DETAILED NON-LTE MODEL ATMOSPHERES FOR NOVAE DURING OUTBURST. I. NEW THEORETICAL RESULTS

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ABSTRACT

We present new, detailed non-LTE (NLTE) calculations for model atmospheres of novae during outburst. This fully self-consistent NLTE treatment for a number of model atoms includes 3922 NLTE levels and 47,061 NLTE primary transitions. We discuss the implication of departures from LTE for the strengths of the lines in nova spectra. The new results show that our large set of NLTE lines constitutes the majority of the total line-blanketing opacity in nova atmospheres. Although we include LTE background lines, their effects are small on the model structures and on the synthetic spectra. We demonstrate that the assumption of LTE leads to incorrect synthetic spectra and that NLTE calculations are required for reliably modeling nova spectra. In addition, we show that detailed NLTE treatment for a number of ionization stages of iron changes the results of previous calculations and improves the fit to observed nova spectra.

Subject headings: novae, cataclysmic variables — stars: atmospheres

1. INTRODUCTION

In a series of papers (Hauschildt et al. 1992, 1994a, 1994b, 1995; Pistinner et al. 1995; Hauschildt et al. 1996a, 1996b; Schwarz et al. 1997a) we have developed detailed spherical, expanding non-LTE (NLTE) model atmospheres to treat the optically thick early stages of nova outbursts and have also analyzed a number of observed nova spectra. The models were computed self-consistently, employing the equation of transfer in a special relativistic framework (Hauschildt 1992), energy conservation in the comoving frame calculated with a modified Unsöld-Lucy method (Allard & Hauschildt 1995), NLTE effects for a large number of atomic and molecular species using numerical methods that we have developed to treat very large and detailed model atoms (Hauschildt 1993; Hauschildt & Baron 1995; Hauschildt, Baron, & Allard 1997), and extensive NLTE and LTE line blanketing by several million lines that were dynamically selected from the Kurucz lists (Kurucz 1994d) and other sources (for molecular lines). These models have been extremely successful in fitting observed nova spectra (Hauschildt et al. 1994b; Schwarz et al. 1997a) and, in particular, have been used to identify the UV signature of the fireball phase of Nova Cygni 1992 (Hauschildt et al. 1994b) and LMC 1991 (Schwarz et al. 1997b).

Although nova atmospheres can be treated as stationary expanding shells (see Bath & Shaviv 1976), the time development of the nova spectra can be simulated by a series of nova atmospheres at constant luminosity and increasing model temperatures during the phase of constant bolometric luminosity of the nova. Therefore, the analysis of a time sequence of observations can provide insight, for instance, into the development of the velocity field of the shell. Such sequences can also be used to check the results of the analysis for consistency and to obtain an estimate on the statistical errors inherent in the analysis process. This means that grids of nova atmosphere models and synthetic spectra are important to investigate the time evolution of a nova outburst.

We present here a new generation of nova atmosphere models and synthetic spectra with a much larger set of NLTE species than any previous calculation. The majority of the line-blanketing opacity in these new models is provided by NLTE lines, constituting a significant advance for nova model atmospheres. In this first paper, we discuss some new theoretical results and their implications. In a companion paper (Schwartz et al. 1997b), we show fits to specific observed novae using these models. Our outline is as follows. In § 2, we briefly discuss the model assumptions and the numerical methods that we use and how we derive our model atoms. The results of the calculations are presented in § 3 and the structure of the atmosphere and the spectra are discussed in § 4. We close with a summary and conclusions.

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2. METHODS AND MODELS

The basic assumptions of our nova models are the same as those used in Hauschildt et al. (1995). The expanding nova shell is assumed to have a power-law density of the form $\rho \propto r^{-N}$ with $N = 3$ for the models presented in this paper. The velocity law is derived from the condition of constant mass-loss rate (in radius) with a prescribed maximum velocity $v_{\text{max}}$ (we use here $v_{\text{max}} = 2000$ km s$^{-1}$), consistent with typical values observed in classical novae. We further parameterize the models with the model temperature $T_{\text{model}}$ through the relation $L = 4\pi R^2 \sigma T_{\text{model}}^4$, where $L = 50,000 L_\odot$ for all models; the absolute value of the luminosity does not affect the spectra: see Pistinerti et al. (1995; Hauschildt et al. 1995). $R$ is the radius of the shell at $t = 1$ in the bound-free (hereafter, b-f) continuum at 5000 Å. The model temperature is comparable to the effective temperature $T_{\text{eff}}$ in that it parameterizes the bolometric flux of the model at any time. However, it should not be confused with the effective temperature, which can be defined only for plane-parallel configurations (Hauschildt et al. 1995).

We solve the radiative transfer equation consistently for lines and continua (allowing for arbitrary overlaps) with the method discussed in Hauschildt (1992) and Hauschildt et al. (1995) rather than employing the Sobolev approximation. Hauschildt et al. (1995) have shown that this simpler method cannot be used in nova atmospheres owing to the large number of overlapping lines as well as the strong coupling between lines and continua. Such complications require that the multilevel NLTE rate equations be solved self-consistently and simultaneously with the radiative transfer and energy equations and that the equations must include the effects of both line blanketing and expansion of the nova atmosphere.

For this analysis, we use our multi-purpose stellar atmosphere code PHOENIX. PHOENIX (version 8.1, Hauschildt et al. 1996a; Hauschildt et al. 1997) uses a special relativistic spherical radiative transfer for nova models and an equation of state (EOS) that includes more than 300 ions of 39 elements (with up to 26 ionization stages). The temperature correction is based on a variety of the Unsöld-Lucy method that has been modified to include NLTE and scattering. This algorithm converges very quickly and is highly stable.

Both the NLTE and LTE background lines (see below) are treated with a direct opacity sampling method. We do not use precomputed opacity sampling tables but instead dynamically select the relevant LTE background lines from master line lists at the beginning of each iteration and sum the contribution of every line within a search window to compute the total line opacity at arbitrary wavelength points. The latter feature is crucial in NLTE calculations in which the wavelength grid is both irregular and variable from iteration to iteration owing to changes in the physical conditions. This approach also allows detailed and depth-dependent line profiles to be used during the iterations. To make this method computationally efficient, we employ modern numerical techniques, e.g., vectorized and parallelized block algorithms with high data locality (Hauschildt et al. 1997; Baron & Hauschildt 1997), and we use high-end workstations or supercomputers for the model calculations.

In the calculations we present in this paper, we have included a constant statistical velocity field, $\xi = 50$ km s$^{-1}$, which is treated like microturbulence. The choice of lines of species not explicitly treated in NLTE (hereafter, LTE background lines) is dictated by whether they are stronger than a threshold $\Gamma \equiv \chi_i / \kappa_i = 10^{-4}$, where $\chi_i$ is the extinction coefficient of the line at the line center and $\kappa_i$ is the local b-f absorption coefficient. This typically leads to about $2 \times 10^6$ LTE background lines. The profiles of these lines are assumed to be depth-dependent Gaussians. We have verified in test calculations that the details of the LTE background line profiles and the threshold $\Gamma$ do not have a significant effect on either the model structure or the synthetic spectra. However, the LTE background lines are included because their cumulative effect can change the structure and the synthetic spectra. In addition, we include about 2000 photoionization cross sections for atoms and ions (Verner & Yakovlev 1995).

Hauschildt & Baron (1995) have extended the numerical method developed by Hauschildt (1993) for NLTE calculations with an extremely detailed model atom of Fe II. In the calculations presented in this paper, we significantly enlarge the set of NLTE species, namely H, He I-II, Mg II, Ca II, Ne I, C I-IV, N I-VI, O I-V, S II-III, Si II-III, and Fe I-III (for a complete list of NLTE species available in PHOENIX 8.1, see Table 1). Note that we do not use the NLTE treatment for Li I, Na I, Co I-III, and Ti I-III because these species are not very important in nova atmospheres and, particularly, treating Co and Ti in NLTE would considerably increase the CPU time for the model calculations with little additional improvement. We thus include a total of 3922 NLTE levels and 47,061 NLTE primary lines in the calculations presented here, nearly a factor of 5 more levels and lines than in our previous nova calculations (Hauschildt et al. 1996a).

2.1. NLTE Calculational Method

The large number of transitions that have to be included in realistic models of nova atmospheres require an efficient method for the numerical solution of the multilevel NLTE radiative transfer and model calculation problem. Simple approximations, such as the Sobolev method, are very inaccurate in situations in which lines overlap strongly and make a significant pseudocontinuum contribution (weak lines), as is the case for nova and supernova atmospheres (see Hauschildt et al. 1996a; Baron et al. 1996). Classical techniques, such as the complete linearization or the equivalent two-level atom method, are computationally prohibitive. In addition, we are modeling moving media (e.g., stellar winds, novae, and supernovae), so that approaches such as Anderson’s multigroup scheme (Anderson 1989) or extensions of the opacity-distribution function method (Hubeny & Lanz 1995) cannot be applied because of the velocity-dependent coupling of different wavelengths. Methods that are based on partial linearization schemes and the use of superlevels tend to be numerically less stable and frequently encounter convergence problems because of the highly nonlinear and nonlocal couplings that dominate these atmospheres.

We use the multilevel NLTE operator-splitting method described by Hauschildt (1993). This method solves the nongray, spherically symmetric, special relativistic equation of radiative transfer in the comoving (Lagrangian) frame using the operator-splitting method described in Hauschildt (1992; see also Cannon 1973). This method has been presented in Hauschildt & Baron (1995), so we do not repeat
the detailed description here. For all primary NLTE lines, the radiative rates and the appropriate rate operators (Hauschildt 1993) are computed and included in the iteration process. Secondary NLTE lines are included for completeness but do not affect either the model structure or the synthetic spectra (in fact, the model atoms have been explicitly constructed so that all important lines are primary lines). This method is flexible, can be parallelized (hereafter, b-b) transitions with log \((gf) \geq -3.0\) as NLTE levels where \(g\) is the statistical weight of the lower level and \(f\) is the oscillator strength of the transition (we have used Kurucz’s data provided on CD-ROMs: Kurucz 1993, 1994a, 1994b, 1994c; Kurucz & Bell 1995). That is, we solve the complete b-f and b-b radiative transfer and rate equations for all levels including all radiative rates of the primary lines. In addition, we treat the opacity and emissivity for the remaining \(\approx 2 \times 10^{6}\) weak secondary b-b transitions in NLTE if one level of a secondary transition is included in the model. A more complete description of the numerical method is presented in & BaronHauschildt et al. and, most importantly, leads to (Hauschildt 1993), where \(\delta\) is the derivative and the NLTE departure coefficients are converged better than 1% in the comoving frame flux and its derivative and the NLTE departure coefficients are converged better than 1% at the same time. We have found in test calculations that this is necessary and sufficient to obtain a converged solution (see also Hauschildt 1993). On a single-processor Cray C90 or a single-processor HP 9000-C180 workstation, a typical model calculation with 10 iterations requires about 18 hr of CPU time. On five thin nodes of an IBM SP2 parallel machine using the parallel version of PHOENIX (Hauschildt et al. 1997), the same calculations also require about 18 hr of wall-clock time.

2.2. The Model Atoms

To construct most of the model atoms, we have included all observed levels that have observed bound-bound (hereafter, b-b) transitions with log \((gf) \geq -3.0\) as NLTE levels where \(g\) is the statistical weight of the lower level and \(f\) is the oscillator strength of the transition (we have used Kurucz’s data provided on CD-ROMs: Kurucz 1993, 1994a, 1994b, 1994c; Kurucz & Bell 1995). That is, we solve the complete b-f and b-b radiative transfer and rate equations for all levels including all radiative rates of the primary lines. In addition, we treat the opacity and emissivity for the remaining \(\approx 2 \times 10^{6}\) weak secondary b-b transitions in NLTE if one level of a secondary transition is included in the model. A more complete description of the numerical method is presented in Hauschildt & Baron (1995). Photoionization and collisional rates for most of the model atoms are not yet available. Thus, we have taken the results of the Hartree-Slater central-field calculations of Reilman & Manson (1979) to scale the ground-state photoionization rate to the species of interest and have then used a hydrogenic approximation for the energy dependence of the cross section. Although this provides only a rough approximation, the exact values of the b-f cross sections are not important for the opacities themselves, which are dominated by known b-b transitions.

A more accurate treatment of these model atoms requires more accurate collisional and photoionization rates, which are not presently available. We have, therefore, been forced to make several simplifying choices. While collisional rates are important in hotter stellar atmospheres with high electron densities, they remain nearly negligible compared to the radiative rates for the low electron densities found in cooler nova ejecta. We have approximated b-f collisional rates using the semiempirical formula of Drawin (1961). The b-b collisional rates were approximated by the semiempirical formula of Allen (1973), while Van Regemorter’s (1962) formula was used for permitted transitions. In the present calculations, we have neglected collisions with particles other than electrons because the cross sections are largely unknown.

3. RESULTS

We have computed a grid of models with 50 radial points to investigate the effects of NLTE on the atmospheric structure and the spectra of novae. All models include the NLTE treatment as discussed above as well as the standard PHOENIX equation of state and additional LTE background lines (about \(2 \times 10^{6}\) atomic lines). The NLTE effects are included in both the temperature iterations (so that the structure of the models includes NLTE effects) and all radiative transfer calculations. For primary NLTE lines we add 3–5 wavelength points within their profiles to the global wavelength grid (the transfer equation, the rate operators, and the approximate rate operators are computed for every wavelength point that falls into the profile of each primary line, resulting in substantially more wavelength points per line due to the line crowding). This procedure typically leads to about 120,000–190,000 wavelength points for the model and the synthetic spectrum calculations. We iterated the models until the radiative energy conservation is fulfilled better than 1% for both the comoving frame flux and its derivative and the NLTE departure coefficients are converged better than 1% at the same time. We have found in test calculations that this is necessary and sufficient to obtain a converged solution (see also Hauschildt 1993). On a single-processor Cray C90 or a single-processor HP 9000-C180 workstation, a typical model calculation with 10 iterations requires about 18 hr of CPU time. On five thin nodes of an IBM SP2 parallel machine using the parallel version of PHOENIX (Hauschildt et al. 1997), the same calculations also require about 18 hr of wall-clock time.
3.1. NLTE Effects on the Concentration of Atoms and Ions

We plot the relative concentration, \( P_i/P_{\text{gas}} \), where \( P_{\text{gas}} \) is the total gas pressure, as a function of the standard optical depth \( \tau_{\text{std}} \) (which we define as the absorption optical depth in the continuum at 5000 Å) for a variety of atoms and ions for both the LTE and the NLTE cases in Figures 1–7. The LTE plots were constructed using the NLTE structure of the model atmosphere but setting all departure coefficients, \( b_n \), to unity. Figure 1 shows the ionization balance for H and He as well as the concentration of free electrons in a nova model with \( T_{\text{model}} = 15,000 \) K. In this model, hydrogen recombines in the optically thinner regions of the atmosphere. Therefore, the NLTE effects lead to changes in the location and size of the recombination zone as compared to the LTE models. In particular, they lead to an earlier recombination of \( \text{H}^{\text{II}} \) to \( \text{H}^{\text{I}} \) at an optical depth of \( \tau_{\text{std}} \approx 10^{-3} \) compared to the LTE location of the H recombination zone around \( \tau_{\text{std}} \approx 10^{-5} \). In the outer atmosphere, however, the NLTE model shows a higher electron density compared to the LTE structure. Here, the NLTE effects cause a slight overionization of hydrogen. To a lesser degree, this is also the case for He. We remind the reader that any one of these models is actually a snapshot of the atmosphere in time, so the differences between the LTE and NLTE models will be important for the comparison between theory and observations in a sequence of spectra for novae in outburst.

In general, the effects of NLTE on the ionization balance are relatively small for C, N, and O. We demonstrate this in Figures 2, 3, and 4, where we plot the CNO ionization balance for those models with the largest NLTE ionization changes for these species. For carbon and nitrogen, the dominant ionization stage in the atmosphere is practically unaffected by NLTE over- or underionization. Less important ionization stages are affected, but their concentration is small compared to the dominant ionization stage. For oxygen, the situation is slightly different, as \( \text{O}^{+} \) recombines to \( \text{O}^{1} \) in the outer atmosphere at low optical depths. The location of the recombination point is now changed by the NLTE effects such that the NLTE models show a higher ionization in the outer atmosphere.

The ionization changes are more pronounced for sulfur and silicon; see Figures 5 and 6. Both elements have recombination zones in the optically thin parts of some nova models, and the location and the extent of these zones are altered by the NLTE effects. For these elements, the NLTE effects are not large enough to change the degree of ionization significantly farther away from ionization/recombination zones in the nova atmosphere. The concentrations of the nondominant ionization stages are influenced by NLTE effects, but the lines of these species are much weaker because of the relatively small number density of their parent ions. For the elements discussed so far, NLTE effects will be mostly present in the line formation rather than in changing the number density of the ions themselves.

For iron, the NLTE effects on the ionization balance are small but significant. We show this in Figure 7 for a model with \( T_{\text{model}} = 20,000 \) K. NLTE reduces the concentration of \( \text{Fe}^{+} \) ions in the \( \text{Fe}^{\text{II}} \) line-forming region \( (10^{-4} \leq \tau_{\text{std}} \leq 10^{-2}) \), thus reducing the overall strength of the \( \text{Fe}^{\text{II}} \) lines compared to the LTE case. These results are different from those we reported previously (Hauschildt et al. 1996a).

\[ \frac{P_i}{P_{\text{gas}}} \]

\[ \tau_{\text{std}} \]

Fig. 1.—Ionization balance for H and He for a nova model with \( T_{\text{model}} = 15,000 \) K. The plot shows the relative concentration \( P_i/P_{\text{gas}} \). Large symbols show the NLTE model; small symbols, the LTE results.
Fig. 2.—Ionization balance for C for a model with $T_{\text{model}} = 25,000$ K. The plot shows the relative concentration $P_i/P_{\text{gas}}$ for some C ions. Large symbols show the NLTE model; small symbols, the LTE results.

Fig. 3.—Ionization balance for N for a model with $T_{\text{model}} = 25,000$ K. The plot shows the relative concentration $P_i/P_{\text{gas}}$ for some N ions. Large symbols show the NLTE model; small symbols, the LTE results.
Fig. 4.—Ionization balance for O for a model with $T_{\text{model}} = 15,000$ K. The plot shows the relative concentration $P_i/P_{\text{gas}}$ for some O ions. Large symbols show the NLTE model; small symbols, the LTE results.

Fig. 5.—Ionization balance for S for a model with $T_{\text{model}} = 30,000$ K. The plot shows the relative concentration $P_i/P_{\text{gas}}$ for some S ions. Large symbols show the NLTE model; small symbols, the LTE results.
Fig. 6.—Ionization balance for Si for a model with $T_{\text{model}} = 25,000$ K. The plot shows the relative concentration $P_i/P_{\text{gas}}$ for some Si ions. Large symbols show the NLTE model; small symbols, the LTE results.

Fig. 7.—Ionization balance for Fe for a model with $T_{\text{model}} = 20,000$ K. The plot shows the relative concentration $P_i/P_{\text{gas}}$ for some Fe ions. Large symbols show the NLTE model; small symbols, the LTE results.
because, in these new models, we also include NLTE effects for Fe$^0$ and Fe$^{+2}$. In particular, the new treatment of Fe$^{III}$ reduces the NLTE effects of the Fe$^+/Fe^{+2}$ ionization balance; the full treatment of Fe$^{III}$ reduces the NLTE overionization for Fe$^{II}$ compared to our previous calculations. We show this in Figure 8, where we compare the full NLTE model (large symbols) with a model where Fe$^{II}$ is the only iron species treated in NLTE (but all other NLTE species are included). This shows that nova atmosphere calculations require a comprehensive NLTE treatment with many ions of the NLTE species. The new models fit the observed spectra of novae better than previous model generations (Schwarz et al. 1997b).

The behavior of the iron ionization balance becomes clearer by looking at the departure coefficients for Fe$^{I-III}$ for the $T_{\text{model}} = 20,000$ K model plotted in Figure 9 (see Hauschildt et al. 1996a for a more detailed discussion of the departure coefficients and source functions). The variations of $b_1$ with optical depth are complicated since their definition explicitly includes the concentrations of both electrons and the ground state of the next higher ionization stage (see Mihalas 1978, p. 219). It can be seen that the $b_1$ of Fe$^{II}$ and that of Fe$^{III}$ are about the same order of magnitude in the outer region of the atmosphere. Therefore, the ionization balance of Fe$^{II}$ to Fe$^{III}$ is comparable to the LTE case, because the ratio of their ground state departure coefficients $b_1$ is roughly unity. Treating Fe$^{III}$ in LTE is equivalent to setting the departure coefficients of Fe$^{III}$ to one. This would change the ratio of $b_1$ for Fe$^{II}$ to that for Fe$^{III}$ by a factor of $10^4$, overemphasizing the change in the ionization balance in the case of pure Fe$^{II}$ NLTE and Fe$^{III}$ NLTE. Therefore, in the full Fe$^{I-III}$ NLTE treatment, the Fe$^{II}$ lines are stronger than in models that treat Fe$^{II}$ as the only NLTE iron ion.

### 3.2. NLTE Effects on the Synthetic Spectra

#### 3.2.1. Overview

In Figure 10 we compare the synthetic spectra of four representative models for $800 \, \AA \leq \lambda \leq 2 \, \mu$m. The figure shows the progressive changes in the spectra with increasing temperature of the atmosphere. The ultraviolet region is particularly sensitive to such changes. In order to understand which lines are responsible for this, we show in Figure 11 synthetic spectra obtained by omitting LTE background lines; only NLTE lines provide line blanketing. The spectra are very similar to the full spectra shown in Figure 10. This indicates that the NLTE lines provide the bulk of the line blanketing and that the LTE background lines, even though numerous, constitute a comparatively small addition to the total line opacity. The fact that our detailed NLTE treatment allows us to handle the majority of the line blanketing in full NLTE is an important feature of the calculations, and the result that they constitute the majority of the line opacity is a basic result of this paper. The LTE background lines are, however, nonetheless still important in localized spectral regions and must be included for the most accurate model and synthetic spectrum calculations.

An additional result is that the NLTE effects on the synthetic spectra are far greater than those of the LTE background lines. In Figure 12, we show the synthetic spectra
Fig. 9.—Departure coefficients for Fe I-III for a model with $T_{\text{model}} = 20,000$ K. The signs indicate the ground state.

Fig. 10.—Comparison of NLTE synthetic spectra for the models. The dotted line gives the Planck function corresponding to the models' model temperature.
Fig. 11.—Comparison of NLTE synthetic spectra where the all LTE background lines have been neglected. The dotted line gives the Planck function corresponding to the models' temperature.

Fig. 12.—Comparison of synthetic spectra where the all NLTE departure coefficients have been set to unity. This corresponds to the pure LTE assumptions for the lines that are normally treated in NLTE. The dotted line gives the Planck function corresponding to the models' temperature.
obtained by setting all departure coefficients to unity, i.e., the pure LTE assumption, and in Figure 13, we show synthetic spectra obtained by using a single scattering line albedo of 0.95 for all lines, i.e., the NLTE lines are artificially treated in the same manner as the LTE background lines. An inspection of the figures shows that these synthetic spectra are very different from the full NLTE results shown in Figure 10. This is particularly true for the infrared lines, which are much stronger in the pure-LTE spectra than in the NLTE spectra. These also change from P Cygni profiles in the NLTE spectra to pure emission lines in the pure-LTE spectra. The scattering-LTE infrared spectra shown in Figure 13 retain the P Cygni profile, but the lines are now weaker than for the NLTE case. For the IR lines, the NLTE case thus falls somewhere in between the pure-LTE and scattering-LTE cases.

The IR lines are mainly isolated, single transitions. The situation is very different in the UV, where the lines overlap strongly due to the level distributions in the iron peak ions and form a pseudocontinuum. Individual lines are frequently so blended that it is impossible to assign a single identification to a feature in the synthetic spectrum (see Hauschildt et al. 1995 for discussion of this effect). Although one might think that the strong line overlap would reduce NLTE effects, the computations show that the LTE and NLTE UV spectra are very different for all models that we have calculated. This can be seen by closer inspection of Figures 10, 12, and 13. In both the pure-LTE and the scattering-LTE spectra, the UV flux blocking is more severe than in the NLTE models. For $T_{\text{model}} \leq 20,000$ K, the LTE spectra show in some regions (bluward of about 1500 Å) more than a factor of 10 less flux than the NLTE spectra. Whereas for $T_{\text{model}} = 15,000$ K, the pure-LTE and scattering-LTE spectra are similar to each other, the pure-LTE spectra show enormous emission lines$^1$ for larger model temperatures ($\approx 23,000–30,000$ K) in the 2000–3000 Å wavelength range that are absent in the NLTE spectra. These features are caused by clusters of iron lines (mostly Fe II) and the Mg II h + k doublet. These lines are much weaker in the scattering-LTE spectra, and they are nearly completely suppressed in the NLTE spectrum. This is extremely important for the evaluation of the optical taxonomy of nova spectra (see Williams et al. 1991) since the Fe II classification is based on the appearance of the optical emission features.

3.2.2. 1200–3200 Å: The IUE Spectral Region

In Figure 14, we show synthetic spectra for models with $T_{\text{model}} = 15,000$ K and $30,000$ K in the spectral range of the International Ultraviolet Explorer satellite (IUE). The spectra have been boxcar-smoothed to mimic the IUE low-resolution mode ($R = 300$). The LTE spectrum shows much less flux than the NLTE model in the short-wavelength end of the range (see below for the same effect in the far UV) for the 15,000 K model, which is typical of the spectral appearance at optical maximum during outburst. There are a number of features that are different between the NLTE

$^1$ Note that these are real emission features, not gaps in the pseudocontinuum.
and either of the two LTE spectra. This difference is even more pronounced in the model with $T_{\text{model}} = 30,000$ K, which is closer to the initial fireball spectrum and also to the appearance of novae near UV maximum during the optical decline. In particular, the pure-LTE spectrum shows very strong true-emission lines that are absent in the NLTE spectrum. Below about 2000 Å, both LTE spectra show less flux than the NLTE spectrum. A large fraction of the absolute flux difference can be traced to the NLTE treatment of CNO in the full NLTE models and thus shows that a detailed NLTE treatment of CNO is important for the short-wavelength band.

The results here have a bearing on the interpretation of the energy budget of the atmosphere during the expansion. Since novae initially evolve at constant bolometric luminosity, the changes we note between different treatments of the radiative transfer affect the interpretation of the physical conditions in the ejecta from observations in relatively small wavelength intervals. It is especially important for the determination of the mass of the white dwarf that the luminosity be accurately obtained from models; abundance determinations from the optically thick stage of the expansion are also dependent upon the correct assessment of the model temperature and other physical conditions within the atmosphere.

The shape of the pseudocontinuum is comparable between the different treatments, as might be expected with the enormous number of overlapping lines (which are essentially the same lines whether LTE or NLTE models are used) in a moving medium. The latter effect also points out an essential difference between static and moving atmospheres. The line overlap in moving media is enhanced and depends on the absolute velocities as well as on the form of the velocity profile, so that NLTE versus LTE differences for relatively weak lines are washed out in moving media while these differences might very well be detectable in static atmospheres. The pseudocontinuum thus gives information about the form of the velocity profile if analyzed in detail.

3.2.3. The Region around the Mg II 2800 Å Lines

In Figure 15, we show the region around the Mg II $h + k$ lines for a nova model with $T_{\text{model}} = 25,000$ K. Since this region is well observed at relatively high resolution ($R = 10,000$ with IUE) during the early stages of many nova outbursts, it is useful to calculate models that can be directly compared with the available data. The upper panel compares the NLTE spectrum with the pure-LTE and scattering-LTE spectra. Clearly, the pure-LTE assumption is very poor. The scattering-LTE and NLTE spectra are similar in small wavelength ranges (i.e., between 2430 and 2480 Å), but there are some significant departures. The emission component of the Mg II $h + k$ doublet is similar, but the absorption trough of the Mg II lines is too redshifted compared to the NLTE spectrum. This shows that, in NLTE, the Mg II line-forming region has shifted to the outer regions of the nova atmosphere. The pure-LTE model shows about the same wavelength shift as the scattering-LTE model but at a much higher flux level.

The bottom panel of Figure 15 compares the full NLTE spectrum with an NLTE spectrum with no LTE background lines (dotted curve). They are very similar, again illustrating that our set of NLTE species and lines is comprehensive enough to describe nearly completely the total opacity due to line blanketing. This panel also displays the result for a model where Fe I and III were kept in LTE (their lines being handled like LTE background lines). This is the spectrum for the model shown in Figure 8. Clearly, the LTE assumption for Fe I and, more importantly for this model,
for Fe III produces a significantly different spectrum. The total line blanketing due to Fe II lines is reduced due to the stronger ionization of Fe II to Fe III (see Fig. 8), which results in a slightly higher flux level. The Mg II \( h + k \) absorption trough is stronger and more blueshifted than in the full NLTE spectrum. This indicates a significant dependence of the Mg II line formation on Fe NLTE caused by line and continua overlaps and structure changes of the atmosphere in the line-forming regions for both Mg II \( h + k \) and the UV Fe II lines.

### 3.2.4. Near-Infrared Spectra

In Figure 16, we show the near-IR spectra (between 0.83 \( \mu m \) and 1.1 \( \mu m \)) for two model temperatures (15,000 K in the top panel and 30,000 K in the bottom panel). Although this part of the spectrum has not been extensively studied in most historical outbursts, it is becoming more accessible at high resolution (see, for instance, Hayward et al. 1996). Because the infrared becomes less opaque far earlier in the outburst than any other wavelength region and is therefore sensitive to the most rapidly moving parts of the ejecta, it is important for studying the initial stages of the expansion and such features as the homogeneity of the ejecta. It is also important for the energetics of the fireball and also for the stages just at and following UV maximum following optical peak. Although there are currently no spectra available in this region, with the exception of some low-resolution \textit{Voyager} 2 data for V1974 Cyg (Shore et al. 1994), this wavelength region will be accessible once the \textit{Far Ultraviolet Spectroscopic Explorer} is launched. We show the same models as in Figure 16 and add the NLTE spectra where all LTE background lines have been omitted (these spectra would have been identical to the full NLTE spectra shown in Fig. 16). Now both LTE spectra show less flux than the NLTE models. This is especially true near \( \lambda \approx 8500 \) \( \AA \), around the Ca II triplet, for the \( T_{\text{model}} = 15,000 \) K model. The pure-LTE lines are actually about a factor of 4 stronger than the NLTE lines in this region and are off the scale. In contrast, the scattering-LTE lines are generally weaker than the NLTE lines in the \( T_{\text{model}} = 15,000 \) K model (the exceptions are two lines at about 8500–8600 \( \AA \)) but are stronger than the NLTE lines in the 30,000 K model. The \( T_{\text{model}} = 15,000 \) K NLTE spectrum shows some lines around 9100 \( \AA \) that are in neither of the LTE spectra. In the same region, however, the scattering-LTE model shows lines in the \( T_{\text{model}} = 30,000 \) K model. There is no easily identifiable correspondence between the two LTE spectra and the NLTE spectrum, but the pure-LTE and scattering-LTE cases seem to bracket the NLTE spectrum for most lines (see also Baron et al. 1996 for a similar result in supernova atmospheres).

### 3.2.5. Far-UV Spectra

The situation in the far-UV (FUV) spectral range is very different from the near-IR (see Figure 17). This region is important for the energetics of the fireball and also for the stages just at and following UV maximum following optical peak. Although there are currently no spectra available in this region, with the exception of some low-resolution \textit{Voyager} 2 data for V1974 Cyg (Shore et al. 1994), this wavelength region will be accessible once the \textit{Far Ultraviolet Spectroscopic Explorer} is launched. We show the same models as in Figure 16 and add the NLTE spectra where all LTE background lines have been omitted (these spectra would have been identical to the full NLTE spectra shown in Fig. 16). Now both LTE spectra show less flux than the NLTE models.

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\textbf{Fig. 15}—Comparison of synthetic spectra for model atmospheres with \( T_{\text{model}} = 25,000 \) K. In the “pure-LTE” spectrum all NLTE departure coefficients have been set to unity, whereas in the “scattering-LTE” spectrum, the lines are assumed to have, in addition, an albedo for single scattering of 0.95. The latter corresponds to the assumptions for the LTE background lines. In the “NLTE, no LTE lines” spectrum, all LTE background lines have been neglected. The “NLTE, LTE for Fe I and II” spectrum uses LTE for Fe I and III (with an albedo for single scattering of 0.95) but includes all other NLTE species, in particular Fe II. This model has been fully iterated with its set of NLTE species. All other spectra use the structure of the full NLTE model.

\[ \text{\textit{Fig. 15}—Comparison of synthetic spectra for model atmospheres with } T_{\text{model}} = 25,000 \text{ K. In the "pure-LTE" spectrum all NLTE departure coefficients have been set to unity, whereas in the "scattering-LTE" spectrum, the lines are assumed to have, in addition, an albedo for single scattering of 0.95. The latter corresponds to the assumptions for the LTE background lines. In the "NLTE, no LTE lines" spectrum, all LTE background lines have been neglected. The "NLTE, LTE for Fe I and II" spectrum uses LTE for Fe I and III (with an albedo for single scattering of 0.95) but includes all other NLTE species, in particular Fe II. This model has been fully iterated with its set of NLTE species. All other spectra use the structure of the full NLTE model.} \]
Fig. 16.—Comparison of synthetic spectra for model atmospheres with \( T_{\text{mod}} = 15,000 \) K and \( T_{\text{mod}} = 30,000 \) K in the near-infrared. In the "pure-LTE" spectrum, all NLTE departure coefficients have been set to unity, whereas in the "scattering-LTE" spectrum, the lines are assumed to have, in addition, an albedo for single scattering of 0.95. The latter corresponds to the assumptions for the LTE background lines. The scattering-LTE spectra have been scaled so that their continua coincide with the NLTE continua. All spectra use the structure of the full NLTE model.

NLTE spectra. The line overlap in this spectral region is so severe that all of the features in the \( T_{\text{mod}} = 15,000 \) K model, and most of the features in the 30,000 K model, are blends. The LTE background lines have only small effects on the NLTE spectra, although they produce some absorption features just above the Lyman edge in the 30,000 K model. Again, practically all of the line blanketing is provided by lines that are treated in NLTE.

Fig. 17.—Comparison of synthetic spectra for model atmospheres with \( T_{\text{mod}} = 15,000 \) K and \( T_{\text{mod}} = 30,000 \) K in the far-ultraviolet. In the "pure-LTE" spectrum, all NLTE departure coefficients have been set to unity, whereas in the "scattering-LTE" spectrum, the lines are assumed to have, in addition, an albedo for single scattering of 0.95. The latter corresponds to the assumptions for the LTE background lines. The spectrum labeled "NLTE, no LTE lines" is identical to the NLTE spectrum but omits LTE background lines. All spectra use the structure of the full NLTE model.
3.2.6. Optical Spectra

We show optical spectra in Figures 18 and 19. Note that in these plots we plot $F_\lambda$ instead of $F_{\lambda}$ in order to flatten the slope of the continuum. Figure 18 demonstrates that the formation of the Balmer and optical Fe II lines cannot be properly calculated by assuming LTE. The Fe II lines are sensitive to NLTE effects and the pure-LTE and scattering-LTE approximations bracket the true NLTE shape of the emission parts of the lines. In addition, their P Cygni profiles cannot be correctly reproduced by LTE models. In the $T_{\text{model}} = 30,000$ K model, the optical Fe II lines are far too strong in the LTE spectra compared to the NLTE spectra.
Figure 19 shows the region around Hz. The Hz profile is very different between the LTE and NLTE spectra. While the NLTE emission strength is intermediate between the two LTE cases, the absorption part of the P Cygni profile is much stronger in the NLTE spectra than in either of the LTE spectra. The LTE background lines have no effect on the optical spectra—all the detectable lines in the NLTE spectrum are NLTE lines. This is similar to the case of the near-IR spectrum.

Thus, pure-LTE is an extremely poor assumption in nova atmospheres, although scattering-LTE is a somewhat better description. However, neither approach can replace a detailed and complete NLTE calculation—the complexity of the line formation in a nova atmosphere can only be adequately described by these detailed NLTE model calculations.

4. SUMMARY AND CONCLUSIONS

In this paper, we have presented a new set of model atmospheres, with significantly improved input physics for novae during the early phase of outburst. Modern numerical methods that allow the detailed treatment of thousands of NLTE levels now make it possible to include the majority of the line-blanketing opacity in detailed NLTE. LTE background lines from species that we do not treat explicitly in NLTE are not important for the structure of the atmosphere. They do, however, contribute some of the opacity and are necessary in order to reproduce some of the details in the synthetic spectra, particularly in the UV.

We have discussed the synthetic spectra for a number of models in detail. The comparison with LTE and simplified NLTE models for a number of specific wavelength ranges shows that (unfortunately) the detailed models cannot easily be approximated by simplified approaches. The addition of a detailed NLTE treatment for Fe i and (more importantly) for Fe iii changes the synthetic spectra compared to our previous results (Hauschildt et al. 1996a), which in turn improves the fits to observed nova spectra (Schwarz et al. 1997b). Therefore, it is important to include a number of ionization stages in detailed NLTE to model the line strengths correctly.

Our models span a wide range of model temperatures. These correspond to different times of the evolution of novae: in the early wind phase, we have \( T_{\text{model}} \approx 10,000-15,000 \) K; while in the later prenebular stage, \( T_{\text{model}} \approx 30,000 \) K. Thus, the analysis of a time sequence of nova spectra can be used to reduce the error bars of, e.g., abundances and to check for the internal consistency of solutions. In the second paper of this series (Schwarz et al. 1997b), we will present fits to observed nova spectra obtained with the models presented in this paper.

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