Papers published in 1996/1997 with support for the grant (for previous years results see the list of publications):

non-LTE model atmosphere analysis
of the early ultraviolet spectra of nova Andromeda 1986
Greg J. Schwarz, Peter H. Hauschildt, S. Starrfield,
E. Baron, France Allard, Steven N. Shore, and G. Sonneborn

We have analyzed the early optically thick ultraviolet spectra of Nova OS And 1986 using a grid of spherically symmetric, non-LTE, line-blanketed, expanding model atmospheres and synthetic spectra with the following set of parameters: $5,000 \leq T_{\text{model}} \leq 60,000\,\text{K}$, solar abundances, $p \propto r^{-3}$, $v_{\text{max}} = 2000\,\text{km}\,\text{s}^{-1}$, $L = 6 \times 10^4\,L_{\odot}$, and a statistical or microturbulent velocity of 50 km s$^{-1}$. We used the synthetic spectra to estimate the model parameters corresponding to the observed IUE spectra. The fits to the observations were then iteratively improved by changing the parameters of the model atmospheres, in particular $T_{\text{model}}$ and the abundances, to arrive at the best fits to the optically thick pseudo-continuum and the features found in the IUE spectra.

The IUE spectra show two different optically thick subphases. The earliest spectra, taken a few days after maximum optical light, show a pseudo-continuum created by overlapping absorption lines. The later observations, taken approximately 3 weeks after maximum light, show the simultaneous presence of allowed, semi-forbidden, and forbidden lines in the observed spectra.

Analysis of these phases indicate that OS And 86 had solar metallicities except for Mg which showed evidence of being underabundant by as much as a factor of 10. We determine a distance of 5.1 kpc to OS And 86 and derive a peak bolometric luminosity of $\sim 5 \times 10^4\,L_{\odot}$. The computed nova parameters provide insights into the physics of the early outburst and explain the spectra seen by IUE. Lastly, we find evidence in the later observations for large non-LTE effects of Fe II which, when included, lead to much better agreement with the observations.

The Effects of Fe II NLTE on Nova Atmospheres and Spectra
Peter H. Hauschildt, E. Baron, S. Starrfield, F. Allard
The atmospheres of novae at early times in their outbursts are very extended, expanding shells with low densities. Models of these atmospheres show that NLTE effects are very important and must be included in realistic calculations. We have, therefore, been improving our atmospheric studies by increasing the number of ions treated in NLTE. One of the most important ions is Fe II which has a complex structure and numerous lines in the observable spectrum. In this paper we investigate NLTE effects for Fe II for a wide variety of parameters. We use a detailed Fe II model atom with 617 level and 13675 primary lines, treated using a rate-operator formalism. We show that the radiative transfer equation in nova atmospheres must be treated with sophisticated numerical methods and that simple approximations, such as the Sobolev method, cannot be used because of the large number of overlapping lines in the co-moving frame.

Our results show that the formation of the Fe II lines is strongly affected by NLTE effects. For low effective temperatures, $T_{\text{eff}} < 20,000 \, \text{K}$, the optical Fe II lines are most influenced by NLTE effects, while for higher $T_{\text{eff}}$ the UV lines of Fe II are very strongly affected by NLTE. The departure coefficients are such that Fe II tends to be overionized in NLTE when compared to LTE. Therefore, Fe II-NLTE must be included with sophisticated radiative transfer in nova atmosphere models in order to reliably analyze observed nova spectra. Finally, we show that the number of wavelength points required for the Fe II NLTE model atmosphere calculations can be reduced from 90,000 to about 30,000 without changing the results if we choose a sufficiently dense UV wavelength grid.

Radiative Transfer in the Co-Moving Frame

*with E. Baron and A. Mezzacapa*

We discuss the formulation of the radiative transfer equation in the co-moving frame. We show that the time-independent or quasi static approximation is adequate for most astrophysical problems including supernovae. We also discuss the form of mean opacity in the co-moving frame and the use of Eulerian approximations such as Sobolev.

We have shown that advection cannot be neglected in the co-moving solution of the radiation transport equation. Its main effect is on the temperature structure through the term it adds to the equation of radiative equilibrium.

We have also shown that the Sobolev approximation is invalid for weak lines in the co-moving frame, since many of these lines overlap.

We have derived an approximate expression (good to $O(\beta)$) for the Rosseland mean opacity which can be used in radiation hydrodynamical calculations. The important effect of the Doppler shift is fully accounted for in this approximation. We have also derived an accurate and easy to implement approximation to the co-moving frame mean opacity.

The Physics of Early Nova Spectra

*with S. Shore, F. Allard, and E. Baron*

We discuss the physical effects that are important for the formation of the early spectra of novae. Nova atmospheres are optically thick, fast expanding shells with flat density profiles, leading to geometrically very extended atmospheres. We show that the properties of early nova spectra can be understood in terms of this basic model and discuss some important effects that influence the structure and the emitted spectrum of nova atmospheres,
e.g., line blanketing, NLTE effects, and the velocity field. The proper modeling of nova atmospheres is discussed and we give some computational details.

**NLTE Effects in Modeling of Supernovae near Maximum Light**  
*with E. Baron, P. Nugent, and D. Branch*

Supernovae, with their diversity of compositions, velocities, envelope masses, and interactions are good testing grounds for probing the importance of NLTE in expanding atmospheres. In addition to treating H, He, Li I, O I, Ne I, Na I, and Mg II in NLTE, we use a very large model atom of Fe II to test the importance of NLTE processes in both SNe Ia and II. Since the total number of potential line transitions that one has to include is enormous (≈ 40 million), approximations and simplifications are required to treat the problem accurately and in finite computer time. With our large Fe II model atom (617 levels, 13,675 primary NLTE line transitions) we are able to test several assumptions for treating the background opacity that are needed to obtain correct UV line blanketing which determines the shape of near-maximum light supernova spectra. We find that, due to interactions within the multiplets, treating the background lines as pure scattering (thermalization parameter $\epsilon = 0$) is a poor approximation and that an overall mean value of $\epsilon \sim 0.05 - 0.10$ is a far better approximation. This is true even in SNe Ia, where the continuum absorption optical depth at 5000 Å (≡ $\tau_{\text{std}}$) is $<< 1$. We also demonstrate that a detailed treatment of NLTE effects is required to properly determine the ionization states of both abundant and trace elements.

**Non-LTE Treatment of Fe II in Astrophysical Plasmas**  
*with E. Baron*

We describe our implementation of an extremely detailed model atom of singly ionized iron for NLTE computations in static and moving astrophysical plasmas. Our model atom includes 617 levels, 13675 primary permitted transitions and up to 1.2 million secondary transitions. Our approach guarantees that the total iron opacity is included at the correct wavelength with reasonable memory and CPU requirements. We find that the lines saturate the wavelength space, such that special wavelength points inserted along the detailed profile functions may be replaced with a statistical sampling method. We describe the results of various test calculations for novae and supernovae.

**Some Remarks About Nova Spectroscopy And Photometry**  
*with S. Pistinner and G. Shaviv*

We explore the proper parameterization of a novae envelopes. Numerical results show that certain regions of the continuum spectra are not sensitive to the input parameters.

We establish that in certain cases nova atmospheres have a continuum extinction coefficient that is dominated by scattering. The continuum scattering and the resulting continuum extinction in these cases are nearly gray. We apply and extend the small parameter Chandrasekhar expansion and use the particular properties of the opacity to study the effect of small absorption in the atmosphere. Two cases are treated, the case of a
static extended atmosphere, and the case of an extended atmosphere in motion. We solve
the transfer equation under the above physical conditions self consistently. The assumption
of radiative equilibrium allows us to obtain a self consistent temperature profile to validate
our approximation a posteriori.

Using this solutions, we a) derive conditions for the required magnitude accuracy
and the required observed frequency range needed to obtain a prescribed accuracy of
a nova parameters from comparison of spectra to models. b) assess and establish the
importance of spectroscopic ( in contrast to photometric ) measurements. c) show that
the use of synthetic spectra calculations are an essential part of any determination of nova
characteristics from the observations performed in the photospheric phase. We find that
the only wavelength region which is not affected by the physical conditions that were used
to arrive at these conclusions is the UV. Therefore, we conclude that the UV serves as the
wavelength region to derive nova parameters in a robust manner, when synthetic spectral
techniques are used.

**Synthetic Spectra and Mass Determination of the Brown Dwarf Gl229B**

*France Allard, Peter H. Hauschildt, Isabelle Baraffe and Gilles Chabrier*

We present preliminary non-grey model atmospheres and interiors for cool brown
dwarfs. The resulting synthetic spectra are compared to available spectroscopic and pho-
tometric observations of the coolest brown dwarf yet discovered, Gl229B (Nakajima et al
1995). Despite the grainless nature of the present models, we find the resulting synthetic
spectra to provide an excellent fit to most of the spectral features of the brown dwarf. We
confirm the presence of methane absorption and the substellar nature of Gl229B. These
preliminary models set an upper limit for the effective temperature of 1000 K. We also
compute the evolution of brown dwarfs with solar composition and masses from 0.02 to
0.065 \(M_\odot\). While uncertainties in the age of the system yield some undetermination
for the mass of Gl229B, the most likely solution is \(m \approx 0.04 - 0.055M_\odot\). In any case, we can
set an upper limit \(m = 0.065M_\odot\) for a very unlikely age \(t = 10\) Gyr.

**Water vapor in the spectra of cool stars**

*with H. Jones et al.*

We present comparisons between observed and synthetic spectra for water vapor tran-
sitions in a range of M dwarfs. The observations were from 2.85–3.40 \(\mu\)m where water vapor
transitions are strong in cool stars but relatively weak in the Earth’s atmosphere allowing
reliable observations to be made. They illustrate the strength of water vapor in cool dwarfs
and prove the ability of the current generation of infrared array spectrometers to take high
quality spectra in this little used spectral region. The synthetic spectra were computed
using PHOENIX and include preliminary ab initio calculations for ro-vibrational bands aris-
ing from water vapor transitions from levels up to \(J=30\) above the ground state. Although
the molecular opacity in the region of comparison is accurate, it is not around the peak of
the flux distribution and so the uncertainties of a reliable model atmosphere structure and
an absolute temperature scale still remain. Both the observed and synthetic spectra are
strongly sensitive to temperature. We find that within the calculational uncertainties the
predicted strengths and positions of the water transitions accord with the observations.
Infrared spectra of low-mass stars: towards a temperature scale for red dwarfs

with S. Leggett et al

We present new low-resolution (R ~ 250) 1.0—2.4 µm spectra for 13 red dwarf stars. The sample size is increased to 16 by including other published infrared spectra. New, as well as published, red spectra are presented for 10 of these 16 stars, and new and published VRIJHKLL' photometry is also presented. Both halo and disk stars are included in the sample, which covers a range of spectral type from dM0 to dM6.5. We derive bolometric luminosities and bolometric corrections from the observational data, finding good agreement with earlier results for the disk stars. We fit synthetic spectra generated by Allard & Hauschildt’s model atmospheres to the observed spectra. Although some discrepancies remain between the theoretical and observed spectra we find that the molecular features give a consistent value for effective temperature across the entire observed wavelength range. The \( T_{\text{eff}} \)'s and radii derived are in good agreement with structural models of low-mass stars. This removes a long-standing discrepancy between the observed and calculated locations of such stars in the HR diagram, for stars more massive than 0.1 M\(_\odot\).

New evolutionary tracks for very-low-mass stars

with I. Baraffe, G. Chabrier, and F. Allard

We present new evolutionary calculations for low-mass and very low-mass M-dwarfs, for a metallicity range \(-2 \leq [M/H] \leq 0\), down to the hydrogen-burning minimum mass \((0.07 < M/M_\odot < 0.6)\). The calculations include the best input physics presently available, i.e. equation of state, enhancement of nuclear reaction rates and atmosphere models. We use the most recent atmosphere models calculated by Allard and Hauschildt (1994), based on synthetic spectra at finite metallicity and grey atmosphere models based on Alexander and Fergusson (1994) Rosseland opacities. Comparisons are made with observational results down to the bottom of the main sequence, for different metallicities, in a magnitude (\( M_V \)) - color (\( V-I \)) diagram, and in color-color \( I, J, H, K \) diagrams. We find an excellent agreement between theory and observations over the whole characteristic temperature/luminosity range. This enables us to determine the mass of the faintest objects observed, which is found to be \( m_{\text{lim}} \approx 0.085 M_\odot \) for [M/H]=0 and -0.5, and \( m_{\text{lim}} = 0.09 M_\odot \) for [M/H]=-1.5, for an age of 10 Gyrs.

NLTE Model Atmospheres for M Dwarfs and Giants

with F. Allard, D.R. Alexander, A. Schweitzer, E. Baron

The atmospheres of M stars are dominated by a small number of very strong molecular compounds (H\(_2\)O, TiO, H\(_2\), CO, VO). Most of the hydrogen is locked in molecular H\(_2\), most of the carbon in CO; and H\(_2\)O, TiO and VO opacities define a pseudo-continuum covering the entire flux distribution of these stars. The optical “continuum” is due to TiO vibrational bands which are often used as temperature indicators for these stars. These may be the depth of the bands relative to the troughs in between them; or the depth of the VO bands; or of the atomic lines relative to the local “continuum”; or even the strength of the infrared water bands; all of these depend on the strength of the TiO bands and the amount of flux-redistribution to longer wavelengths exerted by them. Departures from LTE of the Ti I atom, and thus the concentration of the important TiO molecule,
could, therefore, have severe and measurable consequences on the atmospheric structure and spectra of these stars.

Due to the very low electron temperatures, the electron density is extremely low in M stars; even lower than in novae and SNe. Collisions with particles other than electrons, e.g., the H$_2$ or helium, are by far not as effective as electron collisions, both because of their smaller cross-sections and of their much smaller relative velocities. Therefore, collisional rates which tend to restore LTE, could be very small in cool stars. This in turn could significantly increase the importance of NLTE effects in M stars when compared to, e.g., solar type stars.

In this paper we discuss NLTE effects of Ti I in fully self-consistent models for a few representative M/Brown dwarf and M giant model atmospheres and spectra.

**Spectrum Synthesis of the Type Ia SNe**

*with E. Baron, P. Nugent, D. Branch*

We present NLTE synthetic spectra for the Type Ia supernovae SN 1992A SN 1981B, and SN 1991bg near maximum light. At this epoch both of the normal SNe Ia (SNe 1981b and 1992A) were observed from the UV through the optical. This wide spectral coverage is essential for determining the density structure of a SN Ia. Our fits are in good agreement with observation and provide some insight as to the differences between these supernovae. We show that SNe Ia form a spectral sequence which can be understood in terms of their luminosity. We also discuss the application of the spectral fitting expanding atmosphere method (SEAM) to SNe Ia which gives a distance that is independent of those based on the decay of $^{56}$Ni and Cepheid variable stars.
List of Publications
Peter H. Hauschildt

Publications in refereed journals:


Review Articles:


Selected Publications in conference proceedings:


Selected invited talks

1: “Model atmospheres for M dwarfs”, Colloquium of the Carnegie Observatory, Pasadena, 1995


4: “Model atmospheres for M dwarfs”, Invited colloquium at the Landessternwarte, Heidelberg, 1995


8: “Modeling Stellar Winds with PHOENIX”, Combined Baarsheva-Tel Aviv Astronomical Colloquium, Tel Aviv, 1997