The nebular phase of lanthanide-rich ejecta of a neutron star merger (NSM) is studied by using a one-zone model, in which the atomic properties are represented by a single species, neodymium (Nd). Under the assumption that $\beta$-decay of $r$-process nuclei is the heat and ionization source, we solve the ionization and thermal balance of the ejecta under non-local thermodynamic equilibrium. The atomic data including energy levels, radiative transition rates, collision strengths, and recombination rate coefficients, are obtained by using atomic structure codes, GRASP2K and HULLAC. We find that both permitted and forbidden lines roughly equally contribute to the cooling rate of Nd\textsc{ii} and Nd\textsc{iii} at the nebular temperatures. We show that the kinetic temperature and ionization degree increase with time in the early stage of the nebular phase while these quantities become approximately independent of time after the thermalization break of the heating rate because the processes relevant to the ionization and thermalization balance are attributed to two-body collision between electrons and ions at later times. As a result, in spite of the rapid decline of the luminosity, the shape of the emergent spectrum does not change significantly with time after the break. We show that the emission-line nebular spectrum of the pure Nd ejecta consists of a broad structure from 0.5 $\mu$m to 20 $\mu$m with two distinct peaks around 1 $\mu$m and 10 $\mu$m.

Key words: transients: neutron star mergers

1 INTRODUCTION

Neutron star mergers (NSMs) have been considered as the sites of $r$-process nucleosynthesis (Lattimer & Schramm 1974). In August 2017, the LIGO/Virgo Collaboration (LVC) discovered the first NSM, GW170817, which was accompanied by radiation across the entire electromagnetic spectrum (Abbott et al. 2017; Nakar 2020; Margutti & Chornock 2020). In particular, the spectrum and light curve of the uv-optical-infrared counterpart referred to as ‘kilonova’ or ‘macronova’ indicate that a copious amount of $r$-process elements is produced in this event (Andreoni et al. 2017; Arcavi et al. 2017; Coulter et al. 2017; Cowperthwaite et al. 2017; Drout et al. 2017; Evans et al. 2017; Kasliwal et al. 2017; Pian et al. 2017; Smartt et al. 2017; Tanvir et al. 2017; Utsumi et al. 2017). The amount of the produced $r$-process elements and the event rate estimated from GW170817 suggest that NSMs could provide all the $r$-process elements in the Galaxy (e.g. Hotokezaka et al. 2018; Rosswog et al. 2018).

Lanthanide ions have unique optical properties, which enhance the opacity of the NSM ejecta material (Barnes & Kasen 2013; Kasen et al. 2013; Tanaka & Hotokezaka 2013; Wollaeger et al. 2018; Bulla 2019; Barnes et al. 2020). Thus, the existence of lanthanide ions imprints observable signatures in kilonova light curves and spectra. In fact, the late-time spectra of GW170817 peaking around the near infrared (nIR) band implies that lanthanides exist in the GW170817 ejecta (Kasen et al. 2017; Tanaka et al. 2017b). At the same time, the light curve rises on a short time scale of ~ 0.5 day, suggesting that there is a lanthanide-free ejecta component. Various models have been proposed to explain the coexistence of lanthanide-rich and free components in the GW170817 ejecta (Kasen et al. 2017; Tanaka et al. 2017a; Villar et al. 2017; Waxman et al. 2018; Shibata et al. 2017; Perego et al. 2017; Kawaguchi et al. 2018; Hotokezaka & Nakar 2020).

Recently, Watson et al. (2019) analyzed the observed spectra of GW170817 with an assumption that the spectra from ~ 1 to 5
The question is now - can more elements be identified from kilonova observations? The direct detection of nuclear γ-rays can be one of the most robust identifications of radioactive isotopes (Hotokezaka et al. 2016; Li 2019; Wu et al. 2019b; Korobkin et al. 2020). However, such measurements are very challenging and only weak upper limits were put by NuSTAR in GW170817 (Evans et al. 2017).

Here we consider the nebular phase of kilonovae, where the emergent spectrum is dominated by emission lines, and hence, spectroscopic observations may enable to identify the elements produced in NSMs. Since the slower ejecta component can be observed in the nebular phase than the earlier phases one can expect that the Doppler broadening of lines is weaker so that the spectral structure arising from individual lines may be more pronounced. In GW170817, the Spitzer Space Telescope detected the late-time nebula in $4.5 \mu m$ and put upper limits at $3.6 \mu m$ (Kasliwal et al. 2019; Villar et al. 2018), suggesting that a fraction of the luminosity of the nebula is radiated in infrared with a peculiar spectral shape.

The primary goal of this paper is to address the evolution of thermodynamic quantities and the emerging spectral shape of lanthanide-rich NSM nebulae. The early works on the nebular modelings of kilonovae assume local thermodynamic equilibrium (LTE) for ionization and level population (Waxman et al. 2018; Gillanders et al. 2021). However, the non-LTE effects are crucial for the late-time nebular modelings. Here we develop a NSM nebula model under non-LTE by following the studies of supernova (SN) nebular emission (Axelrod 1980; Fransson & Chevalier 1989; Ruiz-Lapuente & Lucy 1992; Mazzali et al. 2006; Maeda et al. 2006; Botyánszki et al. 2018). The paper is organized as follows. In §2, we describe the heating and ionization rates due to $\beta$-decay of $r$-process nuclei. In §3, we describe the equations and several approximations used in the modeling. In §4, we show the atomic data obtained by using the atomic codes. In §5, we apply our model to a lanthanide-rich NSM nebula and show the time evolution of temperature, ion abundances, and emission spectra. We conclude and discuss our study in §6.

2 TIME SCALE, RADIOACTIVE HEAT, AND IONIZATION

Calculating the nebular emission generally requires radiative transfer computations under non-LTE. However, such computations for NSM nebulae demand a lot of effort. As a first step, we focus here on the nebular phase where the following conditions are satisfied: (i) the ejecta is optically thin and (ii) the recombination and cooling times are shorter than the dynamical time. The former allows us to simplify the treatment of radiative transfer and the latter allows to use the steady-state approximation.
of heat and ionization. Note that the light curve of the GW170817 kilonova is consistent with the picture that β-decay of r-process nuclei predominantly heats the ejecta material over the time scales from 0.5 to 70 day (e.g., Kasliwal et al. 2019). In the nebular phase, the ejecta is optically thin for γ-rays, and hence, we consider only β-decay electrons. We use the heating rate with 130 ≤ A ≤ 209, where A is atomic mass number, provided by Hotokezaka & Nakar (2020). In the following, we describe the characteristic features of the β-decay heating rate relevant to the NSM nebular modelings.

At early times, the heating rate per unit mass approximately follows (Metzger et al. 2010):

$$\dot{Q}_{\text{th}}(t) \propto t^{-1.3}$$  (4)

This power law is valid as long as thermalization of β-decay electrons occurs on a time scale much shorter than a dynamical time. The heating rate starts to deviate from equation (4) around the thermalization time, $t_{\text{th}}$, estimated by $t_{\text{th}} = \frac{C_\rho \kappa_{\text{eff,e}} M_{\text{ej}}}{v_0^3}$,

$$\approx 55 \text{day} \left[ \frac{C_\rho}{0.05} \right]^{1/2} \left[ \frac{M_{\text{ej}}}{0.05 M_\odot} \right]^{1/2} \left[ \frac{v_0}{0.1c} \right]^{-3/2} \times \left[ \frac{\kappa_{\text{eff,e}}}{4.5 \text{ cm}^2 \text{g}^{-1}} \right]^{1/2} \left[ \frac{E_e}{0.25 \text{ MeV}} \right]^{-1/2},$$  (5)

where $E_e$ is the initial energy of β-decay electrons and $\kappa_{\text{eff,e}}$ is an effective opacity of the interaction of β-decay electrons with the ejecta material. Hereafter, we use the one-zone approximation, in which the density at a given time is represented by the mass weighted mean, $\rho_m(t) = C_\rho M_{\text{ej}} t^{-3} v_0^{-3}$, where $C_\rho$ is a normalization constant (Hotokezaka & Nakar 2020).

For $t \gg t_{\text{th}}$, the specific heating rate declines as (Kasen & Barnes 2019; Waxman et al. 2019; Hotokezaka & Nakar 2020)

$$\dot{Q}_{\text{th}}(t) \propto t^{-2.8} \quad (t \gg t_{\text{th}}).$$  (6)

This break in the β-decay heating rate from $\propto t^{-1.3}$ to $\propto t^{-2.8}$ is referred to as the thermalization break, which typically occurs in the nebular phase (see equations 3 and 5).

It is useful to introduce the normalized heating rate:

$$\Gamma = \frac{\rho_m \dot{Q}_{\text{th}}}{n^2} \propto \begin{cases} t^{1.7} & (t \ll t_{\text{th}}), \\ t^{0.2} & (t \gg t_{\text{th}}), \end{cases}$$  (7)

where $\Gamma$ is the heating rate per unit volume and $n$ is the mass-weighted mean atomic number density

$$n \approx 4 \cdot 10^4 \text{ cm}^{-3} \left( \frac{\langle A \rangle}{150} \right)^{-1} \left( \frac{C_\rho}{0.05} \right) \times \left[ \frac{v_0}{0.1c} \right]^{-3} \left[ \frac{M_{\text{ej}}}{0.05 M_\odot} \right] \left( \frac{t}{35 \text{d}} \right)^{-3},$$  (8)

where $\langle A \rangle$ is the mean atomic mass of the ejecta material. As we will see later, the evolution of kinetic temperature and ionization degree roughly follows the evolution of the normalized heating rate.

Figure 1 shows the specific heating rates, $\dot{Q}_{\text{th}}$, and normalized heating rates, $\Gamma/n^2$, with three different combinations of the ejecta mass and velocity. For more massive and slower ejecta, the normalized heating rate at a given time is smaller, corresponding to that the efficiency of ionization and heating is lower. As expected from equation (7), the slope of the normalized heating rates becomes almost flat at later times. For comparison, figure 1 also shows the heating rate of the decay chain powering SNe Ia, $^{56}\text{Ni} \rightarrow ^{56}\text{Co} \rightarrow ^{56}\text{Fe}$, with $M_{56\text{Ni}} = 0.54 M_\odot$, $M_{56\text{Co}} = 1.4 M_\odot$, and $v_0 = 7000 \text{ km s}^{-1}$. Unlike the r-process cases the normalized heating rate of this decay chain turns to decrease around the half-life of $^{56}\text{Co}$. Note that the normalized heating rate of NSMs is much larger than that of SNe Ia because of the difference in the expansion velocity, suggesting that ionization in the NSM ejecta is more efficient.

The ionization rate of an i-th ionized ion, $X^i$, by β-decay electrons is characterized by the work per ion pair $w_i$ (see Appendix A). With this quantity, the ionization rate per unit volume is given by

$$Y_i = \frac{\Gamma}{w_i}.$$  (9)

For the NSM nebulae, we estimate $w_i/l_{i,1} \sim 30$, where $l_{i,1}$ is the first ionization potential of $X^i$. This value indicates that the significant fraction of β-electrons’ energy is deposited to the thermal energy and only ~3% of it is consumed by ionization. Therefore, we neglect the recombination continuum cooling.

### 3 EQUATIONS FOR NEBULA MODELING

In the nebular phase, the ejecta material is in non-LTE, i.e., only free electrons are distributed according to Maxwellian law and atoms are not in equilibrium. Thus, one must solve the ionization and thermal balance to obtain the kinetic temperature, $T_e$, and ionization fractions. Here we use the nebular modeling developed by Axelrod (1980) with some modifications. In this section, we briefly describe the equations used and discuss some generic features of the NSM nebular emission that arise from the characteristic properties of the r-process heating rate (equation 7) without specifying the details of the atomic structure.

We consider the NSM nebular phase where the recombination and cooling time scales are shorter than a dynamical time. This condition allows us to use the steady state approximation. As we will show later, it holds $t \lesssim 100 \text{ day}$ after merger. We assume that the ejecta is composed of a single atomic species, $X$, for simplicity.

Under these conditions, the equation for ionization balance is

$$-Y_i f_i - \sum_{j>i} P_{ij} a_{j+1} \chi f_{j+1} n^2 + (1 - P_{i,i}) a_{i+1} \chi f_{i+1} n^2 = 0$$  for $0 \leq i \leq N - 1$,  (10)

where $f_i$ is the number fraction of $X^i$, $P_{ij}$ is the probability that the photons created by the recombinations of an ion $X^j$ ionize an ion $X^i$, $a_i$ is the recombination rate coefficient for $X^{(i+1)+} \rightarrow X^i$, and $\chi$ is the free electron fraction. This equation can be rewritten in the form (Axelrod 1980)

$$-\frac{\Gamma}{n^2 w_i} f_i - \sum_{j>i} P_{ij} a_{j+1} \chi f_{j+1} + (1 - P_{i,i}) a_{i+1} \chi f_{i+1} = 0$$  for $0 \leq i \leq N - 1$.  (11)

The ion fractions $f_i$ and free electron fraction $\chi$ are obtained by solving equation (11) together with the conditions of $\sum_{i=0}^{N} f_i = 1$.

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1 Spontaneous fission and α-decay of heavy nuclei can also be the energy source (Zhu et al. 2018; Wanajo 2018; Wu et al. 2019a)

2 We consider a single atomic species only for ionization and thermal balances. However we consider that the β-decay heat is produced by many different isotopes.
Therefore the thermodynamic quantities evolve with time according to the \( Z \) numbers, \( \chi n_e \), and the following, we focus on the atomic data of Nd. Before proceeding the details of the atomic data, here, we briefly summarize some spectral properties of lanthanide ions (Goldschmidt 1978). Lanthanide ions, \( \text{Ln} \), are a group of elements with atomic numbers 57 – 71 (\( \text{La} - \text{Lu} \)). Their ions are characterized by the number of electrons in 4f-shell, \( N \) or \( N + 1 \), where we use a number \( N = Z - 57 \), e.g., \( N = 0 \) for \( \text{La} \) and \( N = 14 \) for \( \text{Lu} \). Their configurations lying at low energies often have one to three electrons in the outer shells, 5d and 6s, which means that the energy scales of 4f, 5d, and 6s are similar so that several different configurations with the same parity consists of a group. Figure 2 shows a characteristic spectral structure of first to third lanthanide ions (\( \text{Ln} \) II-IV). For two groups connected by arrows, there are permitted transitions between them. Forbidden transitions between different orbital angular momenta, \( L \), as well as those associated with the fine structure are also important for the cooling rate and the emergent spectra. The characteristic spectra of lanthanides are summarized as follows.

(i) Permitted \( (E1) \) transitions of \( \text{Ln} \) II and \( \text{Ln} \) III exist in the nR and optical bands. These lines lead to the enhancement of absorption and can also be the source of nR-optical emission in the nebular phase.

(ii) Dipole forbidden \( (M1) \) transitions of \( \text{Ln} \) II - \( \text{Ln} \) IV between different configurations or between different total orbital angular momenta produce emission lines in the nR and optical bands.

(iii) Transitions between fine structure levels produce mid-IR lines (\( \lambda \approx 10 \mu m \)).

Note that, among \( \text{Ln} \) II, \( \text{Nd} \) II has resonance lines at the lowest transition energy and more \( E1 \) transitions at longer wavelengths. In fact, \( \text{Tanaka et al.} \) show that the abundance of \( \text{Nd} \) atoms has the most significant effect on the opacity in kilonovae. In the following, we focus on the atomic data of \( \text{Nd} \).

4 ATOMIC PROPERTIES OF NEOODYMIUM

NSM ejecta are composed of atoms with a wide range of atomic numbers, \( Z \geq 30 \), in reality. The experimental atomic data of these heavy elements are largely unavailable. To derive the atomic data necessary for our purpose we use atomic structure codes, General Relativistic Atomic Structure Package (GRASP2K; Jönsson et al. 2013) and Hebrew University Lawrence Livermore Atomic (HULLAC; Bar-Shalom et al. 2001) codes. HULLAC is an integrated code for calculating atomic structures and cross sections for the modelings of atomic processes in plasmas and emission spectra, which employs a parametric potential method for calculations of bound- and free-electron wavefunctions. The GRASP2K code provides more rigorous bound-electron wavefunctions based on the multiconfiguration Dirac–Hartree–Fock method, which enables more ab-initio calculations of atomic structures and bound-bound radiative transition probabilities, and therefore, we use GRASP2K to derive the level spectra and radiative transition rates (see Gaigalas et al. 2019 for details) and compute recombination rate coefficients by using HULLAC.

Lanthanide ions enhance the opacity of NSM ejecta (Kasen et al. 2013; Tanaka & Hotokezaka 2013; Tanaka et al. 2020; Barnes et al. 2020), and thus, they are naturally expected to be strong emitters in the nebular phase. In addition, one may be able to capture, at least qualitatively, some important features of the nebular emission of lanthanide-rich ejecta by using a single element because of the similarity in the spectral structure between lanthanide elements. Motivated by these, we focus on neodymium (\( \text{Nd} \)) in order to qualitatively understand the nebular emission of lanthanide-rich ejecta in this and following sections.
Figure 2. Characteristic structure of the transitions from the lowest configurations for second to fourth lanthanide ions. Ln II: The ground configuration of Ln II is one of the configurations in the two groups \(4f^N(5d + 6s)\). The energy levels of these configurations overlap and there exist permitted transitions between the two groups. This feature causes dense spectra in the nIR band. The transition lines from these lowest energy groups to the second lowest ones are typically in the optical region. Ln III and IV: The ground configurations of Ln III and Ln IV are \(4f^N\), respectively, except for La III, Gd III, and Lu III. The typical energy separations between the ground and the next lowest configurations are in the nIR to optical region for Ln III and in the ultraviolet region for Ln IV. Because only excited configurations overlap their spectra are less dense than those of Ln II.

Figure 3. Number of transition lines per logarithmic interval of energy of excited states \(E_u\) computed by using GRASP2K (top panels). Red and blue histograms show M1 and E1 transitions, respectively. Cooling function of Nd II, Nd III, and Nd IV at an atomic number density of \(10^4 \text{ cm}^{-3}\) (bottom panels). This number density corresponds to \(\sim 40\) day after merger in the case of an ejecta mass of \(\sim 0.05M_\odot\) and expansion velocity of \(\sim 0.1c\). Dotted and dashed curves show the cooling due to M1 and E1 transitions, respectively. For Nd II and Nd III, the contribution of E1 transitions is significant at \(T_e \geq 5000\ K\).
4.2 Radiative transition rate

We include the excited levels of Nd ions up to $\sim 5$ eV (Gaigalas et al. 2019). The numbers of levels included are 1400, 200, 40 for Nd II, Nd III, and Nd IV, respectively. Figure 3 shows the distribution of E1 and M1 transitions. Nd II has more lines than Nd III and Nd IV, suggesting that the cooling of Nd II per ion is the most efficient. Note that radiative transition rates of M1 transitions are lower by a factor of $\sim 10^3$ than E1 transitions. We also examined E2 transitions and found that their contribution to the cooling function is rather minor in the relevant temperature range and therefore we decide not to include E2 transitions.

Note that there are excited states that can decay through E1 transitions down to $\sim 0.7$ eV for Nd II, indicating that the cooling through the E1 lines is important even around 5000 K. This feature is qualitatively different from SN Ia nebulae, where the cooling is completely dominated by forbidden lines of the iron group elements.

Figure 4 compares the line spectra of Nd II and Nd III computed by GRASP2K with those from Den Hartog et al. (2003) and Ryabchikova et al. (2006) in the optical region and that from Hasselquist et al. (2016) in the nIR region. Den Hartog et al. (2003) experimentally measured the wavelengths and oscillator strengths of over 700 lines of Nd II. Here we focus on the intensive lines with $\log g_f > -1.5$, $E_u < 35000$ cm$^{-1}$, and $J > 5/2$ in the range of 4500 < $\lambda$ < 7500. The number of lines satisfying these restrictions is $\sim 180$. The line distribution of GRASP2K statistically agrees with the laboratory-based one. The GRASP2K line distribution is also roughly in agreement with the nIR lines of Nd II identified from the Apache Point Observatory Galactic Evolution Experiment (APOGEE) H-band spectra (Hasselquist et al. 2016).

Because the line spectrum of Nd III is poorly known experimentally, here we compare the GRASP2K result with the line list provided by Ryabchikova et al. (2006), in which they propose the line classification for Nd III based on stellar spectra and a theoretical calculation of atomic structure. In figure 4, we show 23 lines associated with the transitions between 4$^7$P and 4$^4$S$^5$P in the range of 4500 < $\lambda$ < 7500. We note that the wavelength of each line agrees within $\sim 3\%$ level. We consider that the GRASP2K line list is sufficiently accurate at least for E1 transitions to capture the spectral structure of the NSM nebular emission.

4.3 Collisional rate coefficient and critical density

We derive the collisional rate coefficients for the GRASP2K atomic data with the procedure described in Appendix D. Here we discuss the typical critical densities for Nd ions and implications to the evolution of the cooling functions and spectra. The critical density for a given upper level $i$ is estimated as

$$n_{\text{crit},i} = \frac{\sum_{l<k} A_{ul}}{\sum_{l<k} k_{ul}},$$

(16)

$$\sim \begin{cases} 10^5 \text{ cm}^{-3} \quad \text{(E1 transition)}, \\ 10^4 \text{ cm}^{-3} \quad \text{(M1 transition)}, \end{cases}$$

(17)

where we used the typical value of $k_{ul}$ and $A_{ul}$. These critical densities correspond to the critical times:

$$t_{\text{crit}} \sim \begin{cases} 1 \text{ day} \quad \text{(E1 transition)}, \\ 40 \text{ day} \quad \text{(M1 transition)}. \end{cases}$$

(18)

When the NSM ejecta becomes optically thin, the time scale of E1 radiative deexcitation is much faster than that of excitation, i.e., $t_{\text{crit}}(E1) \ll t_{\text{thin}}$. Therefore, the level populations in the nebular phase are always far from those in collisional equilibrium, i.e., the LTE values. For $t > t_{\text{crit}}(M1)$, excited levels predominantly decay through radiative transition. Such a state is referred to as corona equilibrium. In this case, the cooling rate is proportional to $n_{\text{e},\text{HI}}$, i.e., the cooling function, $\Lambda_i/n_{\text{e},\text{HI}}$, is independent of the density, and therefore, the kinetic temperature is expected to evolve very slowly with time after $t_{\text{crit}}(M1)$ because of $\Gamma/n^2 \propto t^{0.2}$. 

Figure 4. Comparison of line strengths of Nd II and Nd III computed by using GRASP2K (Gaigalas et al. 2019) with the experimental results (Den Hartog et al. 2003) and the APOGEE line list (Hasselquist et al. 2016) for Nd II and the Nd III line list based on the stellar spectrum of a strongly magnetic Ap star (Ryabchikova et al. 2006).
4.4 Cooling function

The bottom panels of figure 3 show the cooling functions of Nd II, III and IV ions at an ion density of $10^4$ cm$^{-3}$, corresponding to $\sim 40$ days after merger for $M_{ej} = 0.05 M_\odot$ and $v_0 = 0.1c$. We find the overall trend of the cooling functions, $\Lambda(\nu) < \Lambda(\nu') < \Lambda(\nu)$, which can be understood from the fact that Nd II has more lines in the IR to optical region. M1 transitions dominate the cooling functions of Nd II and Nd III for $T_e < 6000$ K and $< 10000$ K, respectively. This feature is expected from the characteristic lanthanide spectra (figure 2).

Figure 5 depicts the effect of self-absorption (left) and the density effect (right) on the cooling rates. The cooling functions without the trapping effect are calculated with the assumption of $\langle b_{ij} \rangle = 1$. We note that the absorption effect reduces the cooling function of Nd II by $\geq 50\%$ at $\geq 10^4$ K, where E1 transitions dominate the cooling rate. This effect is weaker for Nd III and absent for Nd IV. Note that, however, we likely overestimate the escape probability of lines with $l < 1 \mu m$ because these lines may be absorbed by nearby permitted lines such as resonance lines (see more details in §5). The density effect is quite small at the densities of lanthanide-rich NSM nebulae. Thus, for $n < 10^4$ cm$^{-3}$, the ejecta is in corona equilibrium and the cooling function can be considered to be independent of the density. For the results presented in the following section, the trapping and density effects are accounted for.

The cooling time scale is estimated as

$$t_{cool} \approx \frac{kT_e}{\Lambda/n} \sim 10^2 s \left(\frac{\Lambda/n}{10^{-19} \text{erg cm}^3 \text{s}^{-1}}\right)^{-1} \left(\frac{T_e}{10^4 K}\right) \times \left(\frac{M_{ej}}{0.05 M_\odot}\right)^{-1} \left(\frac{\langle A\rangle}{150}\right) \left(\frac{v_0}{0.1c}\right)^3 \left(\frac{t}{30 \text{day}}\right)^3,$$  

(19)

where $\Lambda$ is the total cooling function. This time scale is much shorter than a dynamical time until $\sim 10$ years after merger, and thus, the steady-state approximation for thermal balance is valid on the time scale, $t < 100$ day, focused in this work.

4.5 Dielectronic recombination

Dielectronic recombination dominates over radiative recombination for lower ionized Nd ions. At nebular temperatures ($\sim 10^4$ K), autoionizing states lying slightly above the ionization threshold contribute to the dielectronic capture process so that resolving fine structure is important here. For this purpose, we use the level model of HULLAC to obtain the energy levels, radiative transition rates, and autoionization rates. With these quantities, we calculate the rate coefficients by following the prescription of Nussbaumer & Storey (1983) (see also Appendix E). We include the following autoionizing states:

- Nd II: $4f^4nl (n \leq 10, l \leq 5)$, $4f^3dnl (n \leq 8, l \leq 5)$, and $4f^66sdl (n \leq 7, l = 4)$
- Nd III: $4f^4nl (n \leq 13, l \leq 5)$, $4f^2dnl (n \leq 8, l \leq 5)$, and $5p^24f^4nl (n \leq 6, l = 3)$
- Nd IV: $4f^2nl (n \leq 11, l \leq 5)$, $4f^4dnl (n \leq 7, l \leq 4)$, $5p^24f^2nl (n \leq 8, l \leq 3)$, and $5p^44f^2nl (n \leq 6, l = 3)$

Here an autoionizing state is denoted by $ynl$, where $y$ denotes the state of the core electrons, $n$ and $l$ denote the principal and orbital angular momentum quantum numbers of the captured electron. We note that the contribution of each configuration with higher $n$ and $l$ that is not included is less than $\sim 1\%$ for $T_e \leq 10^4$ K.

Table 1. Model parameters.

| model                  | $M_{ej} [M_\odot]$ | $v_0 [c]$ |
|------------------------|---------------------|-----------|
| wind (fiducial)        | 0.05                | 0.1       |
| dynamical ejecta       | 0.02                | 0.2       |
| slow wind              | 0.05                | 0.05      |

Figure 6 shows the recombination rate coefficients for Nd II - IV. The contribution of radiative recombination to the total rate coefficient is less than 10\% for all the cases. Note that, for Nd I, we assume that the rate coefficient of dielectronic recombination is 1/4 of that of Nd II because of the limitation of computational time.

The recombination time scale is estimated as

$$t_{rec} \approx \frac{1}{\alpha n_e} \sim 5 \text{ day} \left(\frac{\alpha}{10^{-10} \text{ cm}^3 \text{s}^{-1}}\right)^{-1} \left(\frac{M_{ej}}{0.05 M_\odot}\right)^{-1} \times \left(\frac{\langle A\rangle}{150}\right) \left(\frac{v_0}{0.1c}\right)^3 \left(\frac{t}{40 \text{ day}}\right)^3,$$

(20)

where $\alpha$ is the total recombination rate coefficient. The ionization time scale is estimated from the heating rate (see figure 1):

$$t_{ion} \sim \frac{1}{\langle A\rangle} \sim 5 \text{ day} \left(\frac{t}{40 \text{ day}}\right)^{2.8}$$

(21)

for $t > t_0$. Where we have used $w_i \sim 60$ eV for Nd III. For the fiducial model, $M_{ej} = 0.05 M_\odot$ and $v = 0.1c$, these two time scales become comparable to a dynamical time at $\sim 100$ day. Thus, we consider the nebular phase at $\leq 100$ day after merger, where the steady-state approximation is valid.

5 EVOLUTION OF THERMODYNAMIC QUANTITIES AND EMERGENT SPECTRUM

By solving the equations described in §3 with the atomic data of Nd ions shown in §4, we obtain the evolution of the thermodynamic quantities and emergent spectrum in the NSM nebular phase (see Appendix G for an application of our method to SN Ia nebulae). Table 1 shows the three cases studied here and we choose the wind model, $(M_{ej}, v_0) = (0.05 M_\odot, 0.1 c)$, as the fiducial model.

Figure 7 shows the evolution of the fractional ion abundances and the kinetic temperature in the fiducial case. The temperature slowly increases with time from $\sim 3000 K$ to $5000 K$. We find that the ejecta is predominantly composed of Nd II and Nd III. As we discussed in §2, the evolution of these quantities becomes flat around the thermalization time, $t_{th} \approx 50$ day, where the normalized heating function changes its slope from $\propto t^{-0.2}$ to $t^0$. The fractional ion abundances also very slowly change with time after the thermalization break.

Figure 8 shows the temperature evolution for the dynamical ejecta and slow wind models. The characteristic temperatures for the dynamical ejecta and slow wind models are $\approx 10^4$ K and $3 \cdot 10^3$ K, respectively. The ionization degrees of dynamical ejecta and slow wind models are higher and lower than the fiducial model, respectively.

The individual spectra of Nd II – IV at $n_i = n_e = 1.6 \cdot 10^4$ cm$^{-3}$ and $T = 4500$ K are shown in figure 9. In the nR and optical region, these spectra can be understood qualitatively according to the characteristic spectra of lanthanides discussed in §4. Namely,
these ions have two distinct peaks, one around $5–10\mu m$ produced by fine structure transitions and another around optical-nIR region. Nd II has among the richest spectral structure and its luminosity per atom is the brightest. The dense emission line distribution and the Doppler broadening result in a continuum-like spectrum with some structures. We find that the following transitions predominately produce the Nd II spectrum: $4f^35d^2 \rightarrow 4f^45d$, $4f^35d^6 \rightarrow 4f^46s$, $4f^35d^6 \rightarrow 4f^45d$, $4f^26p \rightarrow 4f^45d$, $4f^26p \rightarrow 4f^46s$, and $4f^45d \rightarrow 4f^46s$. The Nd III and Nd IV spectra are produced by the transitions: $5f^35d \rightarrow 4f^4$, $4f^35d \rightarrow 4f^4$ for Nd III and $4f^3 \rightarrow 4f^4$ for Nd IV. Note that individual M1 lines are more pronounced at $\lambda \lesssim 1 \mu m$ because the line population in this wavelength region is less dense.

There are more E1 transition lines at $\lambda \lesssim 1 \mu m$ for Nd II and Nd III (see figure 3). This implies that these E1 lines may absorb...
Figure 8. Kinetic temperature evolution for the dynamical ejecta model (left: $M_{ej} = 0.02M_\odot$ and $v_0 = 0.2c$) and slow wind model (right: $M_{ej} = 0.05M_\odot$ and $v_0 = 0.05c$). The fiducial model (wind) is also shown as a dash-dotted curve for comparison. The time scales on which the ejecta enters the nebular phase for the dynamical ejecta and slow models are 10 day and 70 day, respectively.

Figure 9. Normalized spectra for Nd II, Nd III, and Nd IV. Here we use a kinetic temperature of $T_e = 4500$ K, an electron density of $n_e = 1.6 \cdot 10^4$ cm$^{-3}$, and electron fraction of $\chi = 1$. These values roughly correspond to those around 40 day after merger in the fiducial model. Solid, dashed, and dash-dotted curves depict the total spectrum, the contribution of E1 transitions, and the contribution of M1 transitions, respectively. Also shown as vertical lines are individual E1 (blue) and M1 (red) lines. The Doppler broadening of each line at a frequency $\nu_l$ is incorporated by using a Gaussian distribution with a standard deviation of $\sigma = (v_0/c)\nu_l = 0.1\nu_l$.

Figure 10. Spectra for the fiducial model at 40 day (left) and 80 day (right) after merger. The contributions of Nd II, Nd III, Nd IV are also shown. Filled circle and triangle are the detection at $4.5 \mu$m and 5$\sigma$ upper limit at $3.6 \mu$m obtained by *Spitzer* telescope at 43 day (left) and 74 day (right) after GW170817 (Kasliwal et al. 2019).
other emission lines and reduce the emission at $\lambda \leq 1 \mu$m. In fact, Nd II and Nd III respectively have $\sim 50$ and $\sim 15$ resonance lines in the range of $0.4 \leq \lambda \leq 1 \mu$m and $0.4 \leq \lambda \leq 0.65 \mu$m. This radiation transfer effect is not accounted for in our modeling, and thus, our modeling likely overpredicts the optical emission.

Figure 10 shows the total spectra at 40 and 80 day for the fiducial model with the fractional ion abundances shown in figure 7. The Nd II lines dominate the total spectrum particularly in the nIR band. The spectral shape does not change significantly from 40 to 80 day while the amplitude decreases by a factor of $\sim 10$. This freeze-out of the nebular spectrum is a characteristic feature of the NSM nebular emission.

The spectra of the dynamical ejecta and slow wind models are shown in figure 11. For dynamical ejecta, each line is significantly broadened because of the fast expansion velocity, $0.2c$. As a result, the structures are completely smeared out. Nevertheless, there are two distinct peaks around the optical and IR bands. On the contrary, for the slow wind model, more lines can be seen in the IR region ($1 \leq \lambda \leq 20 \mu$m) and the optical emission is very weak. The spectral shape does not evolve significantly during the nebular phase in the both models.

We show the detectability of the structure of the nebular spectrum by the James Webb Space Telescope (JWST) for a future kilonova event in figure 12. The JWST is promising to resolve the spectral structure of the nebular emission around 40 day for events out to $\sim 100$ Mpc.

6 CONCLUSION AND DISCUSSION

The emission-line nebular phase of the NSM ejecta is studied by using a one-zone nebula model under non-LTE, in which the ejecta is considered to be composed of one of lanthanide elements, Nd. The atomic data necessary for the modeling are calculated by using the atomic structure codes, GRASP2K and RULLAC. We find that the kinetic temperature and ionization fraction are nearly constant with time after the thermalization break of the beta-decay heating rate. Consequently, the spectral shape of the emergent emission is also expected to be frozen after the break. For the ejecta parameters of $M_{\text{ej}} = 0.05M_\odot$ and $v_0 = 0.1c$, we show that Nd II and Nd III are the most abundant ions and the kinetic temperature approaches $\approx 5000$ K.

The high ionization efficiency of the $\beta$-decay heating rate results in a deviation in the ionization state from LTE. In particular, we find that the neutral fraction is significantly suppressed in the nebular phase. Although we do not account for the velocity distribution in this work, we speculate that this deviation can occur even at the earlier times, e.g., $t < 1$ week, in the outer ejecta, where the expansion velocity is faster. Depending on the mass and velocity, this effect leads to either the enhancement or suppression of singly ionized lanthanides, which has a crucial impact on the ejecta opacity (Tanaka et al. 2020; Barnes et al. 2020) and affects the color evolution of kilonovae (Kawaguchi et al. 2020).

The emergent emission line spectrum of the pure Nd nebula consists of a broad structure from $\sim 0.5\mu$m to $20\mu$m with two distinct peaks around $\sim 1 \mu$m and $\sim 10 \mu$m. Fine-structure transitions produce the mid-IR peak. This spectral structure may be an unique feature of lanthanide-rich nebulae. It is worth emphasizing that individual M1 lines are more pronounced at $\lambda \leq 1 \mu$m because the line population in this wavelength region is less dense. Importantly, the JWST will be able to resolve such structure in the nIR and midIR regions for events at $\sim 100$ Mpc. Note, however, that this structure may be suppressed once more elements are included. Another caveat of our modelling is that we have neglected the absorption due to line overlapping, which may lead to an overestimate of the optical-nIR emission ($\lambda \leq 1 \mu$m), where Nd II and Nd III have a number of permitted lines.

We use a crude approximation for the collisional strength of forbidden lines, i.e., $\Omega_F = 1$, in the case of the GRASP2K calculation.

![Figure 10](image1.png)

Figure 10. Spectrum at 40 day for the fiducial model at a distance of 100 Mpc. Also depicted are the 1σ sensitivity curves of NIRSpec FS and MIRI LRS with 10s integration.

![Figure 11](image2.png)

Figure 11. Same as figure 10 but for the dynamical ejecta model at 20 day (left) and the slow wind model at 80 day (right).

![Figure 12](image3.png)

Figure 12. Spectrum at 40 day for the fiducial model at a distance of 100 Mpc. Also depicted are the 1σ sensitivity curves of NIRSpec FS and MIRI LRS with 10s integration.
While this approximation is statistically consistent with the collisional strengths derived with HULLAC and can reasonably reproduce the cooling rates, the predicted line intensity ratios are by no means accurate. Thus, we need more accurate collisional strengths for the future studies.

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DATA AVAILABILITY

The data underlying this article will be shared on reasonable request to the corresponding author.

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APPENDIX A: WORK PER ION PAIR

The ionization efficiency of fast electrons for a stopping plasma is in principle obtained by solving the Boltzmann equation under some approximations (Spencer & Fano 1954; Kozma & Fransson 1992). Here we take a simple approach employed by Axelrod (1980), which
describes the radioactive ionization rate in terms of work per ion pair. The work per ion pair of $X^{++}$ is defined by

$$w_i = f_i E_{\text{dis}} / N_i,$$  \hspace{1cm} (A1)

where $f_i$ is the number fraction $X^{++}$, $E_{\text{dis}}$ is the total dissipated energy of injected fast electrons and $N_i$ is the total number of ion pairs (ion-electron pairs) of $X^{(i+1)x}$ produced through by the fast electrons. The value of $w_i$ simply represents the amount of energy that is dissipated in each ion-electron pair production.

Let us consider first the work per ion pair for a primary electron with an initial kinetic energy of $E_p$ injected in a stopping plasma. The number of ion pairs of $X^{(i+1)x}$ through the thermalization of the primary is given by

$$N_{i,p} = \int_0^{\ln} n_i \sigma_i(E)(s) ds,$$  \hspace{1cm} (A2)

where $n_i$ is the number density of $X^{++}$, $s$ is the travel distance of the electron, and $\sigma_i$ is the ionization cross section. The energy loss per distance interval is

$$\frac{dE}{ds} = -n \left(L(E) + L_{\text{th}}(E, \chi)\right),$$  \hspace{1cm} (A3)

where $L$ and $L_{\text{th}}$ are the stopping cross sections due to collisional ionization and excitation, and due to the Coulomb collision with thermal electrons, respectively. Equation (A2) is rewritten as

$$N_{i,p} = f_i \int_0^{E_p} \frac{\sigma_i(E)}{L(E) + L_{\text{th}}(E, \chi)} dE.$$  \hspace{1cm} (A4)

The work per ion pair of the primary electron is then

$$w_{i,p} = f_i \frac{E_p}{\int_0^{E_p} \frac{E dN}{\sigma_i(E) L(E) + L_{\text{th}}(E, \chi)}}.$$  \hspace{1cm} (A5)

To evaluate equation (A5), we use the total ionization cross section of $X^{++}$ by electron-ion collision given by Axelrod (1980)

$$\sigma_i \approx \frac{2\pi^2}{m_e v^2} \sum_{j=1}^{N} \frac{q_j}{P_j} \left[ \ln \left( \frac{m_e v^2}{2 P_j} \right) - \ln \left( 1 - \beta^2 - \beta^2 \right) \right],$$  \hspace{1cm} (A6)

where $v$ is the electron's velocity, $\beta = v/c$, $q_j$ and $P_j$ are the number of electrons and the ionization potential of a subshell $j$. We note that this formula (A6) agrees with the experimental data (Yagi & Nagata 2001). The stopping power for electrons for the Bethe formula:

$$L(E) \approx \frac{4\pi Z e^4}{m_e v^2} \ln \left( \frac{\sqrt{m_e v^2 T}}{2^{1/2}(I)(1-\beta^2)} \right)^{1/2},$$  \hspace{1cm} (A7)

$$-\left( 1 - \beta^2 - \frac{1-\beta^2}{2} \ln(2) + \frac{1}{16}(1-\sqrt{1-\beta^2})^2 \right)$$

where $Z$ is the charge of the target ion, $T$ is the kinetic energy of the electron, and $(I)$ is the mean ionization energy of the stopping material. The value of $(I)$ is taken from the ESTAR database. The stopping power of thermal plasma for with thermal velocity $v_{th} \ll v$ is given by (Bohr 1913)

$$L_{\text{th}}(E, \chi) = \frac{4\pi Z e^4}{m_e v^2} \ln \left( \frac{1.123 m_e v^2}{\chi^2} \omega_p \right),$$  \hspace{1cm} (A8)

where $\omega_p$ is the plasma frequency, $n_e$ is the electron number density, and $\chi$ is the electron fraction $n_e/c/n$.

For comparison between different ions, it is useful to define work per ion pair normalized by the first ionization potential, $I_{i,1}$. For instance, in the case of $E_p = 250$ keV and $\chi = 2$, we find $w_{i,p}^{P} / I_{i,1} \sim 45$, 45, 40, and 35 for Nd I, Nd II, Nd III, and Nd IV, respectively. In addition to ionization by primary electrons, secondary electrons may further ionization. This means that the total number of ion pairs $N_i$ in equation (A1) is larger than $N_{i,p}$. Secondaries are ejected with recoil energy typically around the binding energy of the target electron. For a weakly ionized Nd plasma, the stopping power of thermal electrons dominates over the ionization energy loss at electron energies $\leq (I) \sim 0.5$ keV, and therefore, the recoil energy of the secondaries originating from the inner shells (K, L, M) typically exceeds this threshold. Thus, a fraction of the recoil energy of secondaries from the inner shells is lost through ionization and more ion pairs are created. Accounting for the secondary ionization, the ionization efficiency is increased by $\approx 20$–50% corresponding to $w_i/I_{i,1} \sim 30$. In this paper, we use $w_i/I_{i,1} = 30$.

APPENDIX B: PHOTOIONIZATION

The recombination processes emit photons that may be reprocessed by photoelectric absorption. This reprocess reduces the recombination rate. The recombination of $X^{i+}$ may emit ionizing photons for $X^{(i+1)x}$. The number of ion pairs of $X^{(i+1)x}$ and $e^-$ produced by photoionization due to the photons emitted in a recombination process of $X^{(i+1)x} \rightarrow X^{i+}$ is estimated by

$$P_{ij} = \int \left(1 - e^{-\tau(v)}\right) \frac{f_i \sigma_{ph}^i}{\sum_k f_k \sigma_{ph}^k} \frac{dN_{ph}}{dv} d^v,$$  \hspace{1cm} (B1)

where $(dN_{ph}/dv)$ is the number of photons per frequency interval emitted in recombination of $X^{(i+1)x}$. Here the optical depth for photons with frequency $v$ is given by

$$\tau(v) = \sum_{k=0}^N f_k \sigma_{ph}^k \langle v \rangle n_R,$$  \hspace{1cm} (B2)

where $f_k$ and $\sigma_{ph}^k$ are the number fraction and the photoionization cross section of $X^{k+}$, and $R$ is the radius of the ejecta. Because $\sigma_{ph}$ is $10^{15}$ cm$^2$, the optical depth is $\sim 100$ (t/40 day)$^{-2}$ and therefore the ejecta is optically thick for recombination photons in the nebular phase.

As shown in figure 6, Nd ions recombine predominantly through dielectronic recombination, where recombination photons are produced through the radiative cascades of auto-ionization series to the ground state. Therefore, it is not straightforward to determine the recombination photon spectrum $(dN_{ph}/dv)$. For auto-ionization states that have a large radiative transition rate, each auto-ionization state contributes substantially to the rate coefficient even though the number of such states is relatively small. In this channel, auto-ionization states are typically stabilized through the emission of a photon with energy close to the first ionization potential of the recombined ion and therefore this cascade produces one ionizing photon and several low energy photons. At the same time, there are many auto-ionization states that are stabilized through the emission of photons with energy sufficiently lower than the first ionization potential but high enough to ionize ions in lower ionized states. As a result, the recombination photons are likely to have a somewhat flat spectrum per logarithmic frequency interval. Thus, we assume that the number of recombination photons is constant at each energy scale below the sum of the first ionization potential

\[\text{https://physics.nist.gov/PhysRefData/Stardata/Estar/Estar.html}\]
and the thermal energy of free electrons, i.e., \((dN_\text{ph}/d\nu)_j \propto 1/\nu\) for \(h\nu < I_{j,1} + kT_e\) and its normalization is set such that the total energy of recombination photons is \(I_{j,1} + kT_e\).

**APPENDIX C: SELF-ABSORPTION OF STRONG LINES**

The absorption due to strong lines may have significant impacts on the cooling functions and emergent spectra. In general, absorption occurs non-locally so that one must solve radiation transfer, which is beyond the framework of our one-zone modeling. Here we use the escape probability approximation, which allows to include the effects of self-absorption of lines in one-zone modeling (e.g., Chapter 19 of Draine 2011).

In homologously expanding ejecta, the escape probability is approximated by

\[
\beta_{i,j} = \frac{1 - e^{-t_{\text{Sob}}}}{t_{\text{Sob}}},
\]

where \(t_{\text{Sob}}\) is the Sobolev optical depth:

\[
t_{\text{Sob}} = \frac{g_i A_{ij}}{8\pi} \frac{1}{I_{j,1}^{(n)}} \left( \frac{n_j}{n_i - n_i} \right) t \quad (i > j).
\]

For resonance lines, the optical depth is estimated by

\[
t_{\text{Sob}} \approx 10^2 \left( \frac{g_u A_{a0}}{10^8 \text{s}^{-1}} \right) \left( \frac{\lambda_{a0}}{0.05 \text{\mu m}} \right)^3 \left( \frac{M_\odot}{0.05 M_\odot} \right) \times \left( \frac{v_0}{0.1 c} \right)^{-3} \left( \frac{t}{30 \text{ day}} \right)^{-2}.
\]

This suggests that the resonance lines are trapped in the ejecta on time scales focused in this paper, \(\lesssim 100\) day.

**APPENDIX D: COLLISIONAL EXCITATION AND DEEXCITATION**

With the usual convention, the velocity averaged rate coefficient for collisional deexcitation from an upper level \(i\) to a lower level \(j\) is given by

\[
k_{ij} = \frac{8.63 \cdot 10^{-6} \nu E_{ij}(T_e)}{g_j T_e^{3/2}} \text{ cm}^3\text{s}^{-1},
\]

where \(E_{ij}\) is the velocity averaged collision strength connecting levels \(i\) and \(j\). The collisional excitation rate coefficient is given by

\[
k_{ji} = \frac{g_i}{g_j} k_{ij} e^{-E_{ij}/kT_e},
\]

where \(g_i\) is the level degeneracy, \(E_{ij}\) is the energy-level difference.

The collisional strengths are currently not available for the GRASP2K atomic data. Therefore, we use the following approximations for the collisional strengths \(\Omega_{ij}\) for the GRASP2K atomic data. For E1 transitions, we calculate \(\Omega_{ij}\) by using the approximate formula (van Regemorter 1962):

\[
\Omega_{ij} \approx 2.388 P(E_{ij}) \left( \frac{\lambda}{1 \mu m} \right)^3 \left( \frac{g_i A_{ij}}{10^8 \text{s}^{-1}} \right),
\]

where \(P(x)\) is the Gaunt factor integrated over the electron velocity distribution and \(A_{ij}\) is computed with GRASP2K. Here we use \(P(x) \approx 0.2\), which is a good approximation for \(x \lesssim 2\) (van Regemorter 1962). For forbidden transitions, we assume \(\Omega_{ij} = \Omega_F\), where \(\Omega_F\) is a constant value. Figure C1 shows the collisional strengths for M1 transitions at \(T_e = 5000\) K computed by using HULLAC. We find that the averaged values around \(E_{ij} \lesssim 1\) eV, which are the most relevant to the spectrum formation in the nebular phase, is roughly unity. Therefore, we approximate \(\Omega_F \approx 1\) in this work. Figure C2 compares the cooling function of GRASP2K with that of HULLAC. The cooling functions due to M1 transitions derived with the two codes are in a good agreement. This fact justifies our choice of \(\Omega_F \approx 1\). However, the E1 transition cooling of GRASP2K is higher than that of HULLAC, suggesting that the van Regemorter formula slightly overestimates the collisional strengths. Figure C3 shows the spectrum of each ion at \(n = 1.6 \cdot 10^4\) cm\(^{-3}\) and \(T_e = 6000\) K with the atomic data computed with HULLAC. We note that the spectral structures computed with the two codes are qualitatively similar but the Nd II spectrum of HULLAC has significant emission around 3 \(\mu\)m.

**APPENDIX E: DIELECTRONIC RECOMBINATION**

Dielectronic recombination occurs via the following process:

\[
X_p^{(i+1)+} + e^- \rightarrow X_a^{+} \rightarrow X_b^+ + h\nu, \quad (E1)
\]

where \(a\) and \(b\) denote an autoionizing state of \(X^+\) and a bound state of \(X^{++}\), respectively. The bound state, \(X_{b}^{++}\), is stabilized by radiative decays. At the nebular temperature, radiative decays of both the core and captured electrons contribute to the stabilization of \(X_{a}^{++}\) (Beigman & Chichkov 1980; Storey 1981).

The dielectronic recombination rate coefficient of the capture process (E1) is calculated by

\[
a_{\text{dr}}(p,a;T_e) = \frac{N_S(X_a^{++})}{N_e N_S(X_p^{(i+1)+})} \sum_j A_{aj} \sum_k \Gamma_{ac} + \sum_k A_{ak}
\]

where

\[
\frac{N_S(X_a^{++})}{N_e N_S(X_p^{(i+1)+})} = \frac{g_a}{2g_p} \left( \frac{\hbar^2}{2\pi \mu c kT_e} \right)^{3/2} e^{-E_a/kT_e}, \quad (E3)
\]

where \(E_a\) is the energy of a state \(a\) relative to \(X_p^{(i+1)+}\), and \(g_p\) is the statistical weight of the state \(p\), \(\Gamma_{ac}\) is the autoionization rate. Here the sum for \(j\) is over the levels that are stable against autoionization and the sum for \(k\) is over all the lower levels. We assume that the recombinating ion \(X_p^{(i+1)+}\) is in the ground state. Then the total rate coefficient is

\[
a_{\text{dr}}^{\text{tot}}(T_e) = \sum_a a_{\text{dr}}(p,a;T_e). \quad (E4)
\]

This capture is a resonant process such that \(E(e^-) = E(X_a^{++}) - E(X_p^{(i+1)+})\) must be satisfied and the autoionizing states that are accessible via collision with thermal electrons contribute to the capture rate. This indicates that ions with denser autoionizing states such as open f-shell ions have larger recombination rate coefficients. In fact, the measured values of the dielectronic recombination rate coefficient of Au\(^{55+}\), W\(^{20+}\), and W\(^{18+}\), nearly half open f-shell ions, are larger than the radiative recombination rate coefficient by two to three orders of magnitude at nebular temperatures (Hoffnnecht et al. 1998; Schippers et al. 2011; Spruck et al. 2014).

For the nebular temperatures (\(\lesssim 10^8\) K), the kinetic energy of thermal electrons is typically much smaller than the first ionization potential of ions, and therefore, autoionizing states only slightly above the ionization threshold contribute to the recombination process. Thus, levels in a small energy range from \(I_1\) to \(\sim I_1 + 1\) eV must be resolved. For this purpose, we use the level mode of HULLAC that resolves the fine structure.

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**APPENDIX F: RADIATIVE RECOMBINATION**

Radiative (direct) recombination occurs via

\[ \chi_{p}^{i+1+} + e^{-} \rightarrow \chi_{p}^{i+} + h\nu. \]  

(F1)

A photon produced by the recombination of \( \chi^{i+} \) directly to the ground state is most likely absorbed by \( \chi^{i+} \). This rate coefficient of this process is denoted customary as \( \alpha_A \) and that of the recombination to the other states is denoted \( \alpha_B \). Axelrod (1980) provides

\[ \alpha_A(T) = 10^{-13.2} \left( \frac{T}{10^4 \text{ K}} \right)^{-1/2} \text{ cm}^3 \text{ s}^{-1}. \]  

(F2)
APPENDIX G: NEBULAR SPECTRA OF SNE IA

Our nebula modeling is by no means accurate because we use a number of approximations and assumptions. In order to show the ability of our simple modeling, here we apply our method to the nebular emission of SNe Ia for comparison. Here we consider the decay chain of $^{56}$Ni $\rightarrow ^{56}$Co $\rightarrow ^{56}$Fe as the heat and ionization source and the heating rate computed by a code developed by Hotokezaka & Nakar (2020). As we did for NSM nebulae, we assume that the atomic properties are represented by a single atomic species, Fe. The work per ion pair for Fe ions for primary electrons is $\omega_0/I_1 \approx 30$ (Axelrod 1980). Accounting for secondary ionization, we approximate $\omega_0/I_1 \approx 25$. Because the properties of the transition lines of Fe ions relevant to the SN Ia nebula modelings are experimentally known, we use the NIST line list instead of preparing them with the atomic codes. The collisional strengths are computed in the prescription shown in Appendix D. Here we use $\Omega_E = 0.5$ for forbidden transitions, with which the cooling functions agree with those computed by using HULLAC in the relevant temperature range. Note that our one-zone modeling is fully characterized by only two parameters: the total $^{56}$Ni mass, $M_{56}$Ni, and the ejecta velocity, $v_0$.

We discussed in §4.5 that dielectronic recombination dominates over radiative recombination for Nd ions. Likewise, dielectronic recombination is more important for lower ionized Fe ions (see Nahar et al. 1997; Nahar 1997, 1996 for the results of the R-matrix method). We obtain the rate coefficients of dielectronic recombination of Fe ions by using HULLAC. We find that our rate coefficients are higher by a factor of $\sim 3$–10 than those of Nahar et al. (1997); Nahar (1997, 1996).

Figure F1 shows the evolution of ionization fractions in the case of $M_{56}$Ni $= 0.54M_\odot$ and $v_0 = 7000$ km s$^{-1}$. Figure F2 shows the spectrum of pure Fe emission at $\sim 200$ day and $\sim 360$ day. Also depicted is the observed spectrum of a typical SN Ia, SN 2011fe (Mazzali et al. 2015). Our simple one-zone model reproduces the characteristic Fe-line structure (see Mazzali et al. 2015 and Botvinski et al. 2018 for more detailed modelings). Note that our choice of $M_{56}$Ni $= 0.54M_\odot$ agrees with the mass estimate by using the pre-nebular light curve of SN 2011fe (Arnett et al. 2017). At $\sim 360$ day, the value of Fe III/Fe II in our model seems slightly lower than the observed value and the model predictions in the literature. This is because our dielectronic recombination rate coefficients, which are computed with HULLAC, are slightly larger than those used in the literature.

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