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POSTER PAPERS

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Large scale radiative and collisional calculations for Fe II

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Large scale computations are in progress to obtain radiative data for energy levels, oscillator strengths and photoionization cross sections, and for collision strengths of Fe II. Calculations are carried out in the close coupling (CC) approximation using the R-matrix method.

We define the atomic or ionic system as (N+1) electron system, and the residual ion or the target as the N-electron system. In CC approximation, the wave function of the (N+1) electron system is expanded in terms of target states as

$$\Psi^{SL\pi}(E) = A \sum_{i=1}^{I} \chi_i(r^{-1})\theta_i + \sum_{j=1}^{J} c_j\Phi_j, \quad (1)$$

where $\chi_i(r^{-1})$'s are the target states, and $\theta_i(r)$'s are the free electron wave functions, Φ_j's are square-integrable correlation type function for the bound states of the (N+1) electron system, and c_j's are variational parameters.

COLLISIONAL CALCULATIONS: Two sets of CC calculations, (1) a 38-term expansion in LS coupling and (2) a 41-level fine structure calculations in the Breit-Pauli approximation have been carried out for detailed collision strengths, Ω, including resonance structures. The first set includes the quartet and sextet terms and Ω's for 703 transitions in LS coupling are obtained. The second set includes a number of important fine structure levels from the quartet and sextet multiplets and Ω's for 820 transitions are obtained. The autoionizing structures enhance the background significantly. Computations are under progress now to carry out collision strength calculations using the 38-state LS exapnsion split into 142 J values for fine sructure transitions by algebraic transformations. This will result in collision strengths and rates for about 10,000 fine structure transitions of Fe II.

RADIATIVE CALCULATIONS: The complication in computation of Fe II radiative data arises because of large number of closely spaced energy levels of the "target" or residual ion Fe III requiring large CC expansions for Fe II system. Studies of effect of correlations were made using several sets of CC expansions. In the present calculations, a total of 83 Fe III states have been included to carry out CC calculations of Fe II. Table I shows number of target states, N_{CC}, that are included in CC expansion for each type of symmetry. $N_{SL\pi}$, the number of $SL\pi$, that form bound states and total number of corresponding bound states for each type of symmetry of Fe II are also given in the Table. Photoionization cross secitons are obtained for all bound states. Cross sections for photoionization of $3d^5 4s\ ^6D$ ground state of Fe II are presented in Fig. 1.

Present calculations are carried out in LS coupling. Table II shows number of oscillator strengths obtained for allowed bound-bound transitions for each kind of symmetry. The f-values or the oscillator strengths obtained in LS multiplet are now being converted to fine structure transitions using relative line strength scheme. The accuracy of fine structure f-values are improved by use of observed energies in JJ. Present results are compared with the observed values[1] as well as those of Kurucz[2] in Table II.

References:

1. J.R. Fuhr, G.A. Martin and W.L. Wiese, J. Phys. Chem. Ref. Dt. 17 (AIP, 1988).
2. R.L. Kurucz, "Semiempirical calculation of gf values: Fe II", Smithsonian Astrophysical Observatory Special Report 390 (Cambridge, 1981).

Table I: N_{CC} is the number of target states in the CC expansion, $N_{SL\pi}$ is the number of bound symmtries and N_{bnd} is the corresponding number of bound states ($n \leq 10$, $l \leq 7$). N_f is the number of oscillator strengths in LS multiplet. * implies partial data from ongoing work.

Symmetry	N_{CC}	$N_{SL\pi}$	N_{bnd}	N_f	Symmetry	N_{CC}	$N_{SL\pi}$	N_{bnd}	N_f
Octets	2	4	6	8	Quartets	58	19	305	9755
Sextets	21	19	200	4127	Doublets	62	12*	196*	4860*

Table II: Fine structure f-values for allowed transtions of Fe II.

Transition	$2J_i+1$	$2J_f+1$	f_{if} Present (OP)	Expt[1] (NIST)	Kurucz[2] (1981)
$^6D - ^6P^o$			0.12633		
	10	8	0.1264	0.11	0.144
	8	8	0.0449	0.051	0.0624
	6	8	0.0099	0.036	0.0401
	8	6	0.0814	0.091	0.0901
	6	6	0.0771	0.10	0.1035
	4	6	0.0377		
	6	4	0.0396	0.032	0.0437
	4	4	0.0887	0.087	0.1137
	2	4	0.1263	0.13	0.194
$^6D - ^6D^o$			0.2936	0.26	
	10	10	0.2400	0.22	0.262
	10	8	0.0548	0.065	0.0736
	8	10	0.0675	0.043	0.0456
	8	8	0.1313	0.11	0.135
	8	6	0.0948	0.099	0.117
	6	8	0.1248	0.084	0.088
	6	6	0.0502	0.045	0.052
	6	4	0.1176	0.11	0.133
	4	6	0.1748	0.12	0.133
	4	4	0.0032	0.0037	0.004
	4	2	0.1144	0.10	0.119
	2	4	0.2275	0.18	0.187
	2	2	0.0652	0.050	0.059
$^6D - ^6F^o$			0.3976		
	10	12	0.3425		0.37
	10	10	0.0527	0.028	0.038
	10	8	0.0043		
	8	10	0.2888	0.27	0.349
	8	8	0.0968	0.089	0.100
	8	6	0.0122		
	6	8	0.2431	0.20	0.287
	6	6	0.1313	0.12	0.142
	6	4	0.0227	0.019	0.019
	4	6	0.2031	0.19	0.249
	4	4	0.1610	0.14	0.181
	4	2	0.0314	0.031	0.0316
	2	4	0.1747	0.19	0.216
	2	2	0.2199	0.21	0.254

* This work is being carried out on the Cray Y-MP at the Ohio Supercomputer Center and is supported partially by a grant from NSF (PHY- 9115057).

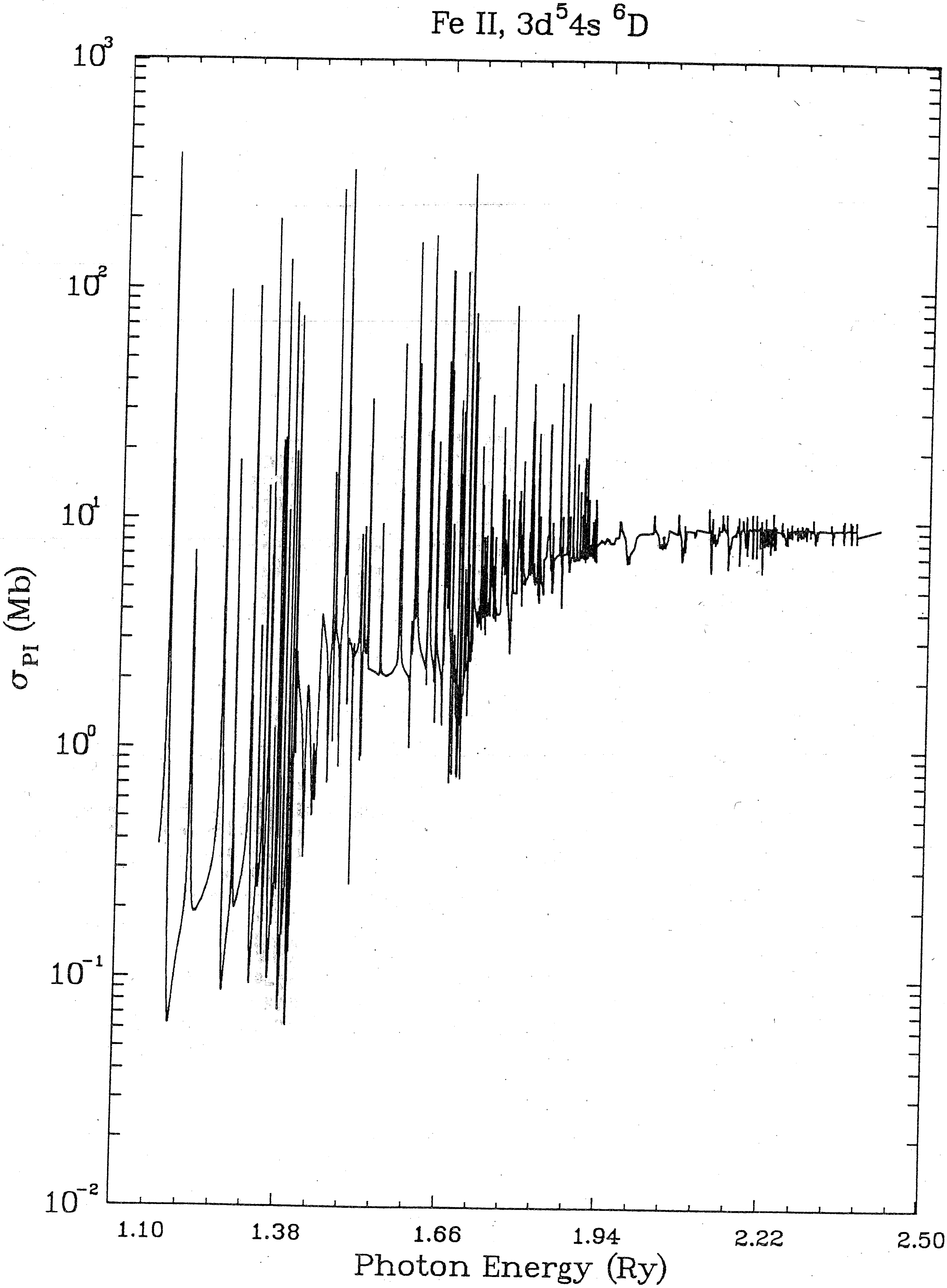

Fig. 1. Photoionization of ^{6}D ground state of Fe II.