Influence of Resonances on Spectral Formation of X-Ray Lines in Fe XVII

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(Received 24 January 2002; published 17 June 2002)

New theoretical results from large-scale relativistic close coupling calculations reveal the precise effect of resonances in collisional excitation of x-ray lines of Ne-like Fe XVII. By employing the Breit-Pauli R-matrix method and an 89-level eigenfunction expansion, including up to $n = 4$ levels, significant resonance enhancement of the collision strengths of forbidden and intercombination transitions is shown. The present results should help resolve long-standing discrepancies; in particular, the present line ratios of three benchmark diagnostic lines $3C$, $3D$, and $3E$ at 15.014, 15.265, and 15.456 Å, respectively, are in excellent agreement with two independent measurements on electron-beam ion traps. Strong energy dependence in cross sections due to resonances is demonstrated.

Prominent Fe XVII x-ray lines have long been observed from laboratory and astrophysical sources (e.g., [1–3], most recently in the *Chandra* and the *XMM-Newton* spectra of active galactic nuclei, x-ray binaries, supernovae, and flaring and nonflaring active stellar coronas [4,5]. In spite of a number of theoretical, experimental, and observational studies over decades there remain outstanding discrepancies related to atomic processes and astrophysical effects responsible for Fe XVII spectral formation in high temperature sources [1–15]. However, the interpretation of experimental and observational ratios of line intensities usually relies on collisional-radiative (CR) models using theoretical cross sections that neglect the fundamental role of resonant excitation, which preferentially affects the forbidden and intercombination transitions as opposed to dipole allowed ones. Of particular interest are three prominent x-ray transitions to the ground level $1s^2 2s^2 2p^6\ ^1S_0$ from excited levels: $3C$ (λ 15.014 Å) $1s^2 2s^2 2p^5[1/2]3d_{3/2}\ ^1P_1^o$ (level 27), $3D$ (λ 15.265 Å) $1s^2 2s^2 2p^5[3/2]3d_{5/2}\ ^3D_1^o$ (level 23), and $3E$ (λ 15.456 Å) $1s^2 2s^2 2p^5[3/2]3d_{5/2}\ ^3P_1^o$ (level 17) (level numbers denote energy order relative to the ground level 1). While the $3C$ is dipole allowed, the $3D$ and $3E$ are spin-forbidden intercombination transitions. All but one of the previous calculations used the distorted wave (DW) approximation that neglects channel coupling and, hence, resonances [8–11]. A point of confusion has been that the only previously coupled channel (CC) calculation [12] also yielded the same results as the DW calculations [11], because the CC R-matrix calculations were at energies *above all target levels in the eigenfunction expansion*; therefore resonances were not included. Since both the DW and the CC results agreed, it has hitherto been assumed that resonance effects are not important, and that the cross sections are relatively constant with energy (e.g., [7,13]). On the other hand, the experiments on electron-beam ion traps (EBIT) at Lawrence Livermore National Laboratory (e.g., [7]) and at the National Institute of Standards and Technology (NIST, [6]) do not measure absolute excitation cross

sections directly. Rather, they measure relative intensity ratios $R1 = 3C/3D$ and $R2 = 3E/3C$ at a few selected energies. Therefore the presence of resonances and, more generally, the energy variations are not readily discernible in experimental data (discussed later). The measured values differ from theoretical ones by up to 50% for $R1$ and a factor of 2 for $R2$ [4,6,7,13,14]. In order to account for these discrepancies several mechanisms based on atomic and astrophysical effects have been put forward, such as polarization, resonance scattering, and dielectronic satellite blending, which may be of varying importance under appropriate conditions [5–7,15].

However, as evident from the results in this Letter, there are extensive resonance structures in cross sections due to many infinite and interacting series of resonances converging onto the $n = 3$ and $n = 4$ levels that must be considered precisely. But for a complex ion such as Fe XVII the number of channels is very large and the CC calculations become enormously difficult, especially since relativistic fine structure must also be considered, in addition to other atomic effects. Using the Breit-Pauli R-matrix (BPRM) method [16,17], we construct a large eigenfunction expansion including 89 levels corresponding to 49 LS terms up to the $n = 3$ and $n = 4$ complexes of Fe XVII. Full details of the calculations will be presented elsewhere, but we briefly outline these below. The coupled-channel wave function expansion for the $(e + $ Fe XVII$)$ system may be expressed as $\Psi(E; e + $ Fe XVII$) = \sum_i \chi_i($Fe XVII$)\theta_e(\ell_i) + \sum_j c_j \Phi_j($Fe XVI$)$, where the Ψ denote the continuum $(E > 0)$ states of given total angular momentum and parity $J\pi$, expanded in terms of the core ion eigenfunctions $\chi_i(S_i L_i J_i)$; the $\theta_e(\ell_i)$ refer to the free-electron partial wave, and the Φ_j are short-range correlation functions that also serve to compensate for orthogonality constraints. The 89 levels belong to the configurations $2s^2 2p^6$, $2s^2 2p^5(3s, 3p, 3d)$, $2s^2 2p^5(4s, 4p, 4d, 4f)$, $2s^1 2p^6(3s, 3p, 3d)$, and $2s^1 2p^6(4s, 4p, 4d, 4f)$. We consider total symmetries $2J \leq 51$ of both parities explicitly in the BPRM calculations. The size of the calculations (possibly the largest $(e + $ ion$)$ scattering calculations to

date) may be gauged by the fact that the dimension of the Hamiltonian matrices ranges up to 10 286, for $J = 3.5$ with 395 free channels and 486 bound channels (Φ_j) (the largest number of free channels per symmetry is 401); 25 continuum basis functions are used to represent the $\Psi(e + \text{Fe XVII})$ in the inner R-matrix region. Relativistic distorted wave (RDW) and Coulomb-Born-Bethe approximations are employed to "top-up" the partial wave summations. Particular attention is paid to the resolution of resonances, with cross sections computed at about 20 000 energies.

Figures 1(a)–1(c) display the dense resonance structures in excitation collision strengths for the 3C, 3D, and 3E transitions, respectively. The results are compared with the RDW values (filled circles, [8]) which essentially represent previous DW calculations (such as from the HULLAC code [9,10]), and the one *nonresonant* value from the previous CC R-matrix calculation (filled square, [12]). As seen from the figures, the other data correspond roughly to the "background" collision strength compared to the present detailed results. The energy behavior of the three transitions may be ascertained from the eigenfunction expansions of the upper levels: 3C, $0.7857|27\rangle + 0.1753|23\rangle + 0.0305|17\rangle$; 3D, $0.7479|23\rangle + 0.2010|27\rangle + 0.0491|17\rangle$;   3E, $0.9150|17\rangle + 0.0767|23\rangle + 0.0030|27\rangle$, where the eigenkets correspond to the energy level indices. As the mixing coefficients indicate, the 3D has a significant component of $|^1P^0\rangle$, but the 3E considerably less so. Therefore the 3D would depart from LS-coupling to intermediate-coupling to jj-coupling schemes along the neon isoelectronic sequence with Z, *and with $\Omega(3D)$ increasing with energy* like $\Omega(3C)$. On the other hand, the 3E remains largely a (spin) forbidden transition and $\Omega(3E)$ decreases with energy. The Einstein A coefficients of the 3C, 3D, and 3E are 2.47×10^{13}, 6.01×10^{12}, and 9.42×10^{10} sec^{-1}, respectively. Other interesting atomic physics aspects of these and other transitions in neonlike ions will be discussed in later publications, with particular reference to laser transitions.

Spectral formations in laboratory and astrophysical plasmas need to be distinguished from each other. While we describe the latter using a CR model for Fe XVII, generally using collision strengths averaged over a Maxwellian characterizing a temperature, the former are measured using a monoenergetic beam with a certain velocity spread assumed to be a Gaussian. We compute the collision strengths averaged three ways: (i) Maxwellian, (ii) Gaussian, and (iii) numerical. Present results for (ii) and (iii) are shown in Figs. 1(a)–1(c). In order to compare with EBIT experiments the Gaussian FWHM is taken to be 30 eV. We note that the energy variations, dependent on resolution and density of resonances in a given energy region, are reflected in the Gaussian averages (ii); the numerical averages are slowly varying. The theoretical line ratios using Gaussian and
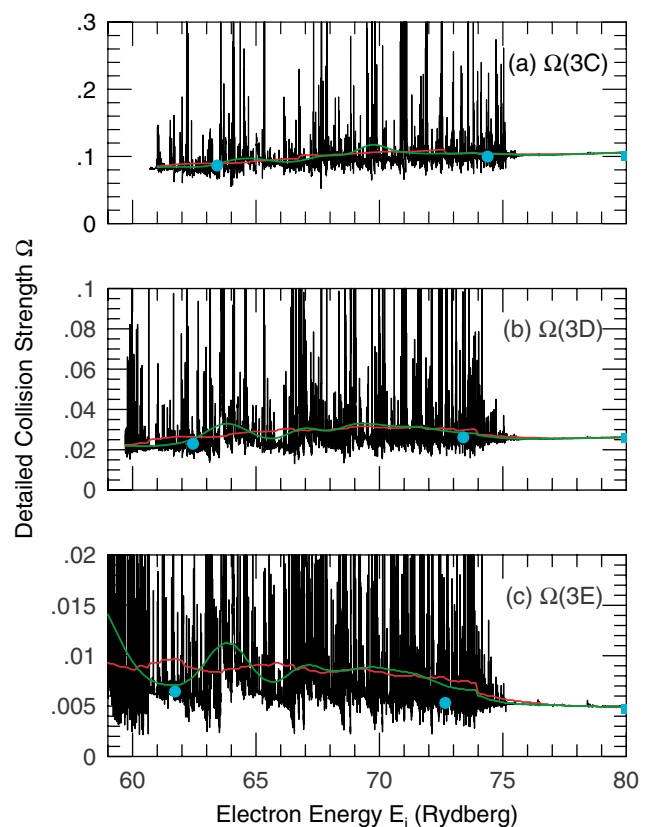

FIG. 1 (color). Breit-Pauli R-matrix collision strengths Ω for the allowed 3C and the intercombination (spin-forbidden) transitions 3D and 3E lines with detailed resonances; filled blue dots and the square are distorted wave results. The Gaussian (FWHM = 30 eV) and numerical averages are the green and red curves, respectively.

numerical averages $\langle\sigma \cdot v\rangle$ (GA and NA, respectively; σ denotes the cross section) are computed by taking account of the radiative branching ratios for 3C, 3D, and 3E which are: 1.0, 1.0, and 0.89, respectively. Therefore we have $R1 = 3C/3D = \langle\sigma_{3C}v\rangle/\langle\sigma_{3D}v\rangle$ and $R2 = 3E/3C = 0.89\langle\sigma_{3E}v\rangle/\langle\sigma_{3C}v\rangle$.   The results are compared with several EBIT measurements in Table I. These direct theoretical results agree with measured values to within experimental errors. Although our calculations extend up to the $n = 4$ levels, the highest threshold (level 89) is at $\sim$84.5 Ry or 1.15 keV; no resonances above this energy are therefore included.   While the line ratios at 0.85 and 0.9 keV are computed directly from the collision strengths as in Figs. 1(a)–1(c), some extrapolation of the averaged values is made to compare with the experimental value at 1.15 keV since we expect similar resonance enhancement above the $n = 4$ due to still higher thresholds. The GA results differ rather more than the NA results but still agree with experiment, in contrast to all other theoretical values. However, there is significant variation with energy in the GA collision strengths as they "oscillate" irregularly with energy depending on the density of resonances prevalent in a given

TABLE I.   Comparison of the present line ratios for $R1 = 3C/3D$ and $R2 = 3E/3C$ with EBIT measurements.

		$E_i = 0.85$ keV	0.9 keV	1.15 keV
$R1 = 3C/3D$	EBIT	2.77 ± 0.19[a]	2.94 ± 0.18[b]	$(3.15 \pm 0.17, 2.93 \pm 0.16)$[a]
	Theory[c]: NA	2.80	3.16	3.05[g]
	Theory[c]: GA	2.95	3.27	3.10[g]
	Other theory	$\cdots$	3.78,[d] 4.28,[e] 3.99[f]	$\cdots$
$R2 = 3E/3C$	EBIT	$\cdots$	0.10 ± 0.01[b]	$\cdots$
	Theory[c]: NA	0.11	0.085	0.07[g]
	Theory[c]: GA	0.11	0.083	0.07[g]
	Other theory	$\cdots$	0.04,[d] 0.05,[e] 0.05[f]	$\cdots$

[a]EBIT experiments at LLNL [7].
[b]EBIT experiments at NIST [6].
[c]Present theory with NA and GA.
[d]See Ref. [8].
[e]See Ref. [11].
[f]See Ref. [12].
[g]Present values with extrapolation of resonance enhancement from *ab initio* collision strengths from $E \leq 1.02$ keV (see text).

range. This appears to be reflected in similar "oscillatory" structure seen in the experimental values reported in [14] throughout the energy range 0.1–4 keV.

We also find that it is the $n = 4$ resonances, rather than the $n = 3$, that dominate the enhancement of electron impact cross sections in Fe XVII. The $n = 4$ resonances begin with resonant configurations $2s^2 2p^5 3\ell 4\ell'$ that manifest themselves from ~47 Ry, considerably *below* the excitation thresholds of the $2p \rightarrow 3d$ lines $3C$, $3D$, and $3E$ at ~60 Ry. Therefore there are relatively fewer $n = 3$ resonances, and the $n = 4$ resonances greatly influence the near-threshold behavior of these cross sections. In the region 75–84.5 Ry the resonances are due to thresholds corresponding to two-electron excitation configurations $2s 2p^6 4\ell$ with weakly coupled channels and resonances. This region is expected to be dominated by $n > 4$ resonances. It might also be mentioned that radiation damping of autoionizing resonances in cross sections of Fe XVII is known to be negligible [18–20].

We note a few specific cases that exemplify the findings in this Letter. Precise estimates of resonance scattering of the 15.014 Å line in the solar and stellar coronas may be made [6,13]. Based on our CR model with the present collisional data and extensive new radiative calculations for Fe XVII transition probabilities, we obtain the $3C/3D$ ratio to vary between 2.63–3.20, which agrees with the values from EBIT and from flaring solar coronas, but is still higher than the observed value [15] of 1.87 ± 0.21 from the nonflaring active region. This further suggests that resonance scattering of $3C$, or possibly some other mechanism, may be operative under astrophysical conditions [6]. Another example is the discussion of the diagnostic utility of the $3C/3D$ line ratio by Brown *et al.* [16] who (A) assume the cross sections to be relatively constant, and (B) multiply the RDW cross section of Zhang and Sampson [8] by 1.25 to agree with the measured value. From this Letter, neither (A) nor (B) is necessary. Furthermore, Brown *et al.* obtain the temperature dependence of $3C/3D$ including an inner-shell satellite line blended with

the $3D$, but using constant cross sections. A revised analysis with the present cross sections should yield a different temperature diagnostics.

More generally, the excitation of most of the $n = 3$ levels of Fe XVII is similarly affected. Using our 89-level CR model, with newly computed collsional and radiative data employing the BPRM method, we investigated the prominent transitions corresponding to the "coronal" x-ray lines $2s^2 2p^5 3s \rightarrow 2s^2 2p^6$ at $\lambda\lambda$ 16.780, 17.055, and 17.100 Å (e.g., [21]). Figure 2(a) shows the detailed collision strength for the forbidden $J = 1 \rightarrow 0$ λ 16.780 Å ($3F$) transition, compared with previous DW values (filled circles [8] and square [11]). The forbidden transitions are expected to be most enhanced by resonances, as in
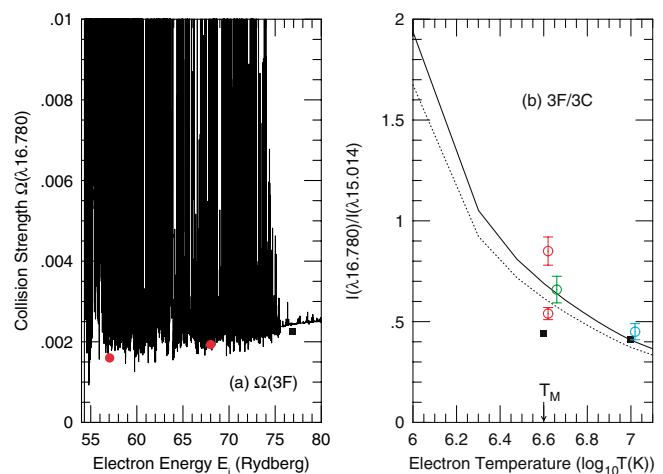

FIG. 2 (color).   (a) Breit-Pauli R-matrix collision strength Ω for the $3F$ line; the filled circles and square are nonresonant DW calculations; (b) line ratio $3F/3C$ vs T from an 89-level CR model. The electron densities for the solid and dotted curves are 10^{13} and 10^9 cm^{-3}, respectively. The four open circles with error bars are observed and experimental values: from the solar corona at $T_m \sim 4$ MK [3], from the corona of solar-type star Capella at ~5 MK [4], and from the EBIT experiment at 0.9 keV (log T = 7) [6]. The filled squares are values using DW results [11].

TABLE II.   Rate coefficients (10^{-13} cm^3 sec^{-1}) at $T_e = 200$ eV for resonant excitation to the $2s^2 2p^5 3s$ levels.

Final state	Present	Smith *et al.* [2]	Goldstein *et al.* [9]	Chen and Reed *et al.* [10]
$2p^5 3s\ ^3P_1^o$	22.7	48.0	15.12	14.2
All $2p^5 3s$ states	70.4	147.0	46.68	42.7

Fig. 2(a), since the background cross sections are much smaller than for allowed transitions. The temperature dependence of the forbidden ($3F$) to the allowed ($3C$) line ratio $R3 = 3F/3C = I(16.780)/I(15.014)$ is demonstrated in Fig. 2(b), and compared with that calculated using DW cross sections (filled squares [11]); at higher temperatures the resonance contribution decreases progressively with energy due to the Maxwellian factor. The electron density dependence is small; solid and dotted lines correspond to 10^{13} and 10^9 cm^{-3}, respectively. The four open circles with error bars are experimental and observed values. At all temperatures $T < 10^7$ K the present line ratio departs considerably from those using DW data without resonances to more than a factor of 3 at about 10^6 K—a fact of considerable importance in photoionized x-ray plasmas that have temperatures of maximum abundance much lower than that in coronal equilibrium $T_m \sim 4 \times 10^6$ K for Fe XVII, as marked.

Resonant excitation may be considered indirectly by approximate methods such as quantum defect theory [20] or isolated resonance approximations (IRA) [2,9,10]. Table II compares the present rate coefficients for the individual $3F$ line, and for all transitons to the $2s^2 2p^5 3s$ levels, with IRA calculations using HULLAC [9], multiconfiguration Dirac-Fock [10], and semirelativistic Hartree-Fock [2] methods. The present data are ~50% higher and differ from [9,10] which (i) neglect interference between resonances and (ii) take limited account of the several infinite Rydberg series of resonances, resulting in a considerable underestimate of resonance enhancement. The imprecision of the IRA is also indicated by more than a factor of 3 discrepancy between [10] and [2], both using IRA but with different decay channels. Our results are about a factor of 2 lower than [2]. Although resonances are generally less important for highly charged ions, the resulting enhancement in the BP R-matrix cross sections for forbidden and intercombination lines, compared to the allowed line, yields the ratios $R1$ and $R2$ closer to experiments compared to other works. We also note that ionization and recombination processes are not included in the present CR model; recombination from Fe XVIII to Fe XVII may also contribute to line emissions.

The main conclusions of this Letter are (I) resonances are present in Fe XVII collision cross sections at all energies, (II) the energy dependence of different types of forbidden, intercombination, and allowed spectral transitions is demonstrated, (III) the effect on diagnostic line ratios is significant, and may be up to several factors compared to previous data neglecting resonance effects, (IV) this work

is expected to be generally applicable to the temeprature and density analysis of many astrophysical and laboratory x-ray sources (especially photoionized plasmas and forbidden lines) not only for Fe XVII but also other neon-sequence ions of importance in x-ray lasers.

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