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Spectroscopy and X-Ray Astronomy

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Abstract. The new x-ray astronomical observatories have sufficient spectroscopic capability to allow the determination of plasma conditions in the form of velocities, temperatures, densities, and turbulence parameters at levels that were previously unattainable. The utilization of these diagnostics are possible only if the atomic and plasma physics are well-enough understood to match the observational sensitivity.

1. Introduction

X-rays provide an undistorted view of the sky. Even if all the mass in the universe was in baryons, and its average density was high enough to eventually halt its expansion (both of which assumptions are inconsistent with recent observations), the universe would still be transparent to X-rays, on average.

The first non-solar X-rays were detected almost 40 years ago (Giacconi et al. 1962), in a rocket flight with Geiger counter detectors that were sensitive to few-keV X-rays but had no spectroscopic capability within its energy acceptance window. Nevertheless, that first detection of X-rays, from both a strong source in the constellation Scorpius (Sco X-1) and a seemingly diffuse component over the whole sky, could be considered to be a spectroscopic measurement of sorts. The very detection of few-kev X-rays virtually demands effective source temperatures of the order of at least tens of millions of degrees. In fact, the argument that such X-rays therefore required a "blue" star (i.e., "hot" stellar counterpart, in relative astronomical terms) was the rationale for the correct identification of Sco X-1 with the blue stellar object in the error box provided by a rotation modulation collimator observation from a subsequent rocket flight (Clark, et el. 1965).

Up until the present time, it is fair to say that the concentration of community effort in X-ray astronomy has been associated with imaging, rather than spectroscopy. This has primarily been associated with the identification of X-ray sources with optical and radio counterparts, and the subsequent determination of class properties. The earliest "imaging" was accomplished by the mechanical restriction of detector fields-of-view, but the subsequent development of true X-ray telescopes with both magnification and fine angular resolution have allowed the true imaging of extended sources and the reduction of observational backgrounds.

Nevertheless, most of the significant breakthroughs in our understanding of the fundamental nature of X-ray sources have come from analyses of aspects of the observations that are other than imaging. Some of the most fundamental have come from timing analyses. For example, the determination of the basic nature of the brightest (in apparent magnitude) X-ray sources was the result of the analysis of temporal variability alone, in much the same way as was the identification of radio pulsars powered by the slowing-down of rotating neutron stars (Gold 1968). X-ray pulsars were found in the early results from the first X-ray astronomical satellite *Uhuru*, but there were two very troubling aspects to the measurements. First, the pulse periods seemed much too long to match the X-ray luminosities (since the radio pulsar explanations required the power to go like the inverse fourth power of the period) and, even more troubling, the putative neutron stars in X-ray sources were speeding up instead of slowing down!

The resolution of this puzzle again came from two complementary temporal measurements on very different timescales: days and seconds (Schreier et al. 1972). The discovery of periodicity in the disappearance of the signal from some X-ray sources on timescales of days suggested to some observers that the signal dropouts might be eclipses in binary systems observed from close to their equatorial planes. This suggestion was clinched when *Uhuru* was able to measure Doppler variations consistent with exactly the day-scale eclipse=orbital periods in their second-scale pulse periods. The total disappearance of the signal was a clear indication that the X-ray source region was much smaller than the ordinary stellar component of the binary system, and the secular speed-up of the pulsations was consistent with the transfer of angular momentum with mass accretion to the neutron star.

New spectroscopic observations are playing an increasingly important role our understanding of the X-ray sky, and our group at the Goddard Space Flight Center has led the community in the development of spectroscopic instrumentation. The new generation of X-ray observatories is providing data of high enough quality that sophisticated modeling is required to use them to full advantage.

2. Some Definitions and Rules of Thumb

X-ray astronomers generally use energy E instead of wavelength λ, and the preferred unit of energy is eV.

The term "energy resolution" δE means the full-width-half-maximum of the detector response at a given energy E. It is also measured in eV.

The dimensionless term "resolving power" R is the ratio of the photon energy E to the energy resolution δE at that energy.

If the temperatures are high enough for the atoms of a specific atomic number to be totally ionized, the only lines that will be observed are those associated with recombination from hydrogenic atoms. Transitions to the ground state from the first excited state (Ly α) produce lines with energies 10.2Z^2 eV, so that the Ly α lines in the span of elements from oxygen to iron cover the energy range 0.65 keV to 6.9 keV, corresponding to most of the bandpass of current X-ray astronomical facilities. In very hot cosmic plasmas, therefore, where even-Z elements are much more abundant than odd-Z elements, an energy resolution of about 370 eV (δE=10.2[(10)^2-(8)^2]) (corresponding to a resolving power of only about 2 near oxygen Ly α) would be sufficient to unambiguously separate all the elemental species of interest. At energies near Ly α for Fe, the required δE would be 800 eV, corresponding to an R of about 9.

At somewhat lower temperatures, lines from helium-like ionization states dominate the emission spectrum over a relatively wide temperature range. Here the resonance line (corresponding to the $1s2p - 1s^2$ transition) for a given element is separated from the Ly α line from the same element by about 10Z eV. Here the δE required to resolve hydrogenic from helium-like oxygen would be about 70 eV (R=10), while 250 eV (R=30) would suffice for iron.

For cold gas, where the atoms are neutral (or low states of ionization), the energy separation between the helium-like resonance line and the K-line produced in the transition to the ground state after an inner-shell electron is removed from a close-to-neutral atom is, similarly, about 10Z eV.

In the spirit of defining a hierarchy of levels of spectroscopic sophistication, the lowest level might be that associated with merely recognizing temperature-equivalent conditions of at least ten million degrees by identifying the mere presence of X-rays above 1 keV. The next level might be the values discussed above that are required to separate elemental species, and the next again might be those required to separate ionization states in atoms into the three categories: cold, hot (helium-like) and very hot (hydrogenic).

Continuing the hierarchy, the next level might be that required to investigate the components of the K-emission from helium-like atoms, and from the satellite lines from slightly lower ionization species. There have been a variety of combinations of the relative strengths of the helium-like resonance, forbidden and intercombination lines that can provide plasma diagnostics (e.g., Bahcall and Sarazin 1978). Here the line separation is approximately Z eV, providing a requirement for δE of <10 eV (R>700) for oxygen and about 25 eV (R>300) for iron.

3. Gas Counter Spectroscopy

The proportional counters used for the earliest X-ray astronomical measurements had resolving powers of no more than 3 at iron, or about a factor of 3 too poor to provide the requirement defined in the previous section to barely be capable of detecting emission from isolated hydrogenic lines. The brightest X-ray sources detected in the first generation of X-ray astronomy, with fluxes of about 10^{-9} erg/(cm^2-s) for the ten brightest, could provide hundreds of detected photons to mechanically-collimated proportional counters in few-minute sounding rocket observations. First-generation "spectroscopy" generally characterized these sources as being consistent with either power laws or bremsstrahlung continua (or both) over a dynamic range similar to the resolving power of these detectors. This was actually a pretty good match, since spectral lines contribute much less to the luminosity than does the continuum at X-ray temperatures, and each of the few independent energy bins accumulated enough counts for about 10% statistical precision, which was not much worse than the detector calibration.

The advent of satellite observations provided the opportunity for deeper observations. This meant not only that the detectors had to be better-calibrated, but that better resolving power could be usefully applied. Several groups worked hard to provide proportional counters with the limiting resolving power of gas amplification systems of about 6 at 6 keV (for good proportional counters, δE is proportional to $\sqrt{E}$). This increased resolving power did not quite meet the definition of the last section that was based upon the separation of even-Z elements, but since iron is much more abundant than other heavy elements it allowed for the unambiguous detection of emission lines in sources with prominent (large equivalent continuum width) Fe-K features like Cas A (Serlemitsos et al. 1973). Careful detector calibration was essential since, in general, both line features and continuum gradients had to be "detected" via the residuals from the inconsistency of data with model spectra rather than from the prominent appearance of line features in the raw data.

4. Some Brief Remarks About Dispersive vs Non-dispersive Spectroscopy

The *Einstein Observatory* provided breakthroughs in spectroscopy as well as imaging. Dispersive grating and crystal spectrometers, which had been used to measure the X-ray spectra of huge solar flare fluxes available in rocket flights, could not easily be made with large enough effective geometric areas or reflection efficiencies to be useful for non-solar X-rays in early satellites. Coupling the dispersive gratings/crystals with the telescope provided large area with small focal plane detectors. The gratings were limited by the fact that the spectra were dispersed on the images of (typically) extended sources, and the crystals were limited by the fact that only a small bite of the whole spectrum could be dispersed (and registered) at any time. Both instruments provided some investigations with dispersed X-ray spectra at a resolving power of about 100, far exceeding what was possible at that time with non-dispersive detectors.

The new *Chandra* and *XMM* observatories have grating spectrometers, which utilize their imaging detectors to obtain resolving powers approaching 1000 at energies less than 1 keV (but <100 at the Fe-K lines). The first results from the *Chandra* gratings presented in this volume are spectacular, and demonstrate the need for careful calculations of the line spectra expected from higher ionization states.

As spectacular as these results are, non-dispersive spectrometers can offer several distinct advantages over dispersive techniques. They can have quantum efficiency approaching unity. They can simultaneously multiplex this efficiency over the entire energy bandpass of the telescope. They can utilize their imaging and spectroscopic capabilities simultaneously without interference. And, while dispersive techniques must have R proportional to wavelength (and therefore inversely proportional to energy), non-dispersive systems can have R increasing with energy faster than $\sqrt{E}$ and can actually provide higher R at higher E.

5. Non-dispersive Spectroscopy

The *Einstein Observatory* also included a new non-dispersive spectrometer that provided somewhat more general capability at a new level of sensitivity. The *Einstein* "solid state spectrometer" was a cryogenically cooled (to about 120 K) non-imaging silicon detector with R= 20 at the K-lines of Si and S (this would have been R=40 at the K-lines of Fe, but Fe-K energies were above the high-energy cutoff of the telescope).

The Japanese-led *ASCA* mission (the name is both a homonym for a fabulous mythic Japanese bird *Asuka* and the acronym for *Advanced Satellite for Cosmology and Astrophysics*; it was called *Astro-D* prior to its launch) carried the first CCD array, which provided true imaging capability with spectroscopic resolving power corresponding to that of the *Einstein* solid state spectrometer. *ASCA* had telescopes with sensitivity out to 10 keV, so that the Fe-K lines could be investigated.

All three of the new generation of X-ray observatories: *Chandra*, *Astro-E* and *XMM* each have imaging arrays of CCDs, with effective areas (at 1.5 keV) of about 500, 1600, and 2500 cm^2, respectively.

The totally new spectroscopic capability of *Astro-E* is the "quantum microcalorimeter." Operating at a temperature of less than 100 mK, the detector "noise" associated with the exchange of phonons between the X-ray absorber and the cold sink can be of the order of 1 eV. This instrument was originally chosen to be part of the complement for *Chandra* (Holt 1987). Practical imaging arrays of 32 detectors have been made for *Astro-E* with the total system "noise" being such that the energy resolution of each of the pixels is <10 eV, so that R at Fe-K is >500.

Such high resolving power makes the microcalorimeter competitive with dispersive techniques, but with the distinct advantages of high efficiency, simultaneous response over the whole available energy range, and no dispersion of the photons in the focal plane that can be confused with source extent. This is especially important in the case of line emission from spatially extended (i.e., larger than about 30 arc-seconds) objects that are rich in line emission, such as supernova remnants and clusters of galaxies.

At the time of this writing, the *Chandra* and *XMM* observatories are operational, while there has just been a tragic launch failure of *Astro-E*. This prevents the eagerly anticipated application of microcalorimeter technology, but it is planned to be the key focal plane instrument for future missions with even better resolution (<2 eV) with the utilization of TES (transition edge sensors) instead of FET (field effect transistor) readouts.

6. Summary

It is hoped that the next generation X-ray observatory *Constellation-X* will be launched before the end of the decade. Its next generation non-dispersive imaging spectrometer, baselined to be a focal plane array of microcalorimeters with TES readouts, will have a resolving power in excess of 3000 for Fe-K lines. *Constellation-X* will be optimized for spectroscopic investigations, but will naturally have large aperture in order to take advantage of its spectroscopic capability. The better the resolution, the larger the necessary aperture in order to assure that the statistical precision of the data is consistent with the calibration accuracy in each resolution element for typical observations. *Constellation-X* is expected to have an effective area in excess of 15000 cm^2 at 1.5 keV. With this aperture, the angular resolution is not expected to match that of *Chandra*, and is baselined at about 1/4 arc-minute. Remembering that X-ray telescopes have grazing-incidence geometries, an aperture this large would require a focal length of order 100 m if accomplished with a single telescope. The word "constellation" in the name derives from the fact that the baseline design includes multiple launches of extendible telescopes in order to achieve the total aperture.

Just as the increased resolving power demands increased aperture, it also demands increased understanding of the spectra associated with all ionization states of elements heavier than carbon.

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