{ij}}{kT} \right]^{-1} T^{-3} e^{-E_{ij}/kT} \text{ s}^{-1}, \text{ (positive ions)} 
\end{cases}$$

(31)

where $f_j$ is oscillator strength, $T$ is temperature in Kelvin, $E_{ij}$ is transition energy in eV, and $n_e$ is electron density in cm$^{-3}$.

In practice, atomic data for $\Upsilon_{ij}$ are often published in a narrow temperature range; for temperatures outside this range, we use the above approximation to fill in the missing data. We scale Equation (31) so that there is no discontinuity in $C_{ij}$.

Forbidden transitions for which atomic data are not available should be treated as a special case, since oscillator strengths for these transitions produce artificially low collisional rates. Axelrod (1980) provides the following formulation for forbidden transitions (defined as $f_{ij} \ll 0.01$):

$$\Omega_{ij, forb} = \begin{cases} 0.00375 g_i g_j, & \lambda \leq 10\mu \\
0.0225 g_i g_j, & \lambda > 10\mu 
\end{cases}$$

(32)

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### C.2. Recombination

Total recombination rates of relevant ions include a sum over all subshells and incorporate both radiative and dielectronic recombination. We assume that recombinations involve only ground states, a good approximation in regimes where collisional excitation dominates the population of excited states. We use the rates published in the CHIANTI database v.8 (Dere et al. 1997; Del Zanna et al. 2015). Although level-specific recombination rates are available for certain ions (Nahar & Pradhan 1992, 1994, etc.), we opt to use a consistent source for recombination rates for this work. We explore the latter data set in Section 4.8 and plan to implement state-specific recombination rates in any future work where recombination lines might contribute significantly.
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