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CLOUDY 94 AND APPLICATIONS TO QUASAR EMISSION LINE REGIONS

Gary J. Ferland

Department of Physics and Astronomy, University of Kentucky, USA

RESUMEN

Se describen los desarrollos recientes del código Cloudy, en su versión 94, realizados a partir de la versión anterior C90 (Ferland et al. 1998), así como su aplicación a regiones de líneas de emisión en cuasares. Este código, desarrollado de la forma en que un observador contruiría un espectrómetro, es una herramienta poderosa para obtener la composición química del gas y la luminosidad de cualquier fuente de líneas de emisión. El avance reciente más importante es el modelo “Locally Optimally-emitting Cloud” (LOC) para la región de líneas de emisión en AGN (Baldwin et al. 1995). Se muestra que varios efectos de selección, junto con la amplia gama de condiciones del gas, impiden obtener información sobre los detalles de los emisores. Esto es un avance importante que permite concentrarnos en la información relevante, como son la luminosidad y composición química de los cuasares.

ABSTRACT

This review discusses the most recent developments of the plasma simulation code Cloudy and its application to the emission-line regions of quasars. The long-term goal is to develop the tools needed to determine the chemical composition of the emitting gas and the luminosity of the central engine for any emission line source. Emission lines and the underlying thermal continuum are formed in plasmas that are far from thermodynamic equilibrium. Their thermal and ionization states are the result of a balance of a vast set of microphysical processes. Once produced, radiation must propagate out of the (usually) optically thick source. No analytic solutions are possible, and recourse to numerical simulations is necessary. I am developing the large-scale plasma simulation code Cloudy as an investigative tool for this work, much as an observer might build a spectrometer. This review describes the current version of Cloudy, version 94. It describes improvements made since the release of the previous version, C90 (Ferland et al. 1998).

The major recent application has been the development of the “Locally Optimally-Emitting Cloud” (LOC) model of AGN emission line regions (Baldwin et al. 1995). Powerful selection effects, introduced by the atomic physics and line formation process, permit individual lines to form most efficiently only near certain selected parameters. These selection effects, together with the presence of gas with a wide range of conditions, are enough to reproduce the spectrum of a typical quasar with little dependence on details. The spectrum actually carries little information to the identity of the emitters. I view this as a major step forward since it provides a method to handle accidental details at the source, so that we can concentrate on essential information such as the luminosity or chemical composition of the quasar.

Key Words: **ATOMIC PROCESSES — LINE FORMATION**

1. INTRODUCTION

Nearly all quantitative information we have about the cosmos, whether H II regions, planetary nebulae, Seyfert galaxies, or high redshift quasars, comes from analysis of spectroscopic observations. Spectra can

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determine the chemical state, source luminosity, or kinematic state, and infer implications for the chemical evolution of the Universe. In all of these cases a compact energy source (whether black hole or star) produces an energetic continuum that is reprocessed into lines and continua by surrounding gas. The thermal and ionization states of the gas are set by a host of microphysical processes, many at the frontier of atomic/molecular physics. Once produced, the incident and emitted radiation must be transferred through opaque media. This set of strongly intercoupled problems must be solved simultaneously. I developed the radiative spectral synthesis code Cloudy, to do just this.

2. CLOUDY 94

Real non-equilibrium plasmas are extremely complicated, with a vast network of interactions between different atomic processes and between the same processes operating at different rates in different regions of the medium. The range of scientific problems that can be tackled depends heavily on the degree of simplification in the code; there are many new lines of research awaiting a better simulation. The fidelity of the simulation increases as the power of the computer makes more things possible, and the accuracy can also be improved as the atomic database advances. Methods to validate predictions must be developed since analytic answers are seldom possible. As a result the development of a simulation code like Cloudy is never complete.

Both the source code and the documentation for Cloudy are openly available on the web at the address http://www.pa.uky.edu/∼gary/cloudy. Other authors use it to produce roughly 100 papers per year. The previous gold version of the code was version 90, reviewed by Ferland et al. (1998). This document discusses improvements made in developing the current version, 94, released in late 1999.

2.1. *Recoding in C*

Cloudy was originally written in FORTRAN 66 and migrated to FORTRAN 77 during the 1980's as compilers became available. It could not go to Fortran 90 or 95 and remain accessible to the Open-Source/Linux community since GNU does not support modern Fortran. Fortran compilers can be purchased but these tend to be expensive.

I moved the code to C to take advantage of strong Open-Source support and to insure the future employability of my graduate students. A person who does not fall into the traditional research career path can easily find programming jobs at major astronomical centers if they are fluent in C. Incoming students often have a strong background in C and retraining them as Fortran programmers is not in their long-term interests. Cloudy is now roughly 160k lines of clean C, meaning that the source files can be renamed to file names ending in "cpp" and then compiled and linked as a C++ code. The code will move to C++ as gcc, its standard libraries, and the ANSI/ISO C++ standard, all mature. This conversion process is discussed further in Ferland (2000).

2.2. *The Ionization/Thermal Kernel*

Cloudy is designed to be both autonomous and self-aware. It will *probably* automatically converge a model and *certainly* complain if it encountered problems.

The code's ionization/thermal balance kernel was rewritten to incorporate all lessons learned from problems encountered. This kernel, the very core of the simulation, is a new code. The rewrite included global changes to make parallel processing possible. MPI, the growing standard for parallel control, is used as an option. C94 is now faster than C90 was, even on scalar machines.

Other changes were possible because of improvements in computers. Cloudy could not use double precision variables when originally written because of the time and memory penalty. Functions like exp and log were also slow. Today's machines are very efficient at evaluating such variables so there is little time penalty. As a result the algorithms could be changed to do better physics without making the code suitable only for supercomputers.

The biggest example of this is in applications to very low-density media. The cooling funciton and its derivative would underflow for a density less than 10^{-4} cm^{-3} when single precision was used. This forced a low density limit for the code. This part of the kernel is now in double precision, and there is no low (or high) density limit.

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2.3. *Automatic Validation of Results*

Reliability in the face of complexity is the single biggest hurdle to developing any large code. Cloudy now consists of over 160,000 lines of code, and a mistake in one of them could invalidate the entire simulation. The community developing such codes like Cloudy has always been highly collaborative, sponsoring meetings on a regular basis to compare predictions of various codes (see Ferland et al. 1995). This provides a framework for verifying overall predictions of any other plasma code.

Anything as large and complex as Cloudy must be thoroughly exercised and its predictions verified every time it is changed. It has always had an extensive set of test calculations, but these were only recomputed and checked several times per year because of the labor involved. As part of the expansion to C94 I developed a set of commands and Perl scripts to automatically confirm that the code obtains expected answers *for all tests every single night*. This already has had payback in the quick and automatic detection of bugs as soon as they are introduced.

The code also conducts a large number of internal checks during a calculation. Important quantities are calculated by two independent routines and their agreement is verified. The goal is to make the code wise enough to automatically catch errors or questionable results (Maguire 1993), and this is often the case today.

2.4. *All Emission Lines in a Common Data Format*

Emission lines were originally added as idiosyncratic individuals. This organization became impossible as the number of lines grew—there are now well over a million spectral lines. All lines, whether H I 21 cm or Fe Kα, have common data handling needs. A single emission line data structure was created, and all lines moved into this form. For internal book keeping purposes, there is really only one emission line, but there are a million instances of it. This coding is ANSI C but is only a few keystrokes from becoming a C++ class. This is an important foundation for the move to exact line radiative transport methods, the next step in Cloudy's development.

2.5. *Charge Transfer*

Charge transfer rates are needed for all ions of the first 30 elements. Previous work had supplemented existing CT calculations with Landau-Zenner estimates for ions lacking accurate data (Kingdon & Ferland 1996). Ferland et al. (1997) extended this data set to include highly charged ions. The needed data are now complete, although of modest quality. Charge transfer also affects the thermal balance of the gas. The post-transfer species fly apart with kinetic energy equal to the difference in the ionization energies of the species. Kingdon & Ferland (1999) showed that this could affect some clouds and provided extended numerical fits to include all thermal effects.

3. THE LOC APPROACH TO ACTIVE NUCLEI

3.1. *Locally Optimally-Emitting Clouds*

Plasma simulations were one of the very first large-scale applications of computers to astronomy (Bahcall & Kozlovsky 1969; Davidson & Netzer 1979). Machines were slow and allowed only modest exploration of parameters, but showed that the spectrum was quite sensitive to the ionization parameter, the ratio of ionizing photon to hydrogen densities. The homogeneity of quasar spectra was taken as an indication that an unknown agent adjusted clouds so that they had similar parameters. Why are quasar spectra so homogeneous?

We developed the Locally Optimally-Emitting Cloud (LOC) model of the BLR (Baldwin et al. 1995) as a simple solution. ("Cloud" in this context is any thermal material, including winds such as Murray & Chiang 1998 or Bottorff et al. 1997). Baldwin et al. show the predicted equivalent width of some of the strongest AGN emission lines as a function of cloud parameters. Line emission peaks at some values of the parameters: powerful selection effects are at work. A particular line only radiates efficiently for parameters essentially determined by the atomic physics, and peaks at the "classical" cloud parameters deduced long ago. The spectrum is consistent

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with no preferred parameters at all—simply a mix of clouds with a very broad range of properties and atomic physics selection effects.

Inhomogeneities clearly exist across most emission-line regions, as can be inferred directly from reverberation mapping and from differences between the profiles of emission lines from different ions. Any realistic model must consider this structure. The LOC approach parameterizes this in a general way. First, large grids are generated for each emission line (Korista et al. 1997 shows many examples). Then, we integrate over this data cube using distribution functions, the goal being to understand what distributions are permitted or excluded. Distribution functions can take many forms including power laws or fractal-like chaos, but reflect the distribution of inhomogeneities. In our tests, the selection effects introduced by the atomic physics are so powerful that almost any function that is flat enough to give some weight to all parts of the plane will work. Questions concerning clouds or their origin no longer enter—the spectrum is mainly sensitive to ensemble properties like metallicity or the shape of the ionizing continuum.

3.2. *Quasars as Probes of Massive Galaxy Evolution*

The ultimate goals are to use quasars as probes of the early evolution of massive galaxies and the $z < 6$ universe. Baldwin and I organized a workshop ("Quasars and Cosmology", ASP Vol. 162) on this topic to summarize current knowledge, and to promote new work.

Our interpretation is that known correlations between quasar emission line properties and luminosity are caused by correlations between the luminosity and properties of the host galaxy, especially the metallicity. The theme is reviewed in a recent article (Hamann & Ferland 1999).

Korista, Baldwin, & Ferland (1998) shows that known correlations between metallicity, continuum shape, and luminosity can reproduce the Baldwin effect—the inverse correlation between C IV equivalent width and quasar luminosity. After this paper was in press, Espey & Andreadis (1999) discovered a correlation between an ion's ionization potential and the slope of the line's Baldwin effect. They showed that Korista et al. had predicted this correlation (although we did not realize it). That this was well fitted by the LOC confirms the predictive power of the model, and is highly suggestive that this physical picture is generally valid.

4. THE FUTURE

The improvements in astronomical instrumentation promised in the near future will be a major revolution. It will be possible to routinely obtain spectra from X-ray through IR wavelengths. The challenge will be to develop the analysis tools needed to fully interpret these observations.

Numerical simulations of plasmas have always been limited by the available computer power. This caused workers to take one of two approaches—either do a complete job on the microphysics or the radiative transport. Cloudy has always taken the first approach—the microphysics is as complete as possible, but all lines are transferred with escape probabilities. The escape probability formalism is known to give exact results when the line source function does not vary across the forming region (Elitzur 1992). Conditions do vary, of course, and it is simply not known how strongly this affects predictions. Today, there is no definitive calculation that does both the microphysics and the radiative transport exactly.

The incorporation of exact radiative transport methods into Cloudy will be the next major improvement. The kernel and emission line structure rewrite described in section 2 above was done with this in mind. The combination of ever-faster processors, with the development of the accelerated lambda operator method (Rybicki & Hummer 1994 and references cited there), both make this possible and timely.

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Gary J. Ferland: Dept. of Physics and Astronomy, University of Kentucky, Lexington, KY 40506-0055, USA (gary@cloud9.pa.uky.edu).