NASA-CR-203971

FINAL REPORT NAGW-3315

Quasars are the most luminous objects in the universe and the highest redshift objects we can observe spectroscopically. Understanding their emission lines has a cosmological imperative since their spectra depend on luminosity. Once we can directly measure their luminosity the quasars will gauge the expansion of the universe at redshifts $z \lesssim 5$. At the same time, the origin of the chemical elements remains a central theme across much of stellar, galactic, and extragalactic astrophysics. Quasars probe early epochs in the formation of massive galaxies and their emission lines can reveal the composition of the interstellar medium (ISM) when the universe had an age well under a billion years.

Deducing reliable abundances and luminosities of galactic and extragalactic emission line objects is the central theme of this proposal. These lines are produced by warm ($\sim 10^4$ K) gas with moderate to low density ($n \leq 10^{12}$ cm^{-3}). Such gas is far from thermodynamic equilibrium and its physical conditions cannot be known from analytical theory. Rather, the observed spectrum is the result of a host of microphysical processes that must be numerically simulated in detail.

This grant supported the development of Cloudy, a large-scale code designed to simulate non-equilibrium plasmas and predict their spectra. My goals are to apply it to studies of emission line objects, but others have used it to study absorption line regions as well. The ionization, level populations, and electron temperature are determined as a function of depth by self-consistently solving the equations of statistical and thermal equilibrium. Lines and continua are optically thick and their transport must be treated in detail. Predictions of the intensities of thousands of lines and the column densities of all constituents result from the specification of only the incident continuum, gas density, and its composition. By their nature, such calculations involve enormous quantities of atomic/molecular data describing a host of microphysical processes, and the codes involved are at the forefront of modern computational astrophysics. Although the task is difficult the rewards are great, since numerical simulations make it possible to interpret the spectrum of non-equilibrium gas on a physical basis. I have developed Cloudy as an aid to this interpretation, much as an observer might build a spectrometer.

1.1. Extensions to the simulations

The code has been extended to include $\sim 10^4$ resonance lines from the 495 possible stages of ionization of the lightest 30 elements, an extension that required several steps. The charge transfer data base was expanded to complete the needed reactions between hydrogen and the first 4 ions and fit all reactions with a common approximation. Radiative recombination rate coefficients were derived for recombination from all closed shells, where this process should dominate . Analytical fits to Opacity Project (OP) and other recent photoionization cross sections were produced . Finally, rescaled OP oscillator strengths were used to compile a complete set of data for 5971 resonance lines.

Figure 1 shows a partial indicator of the scope of this activity, the number of lines of executable Fortran, as a function of time.

*1.1.1. **Community use*** Cloudy is widely used by others in their analysis and theory of spectroscopic observations. Figure 2 shows the number of refereed papers acknowledging the use of Cloudy through 1995. At least 138 papers were published in 1993 –1995, on subjects ranging from the intergalactic medium to inner regions of quasars. Although I was not a co-author on these projects, the code did play some role in their execution.

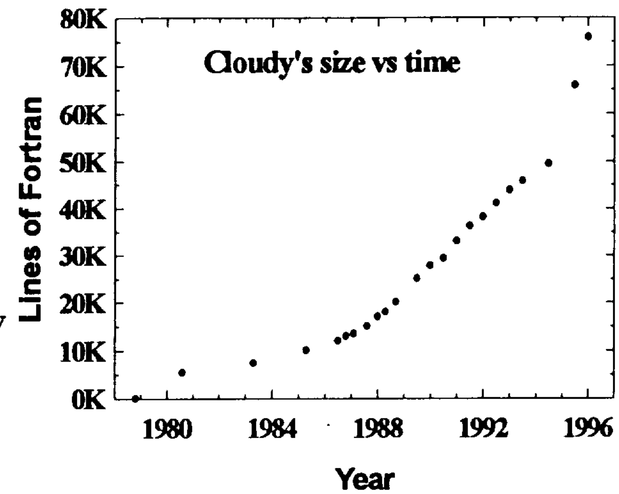

Figure 1 Cloudy's size as a function of time. This shows only the number of executable lines of Fortran. The total distributed source now constitutes ≈110,000 lines of code.

1.2. Active Galactic Nuclei

*1.2.1. **Narrow-lined objects*** Narrow emission lines of AGN form well away from the central engine, and their study can reveal much about the galactic environment. We examined the conditions within a cooling flow filament exposed to the radiation field of its environment, and followed the conversion of the grain-free gas from fully ionized to a fully molecular state. Ref 14 simulated conditions in gas near the center of the Milky Way, and predicted our *optical* emission line spectrum by matching the IR lines. Our galaxy would be classified as an HII galaxy by observers at the Virgo cluster. We showed that very high excitation lines detected by the Hopkins Ultraviolet Telescope (HUT) in NGC 1068 did not require very high (shock-like) temperatures. A photoionized gas produces these lines by a combination of continuum pumping and dielectronic recombination, and fits the NGC 1068 observations quite well.

*1.2.2. **Geometry of the broad line region*** The old picture of the broad line region (BLR) was a set of clouds with a homogeneous column density and ionization parameter (a picture shown to be incorrect by reverberation mapping . We showed that a population of low column density, optically thin, clouds must be present to explain the types of variability. We detected Ne VIII 774 and showed that this required a new population of very high ionization clouds. Distributed emission is further suggested by the delayed responses to continuum variability. The result of these studies is a picture of clouds with a very broad range of distances from the continuum source, densities, and levels of ionization.

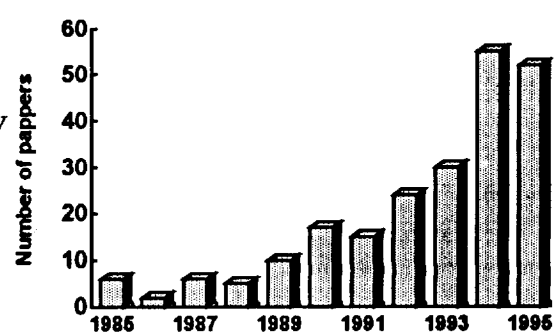

Figure 2 Refereed papers acknowledging Cloudy.

We analyzed high resolution line profiles of high luminosity and high redshift quasars. Lower ionization lines such as Al III] and Mg II form at high density, and were much sharper than high ionization lines such as NV. Radiative acceleration driving the 10^4 lines in Cloudy could push a wind from main sequence stars and produce the observed gas. This work was synthesized in the "locally optimally-emitting clouds" (LOC) model in which the line emitting environment has a wide range of properties but a uniform spectrum because of selection effects. The model will be developed to predict line variability, profiles, and intensities.

*1.2.3. **Metallicities in quasars*** This has been a major emphasis. These papers established that the NV/CIV ratio increases with luminosity, which we interpreted as a metallicity – luminosity relation. We carried out extensive calculations to reproduce observed limits to NV/CIV and NV/HeII in high luminosity high redshift quasars. Gas in the most luminous quasars had metallicities of at least 5 times solar. These metallicities are similar to those present in the ISM of massive galaxies during early epochs of rapid star formation. We examined implications of spectroscopy of broad absorption line gas and concluded that the absorbing gas has an enrichment consistent with the emitting gas, about 5–10 times solar.

1.3. Publications Supported by NAGW-3315

1.3.1. *Refereed publications*

1. *Atomic Data for Astrophysics. I. Radiative Recombination Rates for H-like, He-like, Li-like, and Na-like Ions over a Broad Range of Temperature*. D. A. Verner and G. J. Ferland. 1996, ApJS, 103, 467-473.
2. *Atomic Data for Astrophysics. II. New Analytic Fits for Photoionization Cross Sections of Atoms and Ions.* D. A. Verner, G. J. Ferland, K. T. Korista, and D. G. Yakovlev. 1996, ApJ, 465, 487-498.
3. *Atomic Data for Permitted Resonance Lines of Atoms and Ions from H to Si, and S, Ar, Ca, and Fe.* D. A. Verner, E. M. Verner, and G. J. Ferland. 1996, Atomic Data Nucl. Data Tables, 64, 1-180.
4. *Rate Coefficients for Charge Transfer Between Hydrogen and the First 30 Elements.* J. B. Kingdon and G. J. Ferland. 1996, ApJS, in press (August).
5. *Collisional Effects in He I: An Observational Analysis.* J. B. Kingdon and G. J. Ferland. 1995, ApJ, 442, 714-725.
6. *Theoretical He I Line Intensities in Gaseous Nebulae: NGC 1976, NGC 6572, and IC 4997.* J. B. Kingdon and G. J. Ferland. 1996, MNRAS, in press.
7. *Grains in Ionized Nebulae: Spectral Line Diagnostics.* J. B. Kingdon, G. J. Ferland, and W. A. Feibelman. 1995, ApJ, 439, 793-799.
8. *Grains in Gaseous Nebulae II: Heavy Element Depletions* J. B. Kingdon and G. J. Ferland. 1996, ApJ, in press.
9. *Temperatue Fluctuations in Photoionized Nebulae,* J.B. Kindgon and G.J. Ferland, 1995, ApJ 450, 691-704
10. *Physical Conditions in the Low Ionization Regions of the Orion Nebula.* J. Baldwin, A. Crotts, R. Dufour, G. Ferland, S. Heathcote, J. Hester, K. Korista, P. Martin, C. O'Dell, R. Rubin, A. Tielens, D. Verner, E. Verner, D. Walter, and Z. Wen. 1996, ApJ Letters, in press (Sept 10).

11. *[Fe IV] in the Orion Nebula.* R. H. Rubin, J. A. Baldwin, R. J. Dufour, G. J. Ferland, J. J. Hester, P. G. Martin, C. R. O'Dell, D. K. Walter, and Z. Wen. 1996, ApJ Letters, submitted.

12. *Reprocessing by Hot Gas in the Shell of Nova QU Vul 1984.* P. Saizar and G. J. Ferland. 1994, ApJ, 425, 755-766.

13. *The Physical Conditions Within Dense Cold Clouds in Cooling Flows.* G. J. Ferland, A. C. Fabian, and R.M. Johnstone. 1994, MNRAS, 266, 399-411.

14. *Nebular Properties and the Ionizing Radiation Field in the Galactic Center.* J. C. Shields and G. J. Ferland. 1994, ApJ, 430, 236-261.

15. *The Origin of NIII λ990 and CIII λ977 Emission in AGN Narrow Line Region Gas.* J. W. Ferguson, G. J. Ferland, and A. K. Pradhan. 1995, ApJ, 438, L55-L58.

16. *Optically Thin Broad-Line Clouds in Active Galactic Nuclei.* J. C. Shields, G. J. Ferland, and B. M. Peterson. 1995 ApJ, 441, 507-520.

17. *The HST Sample of Radio-loud Quasars Ultraviolet Spectra of the First 31 Quasars.* B. J. Wills, K.L. Thompson, M. Han, H. Netzer, D. Wills, J. Baldwin, G. Ferland, I. Browne, and M. Brotherton. 1995, ApJ, 447, 139-158.

18. *The HST Sample of Radio-loud Quasars The Lα/Hβ Ratio.* H. Netzer, M. Brotherton, B. Wills, M. Han, D. Wills, J. Baldwin, G. Ferland, and I. Browne. 1995, ApJ, 448, 27-40.

19. *Broad Ne VIII λ774 Emission from the Quasar PG 1148+549.* F. Hamann, J. C. Shields, G. J. Ferland, and K. T. Korista. 1995, ApJ, 454, 688-697.

20. *Locally Optimally-emitting Clouds and the Origin of Quasar Emission Lines.* J. Baldwin, G. Ferland, K. Korista, and D. Verner. 1995, ApJ, 455, L119-122.

21. *The Geometry and Kinematics of the Broad-Line Region in NGC 5548 from HST and IUE Observations.* I. Wanders, M. Goad, K. Korista, B. Peterson, K Horne, G. Ferland, A. Koratkar, R. Pogge, and J. Shields. 1995, ApJ, 453, L87-L90.

22. *The Chemical Enrichment of Gas in BALQSOs: Rapid Star Formation in the Early History of Galaxies.* K. Korista, F. Hamann, J. Ferguson, and G. Ferland. 1996, ApJ, 461, 641-656.

23. *Very High Density Clumps and Outflowing Winds in QSO Broad-Lined Regions.* J. A. Baldwin, G. J. Ferland, K. T. Korista, R. F. Carswell, F. Hamann, M. M. Phillips, D. Verner, B. J. Wilkes, and R. E. Williams. 1996, ApJ, 461, 664-682

24. *High Metal Enrichments in Luminous Quasars.* G. J. Ferland, J. A. Baldwin, K. T. Korista, F. Hamann, R. F. Carswell, M. Phillips, B. Wilkes, and R. E. Williams. 1996, ApJ, 461, 683-697

25. *An Atlas of Computed Equivalent Widths of Quasar Broad Emission Lines.* K. Korista, J. Baldwin, G. Ferland, and D. Verner. 1996, ApJS, in press.

26. *Accurate Hydrogen Spectral Simulations with a Compact Model Atom.* J. W. Ferguson and G. J. Ferland. 1996, ApJ, submitted.

27. *Physical Conditions of the Coronal Line Region in Seyfert Galaxies.* J. W. Ferguson, K. T. Korista, and G. J. Ferland, 1996, ApJ, submitted.

28. *Cloudy 90.* G. J. Ferland, K. T. Korista, D. A. Verner, J. W. Ferguson, J. B. Kingdon, and E. M. Verner. 1996, PASP, to be submitted Sept 1996.

1.3.2. *Internal Reports*

29. *HAZY, a Brief Introduction to Cloudy.* G. J. Ferland, University of Kentucky Physics and Astronomy Department Internal Report, URL http://www.pa.uky.edu/~gary/cloudy, 461 pages.

1.3.3. *Invited Reviews*

30. *The Lexington Benchmarks for Numerical Simulations of Nebulae*. G. Ferland, L. Binette, M. Contini, J. Harrington, T. Kallman, H. Netzer, D. Pequignot, J. Raymond, R. Rubin, G. Shields, R. Sutherland, and S. Viegas. 1995, in The Analysis of Emission Lines, Space Telescope Science institute Symposium Series, R. Williams and M. Livio, editors (Cambridge University Press), pp 83-96.

31. *Grains and the Origin of NLR Gas*. G. J. Ferland. 1993, in *The Nearest Active Galaxies*, (J. Beckman, L. Colina, and H. Netzer, Coordinadores) Consejo Superior de Investigaciones Cientificas), pp 75-82.

32. *Advances in Numerical Simulations of Nebulae*. G. J. Ferland. 1993, pp 123-130, *Planetary Nebulae*, IAU 155, R Weinberger and A. Acker, eds.

33. *Quasars, the Birth of Galaxies*. F. Hamann and G. J. Ferland. 1993, Séptima Reunión Regional Latinoamericana de Astronomía, Rev. Mex. Ast Ap 26, 53-63.

34. *The Metallicity-Luminosity Correlation in Quasars*. G. J. Ferland. 1994, in "Violent Star Formation from 30 Doradus to QSOs", La Palma, Spain.

35. *Photoionization Analysis of Emission Lines of Active Galaxies*. G. J. Ferland, 1994, in Indo-US Workshop on AGN and Quasars.

36. *Spectral Signatures of Rapid Star Formation*. G. J. Ferland, 1996, in Starburst Activity in Galaxies, International Program on Advanced Astrophysical Research, Puebla, Mexico, April 29-May 3, 1996.

1.3.4. *Contributed Abstracts*

37. *The Broad Line Region of Radio-Loud Quasars: New Hubble Space Telescope & Ground-Based Spectroscopy*, by H. Han, B. Wills, M. Brotherton, D. Wills, J. Baldwin, H. Netzer, G. Ferland, and I Browne, 1993 Bul AAS 25, 792.

38. *Implications of Nonlinear Line Response in Variable Seyfert Nuclei*, by J.C. Shields, G. Ferland, and B.M. Peterson, 1993 Geneva IAU AGN Meeting.

39. *A New GHRS Spectrum of the Orion Nebula*, by D. Walter, R. Rubin, R. Dufour, C.O'Dell, J. Baldwin, G. Ferland, J. Hester, and P. Martin, 1994 HST summer Conference.

40. *The Origin of NIII λ990 and CIII λ977 Emission in NGC 1068* by J. W. Ferguson, G. J. Ferland, 1995, Bull. Amer. Astron. Soc 26, 1339.

41. *HST - Ground-base Spectrophotometry of a Quasar Sample: Emission Line Profiles, Radio Emission, and Orientation?* by B. Wills, M Brotherton, D. Wills, K. Thompson, H. Netzer, J Baldwin, G. Ferland, R. Carswell, and M Han, 1995, Bull. Amer. Astron. Soc 26, 1340.

42. *New Atomic Data for Astrophysics* by D. Verner, G. Ferland, K. Korista, 1995, Bull. Amer. Astron. Soc 26, 1371.

43. *Grains in Ionized Nebulae: Spectral Line Diagnostics* by J. Kingdon, G.J. Ferland, and W.A. Feibelman, 1995, Bull. Amer. Astron. Soc 26, 1392.

44. *HST Spectroscopy of the Orion Nebula* by R.H. Rubin, G.J. Ferland, R.J. Dufour, D. Walter, C. O'Dell, J. Baldwin, J. Hester, and P.G. Martin, "Unsolved Problems of the Milky Way (IAU Symposiun No 169, The Hague, August 23-27, 1995), L. Blitz Editor.

45. *HST FOS Spectroscopy of the Orion Nebula*, by R.H. Rubin, D. Walter, R.J. Dufour, C. O'Dell, J. Baldwin, G.J. Ferland, J. Hester, and P.G. Martin, 1996, in The Analysis of Emission Lines, Poster Papers from the Symposium in Honor of the 70th Birthdays of D. E. Osterbrock and M. J. Seaton, p 66.

46. *A GHRS Spectrum of the Orion Nebula*, by D. Walter, R.H. Rubin, R.J. Dufour, C. O'Dell, J. Baldwin, G.J. Ferland, J. Hester, and P.G. Martin, 1996, in The Analysis of Emission Lines, Poster Papers from the Symposium in Honor of the 70th Birthdays of D. E. Osterbrock and M. J. Seaton, p 81.

47. *From Ly α to the Hydrogen Balmer Lines: Quasi-Simultaneous HST-Ground-Based Spectrophotometry of a Quasar Sample*, by B. Wills, J. Baldwin, D. Wills, H. Netzer, G. Ferland, I, Browne, M. Brotherton, R.F. Carswell, and H. Han, 1993 , 1996, in The Analysis of Emission Lines, Poster Papers from the Symposium in Honor of the 70th Birthdays of D. E. Osterbrock and M. J. Seaton, p 90.

48. *Models of FeII emission in infrared and optical wavelength range*. E. M. Verner, G. J. Ferland, K. T. Korista, D. A. Verner. 1995, Bull. Amer. Astron. Soc. 27, 840.

49. *Analytic fits for photoionization cross sections of atoms and ions.*, D. A. Verner, G. J. Ferland, K. T. Korista, D. G. Yakovlev. 1995, Bull. Amer. Astron. Soc. 27, 859.

50. *Metallicity of AGN Emission Line Regions - problems and pitfalls*, G. J. Ferland, 1995, Bull. Amer. Astron. Soc. 27, 871.

51. *The Chemical Enrichment of Gas in BALQSOs: Rapid Star Formation in the Early History of Galaxies*, K. Korista, F. Hamann, J. Ferguson, and G. J. Ferland, 1995, Bull. Amer. Astron. Soc. 27, 872.

52. *Fitting of atomic data for astrophysical applications*, D. A. Verner, G. J. Ferland, K. T. Korista, E. M. Verner, and D. G. Yakovlev 1995, Meudon Meeting on Atomic Needs for Astrophysics

53. *Locally Optimally Emitting Clouds and the Origin of Quasar Emission Lines*, K.T. Korista, J. A. Baldwin, and G.J. Ferland, 1995, Bull Amer Astron Soc 27, 1410.

54. *FeII Emission as a Probe in Radio Loud Quasars*, K. L. Thompson, B.J. Wills, M.S. Brotherton, D. Wills, H. Netzer, J. Baldwin, R. Carswell, and G.J. Ferland, 1995, Bull Amer Astron Soc 27, 1411.

55. *Effects of Extinction on Broad Band Spectra of HII Regions*, G.J. Ferland, R.H. Rubin, P.G. Martin, R. Dufour, C. O'Dell, Z. Wen, J. Baldwin, J. Hester, and D. Walter, Bull Amer Astron Soc 27, 1439.

56. *The N/O Abundance Ratio in the Orion Nebula from UV Lines*, R.H. Rubin, G.J. Ferland, P.G. Martin, R. Dufour, C. O'Dell, Z. Wen, J. Baldwin, J. Hester, and D. Walter, Bull Amer Astron Soc 27, 1439

57. *Locally Optimally Emitting Clouds and the Origin of Narrow Line Region Emission*, by J.W. Ferguson, K.T. Korista, G.J. Ferland and D.A. Verner, Bull. Amer Astron Soc, 28, 825.

58. *Locally Optimally Emitting Clouds and the Origin of AGN Broad Emission Lines*, by K.T. Korista, J.A. Baldwin, G.J. Ferland D.A. Verner and J. W. Ferguson, Bull. Amer Astron Soc, 28, 825.

59. *FeII Emission from the Orion Nebula*, by E.M. Verner, G.J. Ferland, K.T. Korista, and D.A. Verner, Bull. Amer Astron Soc, 28, 833.

60.*Quantitative Spectroscopy of High Redshift Quasars*, by G. Ferland, J. Ferguson, K. Korista, D. Verner, and K. Verner, Bull. Amer Astron Soc, 28, 866.

61.*Atomic Data for Permitted Resonance Lines*, by D. A. Verner, E.M. Verner, and G.J. Ferland, Bull. Amer Astron Soc, 28, 907.