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Electron distributions in X-Ray plasmas: spectral diagnostics with the 3s/3d line ratio in Fe XVII

Guo-Xin Chen[1] and Anil K. Pradhan[2]
[1] *ITAMP, Harvard-Smithsonian Centre for Astrophysics, 60 Garden St., Cambridge, MA 02138, USA,*
[2] *Department of Astronomy, The Ohio State University, Columbus, OH 43210, USA*

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ABSTRACT
Efforts to benchmark astrophysical observations with X-ray laboratory measurements have been stymied by observed and measured differences of up to a factor of two in the ratio '3s/3d' of Fe XVII lines at $\lambda\lambda \sim 17\AA$ and $\sim 15\AA$ respectively. Using the electron distribution function (EDF) as a new physical parameter, we compute the Fe XVII line ratios and account for these differences. Based on large-scale relativistic close coupling calculations using the Breit-Pauli R-matrix method, revealing the precise effect of resonances in collisional excitation, we employ collisional-radiative models using cross sections convolved with both the Gaussian and the Maxwellian EDF. Comparison with astrophysical observations and laboratory measurements demonstrates that (a) the 3s/3d line ratio depends not only on the EDF but also on the electron temperature/energy of the source, and (b) plasma conditions in experimental measurements and astrophysical observations may be quite different, and (c) departure from a Maxwellian should manifest itself in, and be used as a diagnostics of, particle distributions in plasmas.

Key words: Gaseous Nebulae – Optical Spectra: H II Regions – Line Ratios: Atomic Processes – Atomic Data

1 INTRODUCTION

Astrophysical X-ray sources cover a wide range of physical conditions in objects as diverse as stellar coronae, active galactic nuclei, X-ray binaries, supernovae, and afterglows from gamma-ray bursts. In principle, spectral diagnostics should provide accurate information on the particular plasma conditions, particularly from high-resolution observations possible with X-ray satellites Chandra and XMM-Newton (Canizares *et al.* 2000; Huenenmoerder *et al.* 2001; Saba *et al.* 1999). However, the diagnostics are contingent upon accurate theoretical models calibrated against precise experimental measurements. Several spectral lines from neon-like Fe XVII are prominent constituents in the soft X-ray region ∼15–17 Å, and have long been observed as potential diagnostics (Fig. 1). Recent electron beam ion trap (EBIT) experiments on Fe XVII line intensity ratios at the Lawrence Livermore National Laboratory (LLNL) (Beiersdorfer *et al.* 2002), and at the National Institute for Standards and Technology (NIST) (Laming *et al.* 2000), may establish these diagnostics, provided the experimental results, theoretical calculations, and astrophysical observations can be interpreted consistently. But the diagnostic capabilities of the Fe XVII X-ray line ratios have so far been limited because the line-formation mechanism is not well understood, and all spectral modeling codes carry large uncertainties.

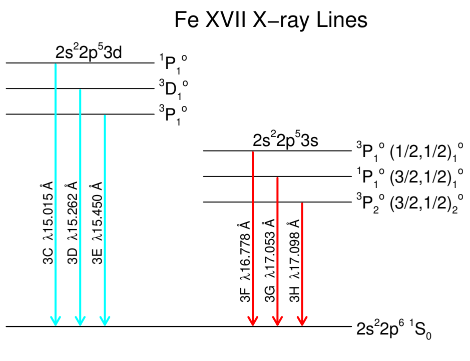

Figure 1. Schematic Fe XVII transitions for three 3s X-ray lines (3F, 3G, and 3H) and three 3d X-ray lines (3C, 3D, and 3E).

A schematic representation of the lines of interest in this Letter is given in Fig. 1. Excitation of the closed-shell

$2p^6$ ground configuration of neon-like Fe XVII to the $2p^5$ $3s$ and $2p^5$ $3d$ configurations corresponds to sets of 3 lines each at $\sim$ 17$\AA$ and $\sim$ 15$\AA$, respectively labeled as the '3s' and the '3d'. The interpretation of the 3s/3d ratios in Fe XVII from current EBIT and tokamak experiments, and astrophysical observations, are perplexing. Basically, there are two long-standing problems in Fe XVII spectra: the so called 3C/3D ratio and the 3s/3d ratio in Fe XVII (Laming *et al.* 2000; Beiersdorfer *et al.* 2002). The 3C/3D is the line intensity ratio of transitions labeled as 3C (λ 15.015 Å) and 3D (λ 15.262 Å). The ratio 3s/3d=$\frac{\mathrm{I(3F+3G+3H)}}{\mathrm{I(3C+3D+3E)}}$ (line 3H is sometimes labeled as M2), is the intensity ratio of three lines at $\lambda\lambda$ 17.098, 17.053 and 16.778 Å with one 3s electron in upper levels, over another set of three lines at $\lambda\lambda$ 15.015, 15.262 and 15.450 Å with one 3d electron in upper levels.

In the past theoretical predictions of the X-ray line intensity ratio 3C/3D were about 50% or more higher than astronomical observations or laboratory experiments. Yet, the EBIT measurements were in agreement with each other and with observations. This problem has been addressed in our recent calculations (Chen and Pradhan 2002; Chen *et al.* 2003; Chen 2005) in the low electron impact energy region. In this low energy region, we carried out ab initio calculations using the Breit-Pauli R-matrix (BPRM) method (Berrington *et al.* 1995) including electron-impact excitation (EIE) resonances up to $n = 4$ levels (n is the principal quantum number), which play a key role in the solution of the 3C/3D problem. The resonance enhancement is extrapolated from $n = 4$ to $n = 5$ for the higher electron-energy (temperature) region (this extrapolation needs to be verified by further calculations). Similarly, the 3s/3d problem pertains to nearly a factor of 2 difference in the intensity ratio between the two sets of EBIT measurements (Beiersdorfer *et al.* 2002; Laming *et al.* 2000). Moreover, there is very large scatter in the 3s/3d ratios from all previous theoretical calculations and observations. However, this case is more complicated than the 3C/3D problem for two reasons. First, at low electron densities cascade effects have important or dominant contributions to the formation of some or all 3s X-ray lines; while the 3C and 3D lines are formed predominantly by EIE. Second, the 3s/3d ratio is very sensitive to plasma conditions under which these X-ray lines are formed. In contrast, the 3C/3D ratio is not very source sensitive i. e. it is determined mainly by atomic micro-processes. It is due to these two reasons that the measured and observed 3s/3d ratios for given temperature and density may differ by up to a factor of two — a difference that is a major unresolved problem in X-ray astrophysics.

One of main goals in this paper is also to introduce electron distribution functions (EDF) (e. g. Maxwellian and Gaussian EDF) as a new physical parameter for the study of X-ray formation mechanism. As evident from the results in this Letter, this new approach is essential to solve the long-standing 3s/3d problem in Fe XVII. The main point is that plasmas in EBITs and astrophysical sources may have different beam/particle distributions. In some laboratory plasmas e. g. EBIT experiments, the electron beam width may be Gaussian or non-Gaussian (non-Maxwellian). In astrophysical objects on the other hand the EDF is normally a Maxwellian, but there are important cases (such as magnetically driven plasmas) where the source may display a bi-Maxwellian character, or a non-Maxwellian component of electron fluxes with high-energy tails. The precise convolution of cross sections with velocity distributions must therefore be generally source-specific.

2 THEORY AND COMPUTATIONS

The extensive calculations of the Fe XVII collision strengths using the BPRM method and a 89-level close coupling expansion up to the $n = 4$ levels is described in earlier works (Chen and Pradhan 2002; Chen *et al.* 2003). Resonance structures in the collision strengths are delineated; the positions, strengths, and distribution of resonances have been illustrated in detail for many of the transitions of interest in this work. Considerable differences are found with respect to previous calculations that neglect resonances, such as several distorted wave results available in literature. The energy dependence of the collision strengths due to resonances introduces a temperature dependence in the averaged collision strengths with temperature dependent EDF's such as a Maxwellian. Moreover, the many Rydberg series of resonances, converging on to most of the 89 levels in the wavefunction expansion, are not uniformly distributed in energy. Therefore a Gaussian average yields significantly different values, depending on the assumed energy widths, than a Maxwellian average.

In the present work, in order to address the issue of EDF influence on line ratios in general, we recalculate the averaged collision strengths, or rate coefficients, and reconstruct the collisional-radiative model. We carry out separate convolutions of our detailed close-coupling cross sections with specific beam distributions e. g. a Gaussian average (GA) and a Maxwellian average (MA), *before* the construction of the collisional-radiative model. The Maxwellian averaged rate coefficients are computed for all transitions as

$$q_{ij}(T) = \frac{8.63\times10^{-6}\mathrm{cm}^3/\mathrm{s}\cdot\exp(-E_{ij}/kT_\mathrm{e})}{g_i\sqrt{T_\mathrm{e}/\mathrm{K}}}\Upsilon_{ij}(T_\mathrm{e}), \qquad (1)$$

where g_i is the statistical weight of the initial level and the quantity Υ_{ij} is the Maxwellian averaged collision strength:

$$\Upsilon_{ij}(T) = \int_{E_j}^{\infty}\Omega_{ij}(E)\exp(-E/kT_\mathrm{e})\ \mathrm{d}(E/kT_\mathrm{e}). \qquad (2)$$

In addition, calculation for all rate coefficients are repeated with Gaussian EDF's obtained using a specified energy spread ΔE to simulate different beam widths in EBIT experiments. The collisional-radiative model for the Fe XVII lines includes 3,916 transitions associated with the atomic model, which also employs new allowed and forbidden transition probabilities for Fe XVII recently computed by Nahar *et al.* (2003).

3 RESULTS AND DISCUSSION

The main results of the calculations and modeling of the 3s/3d line ratio are summarised in Fig. 2. The black arrow marks $T_\mathrm{M} \sim 4\times10^6$ K, the value of Fe XVII maximum abundance in coronal equilibrium. The red arrows mark different highest target thresholds that may be included in CC calculations. Although this study is based on one of the largest and most computer intensive BPRM close coupling calculations, we could only include target levels up to $n = 4$. Comparison with the two experiments shows that NIST EBIT data mimic our calculation assuming a Maxwellian averated EDF (MA), and LLNL data are in basic agreement with the GA results. However, there is some discrepancy with the LLNL results at the higher temperature end. The target levels with $n \geqslant 5$ are currently neglected in the 89CC BPRM calculations. This limitation could result in some cascade contribution to the 3s/3d X-ray line ratios (Liedahl 1999), as well as some missing resonance structures. We have used an EBIT electron beam distribution with FWHM (full width at half maximum) of 30 eV in our GA modeling.

Fig. 2 shows two sets of 3s/3d intensity ratios as functions of electron temperature or electron beam energy. The first set of calculations using MA collision strengths in the 89-level CR model appear as the black curve, calculated at two electron densities 10^{13} cm^{-3} (black solid line) and 10^{9} cm^{-3} (black dotted line); dependence upon electron density is negligible. The second set of data are shown by the blue solid curve with 3s/3d ratios using GA collision strengths with a FWHM of 30 eV (blue dotted curve is obtained with a 50 eV convolution which gives essentially the same results); the further calculation with a 5 eV convolution is also shown by the red solid curve. The oscillations in the 3s/3d values in the GA model are clearly seen. They are due to the distribution, strength, and the density of resonances in the collision strengths in different energy regions as sampled by the convolution function centered around a 30 eV or 5 eV FWHM Gaussian. This oscillation behavior is crucial in explaining accurately the energy (temperature) dependence of 3s/3d ratios in the EBIT experiments. All previous calculations either fail to get the correct 3s/3d line ratios, or fail to obtain their right temperature dependence. The observed 3s/3d ratios from the solar corona are marked with red circles. The open and filled blue circles with error bars mark in particular the coronal spectra of the solar-type star Capella, observed from Chandra and XMM-Newton respectively (Canizares *et al.* 2000; Audard *et al.* 2001). The LLNL EBIT experimental values are shown as green filled circles with error bars, and the NIST EBIT experimental values as two black open circles (without polarization corrections (Laming *et al.* 2000)) or two green open circles (with polarization corrections (Gillaspy *et al.* 2004)). N. B. NIST data in (Laming *et al.* 2000) are reported without polarization corrections while all the LLNL data in (Beiersdorfer *et al.* 2002) are reported with polarization corrections. Also shown for comparison are the very scattered 3s/3d ratios from the long history of various observations of solar, stellar, and disk coronae (corresponding references are given in the caption of Fig. 2).

The 3s/3d problem arises mainly from the factor two difference in the two EBIT experiments at the lower energy, and partly from the large scatter in other observations. This problem is more serious than the 3C/3D problem, as mentioned above, because the two EBIT group are in good agreement for the 3C/3D ratio. Also, the 3s/3d ratio is complicated by a complex line formation mechanism in the three 3s X-ray lines. Both, the cascade effects from high-lying levels and resonance effects, are important and need to be calculated accurately. First of all, we need to understand the difference in EBIT experimental values. We note that the 3s/3d values from EBIT measurements need to be interpreted with care in order to compare directly with astronomical observations because of different plasma conditions and/or different EDF. This point does not bear strongly on the 3C/3D problem, but for the 3s/3d problem it is critical in order to derive a correct interpretation. For example, a recent work (Beiersdorfer *et al.* 2004) reports *similar* values for the line ratio 3s/3C (which differs slightly from the ratio 3s/3d in the denominator) from two different sources, the LLNL EBIT and the tokamak Princeton Large Torus (Beiersdorfer *et al.* 2004). However, this kind of agreement as detailed in Fig. 7 of (Beiersdorfer *et al.* 2004) is most likely fortuitous. This difference in magnitude for GA results, decreasing monotonically with temperature over extended ranges but attenuated by oscillations due to resonances in specific energy regions, is clearly seen in Fig. 2 and is the general feature established in this work. At lower energies the effect of resonances belonging to low-lying levels is more pronounced, and decreases with successively higher levels. This asymmetry in the distribution of resonance strengths with energy is responsible for the overall behavior of the line ratio in Fig. 2.

Fig. 2 apparently shows that the NIST data at the lower energy agrees better with the primary MA calculations, although the EDF inside both the NIST and the LLNL EBITs is quite different from a Maxwellian. The dichotomy inherent in these results reveals the importance of precise determination of experimental beam energies and widths. The NIST data point at the lower energy could possibly correspond to the minimum in the fundamental oscillations of the 3s/3d line ratio, with a narrower EDF than the LLNL EBIT (Gillaspy *et al.* 2004). We further illustrate this by calculating a GA 3s/3d line ratio with a FWHM of 5 eV as shown in the oscillating red solid curve in Fig. 2. We find that indeed the NIST data (the green open circle with polarization correction) at the lower energy is located very close to a minimum in this red curve. The NIST data point (with polarization correction) at the higher energy is in agreement with our GA result. While at present the two sets of experimental data do not fully trace the theoretically predicted oscillations, the present results show that a much more detailed investigation of the fundamental nature of the measurements is required in order to reconcile the two sets of EBIT measurements, assuming that both are of claimed accuracy. Accurate measurements of beam widths are crucial, but to our knowledge have not been accurately determined or reported. The EDF, in turn, bears on physical effects such as space charge potential, beam currents, polarization corrections etc. (Gillaspy *et al.* 2004). Nevertheless, the theoretical sets of 3s/3d ratios clearly demonstrate that they are sensitive to the plasma conditions in the source (c. f. (Beiersdorfer *et al.* 2002; Beiersdorfer *et al.* 2004)). In order to interpret additional experimental information on these issues, the theoretical results will also need to be extended to other EDF to elicit a more complete description of resulting variations in line intensities.

The large-scale relativistic CC calculations for EIE of X-ray lines in Fe XVII (Chen and Pradhan 2002; Chen *et al.* 2003), and the study of different electron distribution functions in plasmas *via* CR models, appear

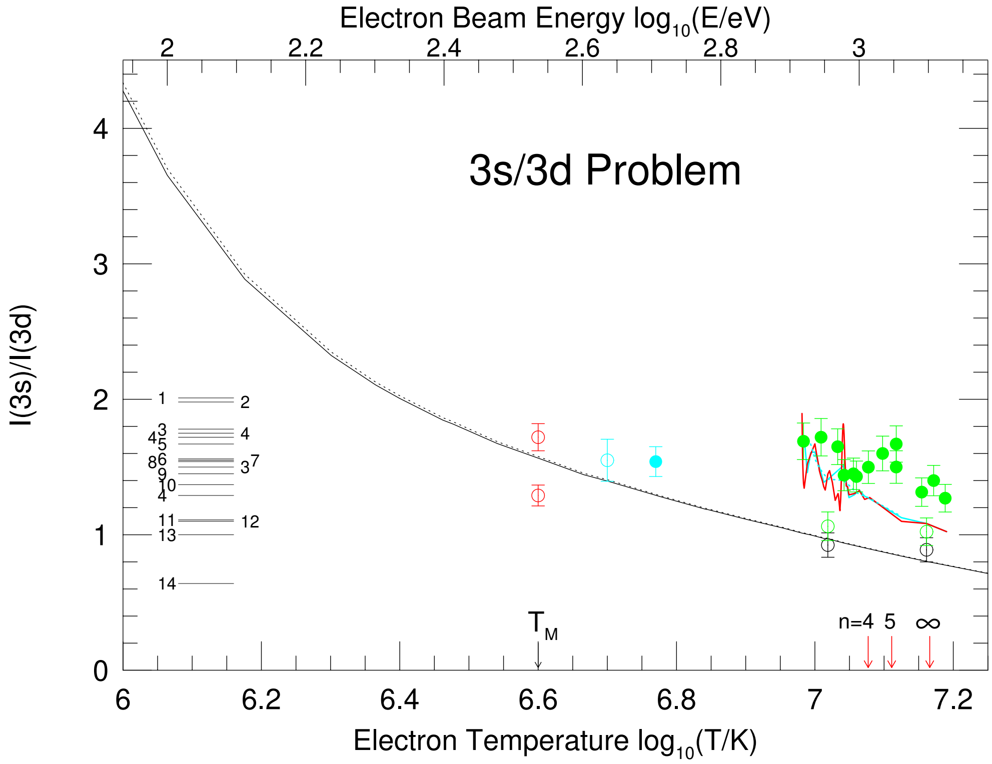

Figure 2. Theoretical X-ray line ratios 3s/3d as a function of electron temperature, or electron beam energy E = kT, are compared with observations from the corona of solar-type star Capella at $\sim$ 5–6 MK from Chandra (open blue circle) (Canizares *et al.* 2000) and XMM-Newton (filled blue circle) (Audard *et al.* 2001), from solar coronae at $T_{\rm m} \sim 4$ MK (red open circles) (Hutcheon *et al.* 1976), and from the LLNL and NIST EBIT experiments (filled and open green circles respectively) (Beiersdorfer *et al.* 2002; Laming *et al.* 2000)). See text for more discussions about the details of the 3s/3d problem. The scattered data for 3s/3d line ratios with labels 1–14 are for various types of observed values from solar, stellar and disk coronae (Mckenzie *et al.* 1980; Huenenmoerder *et al.* 2001; Ness *et al.* 2003; Mewe *et al.* 2001; Brinkman *et al.* 2000; Raassen *et al.* 2002; Phillips *et al.* 1997; Kahn *et al.* 2001; Xu *et al.* 2002).

to have resolved long-standing problems. The relativistic atomic calculations of Fe XVII and the line ratios among its diagnostic X-ray lines are in agreement with two independent measurements on EBIT (Beiersdorfer *et al.* 2002; Laming *et al.* 2000). It follows that the line ratios from the present 89CC CR model may be further applied to interpret X-ray spectra from a variety of X-ray sources observed from current space observatories, Chandra and XMM-Newton, and the upcoming next generation ones with greater spectroscopic capabilities, such as Constellation-X. Towards this goal additional calculations are in progress to calculate level-specific and total recombination rates from from Fe XVIII to Fe XVII , including radiative and dielectronic recombination in a unified scheme (Nahar and Pradhan 2004), and photoionization rates from Fe XVI to Fe XVII. However, astrophysical environments and plasma conditions may be different from those in EBIT plasmas. It is our goal to apply our 'calibrated' atomic data to interpret observed stellar and cosmic X-ray spectra of coronal or collisionally ionized plasmas such as stellar coronae, and photoionized or hybrid plasmas in, for example, from active galactic nuclei (AGN), quasars, disk coronae etc.

In summary, the new results for Fe XVII structure, collision dynamics, and spectral diagnostics reveal not only the effect of resonances and cascades, but also present a challenge for the study of source-specific effects of electron distributions and other conditions prevalent in EBIT, tokamak, laser-produced, and astrophysical plasmas. The present GA and MA averaged CR models should offer possible solutions to obtain more precise information on the physical parameters in the beam and the trap in EBIT experiments. We demonstrate that 3s/3d X-ray line ratios are not a universal constant in an optically thin plasma excited by electron impact, but instead depends sensitively on both the characteristic electron energy (temperature) and the detailed distribution of the electron energies about that characteristic value. Furthermore, the present results should be of general astrophysical importance for objects in a variety of equilibrium or non-equilibrium conditions. A direct physical consequence of this work is that the departure from a Maxwellian should manifest itself in, and be used as a diagnostics of, particle distributions in plasmas. In photoionization equilibrium (as opposed to coronal) we also need level-specific recombination cross sections and rates in order to compute emission line intensities (work in progress). Finally, the results in this Letter should be applicable to other neon-like ions of importance in X-ray lasers (Rosen *et al.* 1985), with population inversion among the upper n=3 levels due to EIE and/or electron-ion recombination.

4 CONCLUSION

The main conclusions of the present study are:

- Line intensities and ratios of the 3s and 3d line-complexes at $\sim 17\AA$ and $\sim 15\AA$ depend on electron distribution functions. The 3s/3d ratio can be a potential diagnostics of temperature, particularly for T $\leqslant T_m$ in astrophysical sources with Maxellian EDF's, and of energy, particularly at $E > kT_m$ in non-Maxwellian plasmas such as laboratory sources.
- The Maxwellian and Gaussian simulations of Fe XVII X-ray line ratios provide an indication of diffrerences in the conditions in the interaction regions of Electron-Beam-Ion-Traps; however, more experiments are needed to fully understand the physical factors involved.
- X-ray line ratios are a potential diagnostic of non-maxwellian astrophysical and laboratory sourcs, such as accretion discs, X-ray flares and bursts, and magnetically or inertially confined fusion plasmas.

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