

Relativistic calculations for Fe XXIII: Atomic structure

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(Received 9 December 1997)

Relativistic multiconfiguration Dirac-Fock theory was applied in calculating the atomic structure of Fe XXIII. These calculations are needed in solar-flare spectra and laboratory plasma modeling and diagnostics, as well as the relativistic distorted-wave calculation of electron impact excitation. For Fe XXIII, relativistic effects begin to show a more or less significant influence on the radial wave function and atomic structure in contrast to a lower- Z Be-like ion. In the present calculation, a large-scale configuration expansion was used in describing the target states. These results are extensively compared with those of nonrelativistic and other calculations. Large differences are found in these comparisons. Comparisons with experimental and observed values, wherever available, are also made. Because more relativistic effects and correlation effects are caught than before, the present results should be more accurate and reliable. [S1050-2947(98)03608-7]

PACS number(s): 31.25.-v, 02.70.-c, 31.30.Jv

I. INTRODUCTION

Accurate atomic data for Fe XXIII are becoming of increasing interest in identifying the solar spectra. In addition, accurate atomic structure is one of the most important input factors for improving the present stage of electron impact excitation calculations. To get accurate atomic structure, relativistic and correlation effects must be appropriately described. Relativistic effect begins to demonstrate great influence on the atomic structure for Fe XXIII in contrast to lower Z Be-like ions. The electron undergoes relativistic interaction with the target nucleus and other bound electrons, such as spin-orbit, spin-spin, and spin-other-orbit interactions, etc. The use of Dirac-Coulomb Hamiltonian H^{DC} will adequately describe these relativistic interactions [1,2]. The GRASP² code [3] based on multiconfiguration Dirac-Fock (MCDF) theory was used in the present calculations. We shall only consider excitations of L -shell electrons in contrast to a previous investigation which was mainly concerned with excitations of a K -shell electron to study satellite transitions [4]. Hence our MCDF configuration-expansion (CE) basis set is quite different from that in Ref. [4]. To catch as much correlation effect as possible, 133-level MCDF CE is used to describe the target states. The resulting atomic structure is compared with that from 20-level MCDF CE in the present calculation and that from 20-level or 46-level nonrelativistic CE by Bhatia and Mason [5,6]. Where possible, comparisons with other theoretical and experimental values are also made. Because we used MCDF theory which caught more correlation and relativistic effects, the present results should be more accurate and reliable.

A brief review of the theory underlying our method is given in Sec. II. In Sec. III the atomic structure calculation and results are presented. First, the level designations and mixing coefficients of the first 46 levels are listed and analyzed and some previous confusions are rectified. Then, the energy levels and wavelengths in the present calculation are compared with other calculations and available experimental data. Finally, oscillator strengths are presented for transitions from a level in the first 20 levels to one in the first 46 levels.

II. THEORY

Standard MCDF theory can be found in a review paper by Grant [7]. Here, we only restate some main points to establish convention and concept. The whole many-body system is described by H^{DC} , which is constructed from the one-body Dirac Hamiltonian H^D and the two-body Coulomb interaction Hamiltonian $H^C(i,j) = 1/|r_i - r_j|$,

$$H^{DC} = \sum_i H^D(i) + \sum_{i < j} H^C(i,j), \quad (2.1)$$

where $H^D(i) = c \vec{\alpha}_i \cdot \vec{p}_i + (\beta - 1)c^2 + V_{\text{nuc}}$, $c \sim 137.036$ is light speed in a.u., $\vec{\alpha}, \beta$ are the usual Dirac matrices, and V_{nuc} is the nuclear potential, modeled as a spherically symmetric distribution of nuclear charge [8], for which nuclear volume effect is considered. The transverse photon interaction is added to the two-body operator. It is perturbatively calculated after the radial orbitals have been solved. Generalized Breit interaction in Coulomb gauge for a photon propagator in the context of a QED picture is

$$H^B(1,2) = -(\vec{\alpha}_1 \cdot \vec{\alpha}_2) \frac{\exp(i\omega r_{12})}{r_{12}} + (\vec{\alpha}_1 \cdot \vec{\nabla}_1) \times (\vec{\alpha}_2 \cdot \vec{\nabla}_2) \frac{\exp(i\omega r_{12}) - 1}{\omega^2 r_{12}}, \quad (2.2)$$

where ω is the wave number of the virtual photon exchanged between the two electrons. The vacuum polarization potential of Fullerton and Rinker [9] is calculated via perturbation-theory (i.e., added to the matrix elements of the Dirac-Coulomb Hamiltonian prior to diagonalizing the resulting matrix). The self-energy is estimated by interpolation of the screened hydrogenic self-energy [10,11]. With the addition of a transverse photon interaction, the mixing coefficients may be somewhat changed. We will discuss this important point further in the next section.

Atomic orbitals are taken to be four-component spinors. Multiconfiguration self-consistent-field (SCF) calculations are based on the Dirac-Coulomb Hamiltonian. In MCDF CE

theory, the atomic-ion state functions (ASF's) Ψ_μ are a linear combination of configuration state functions (CSF's) Φ_ν , sharing common values of parity P and total angular momentum J ,

$$\Psi_\mu = \sum_\nu c_{\mu\nu} \Phi_\nu, \quad (2.3)$$

where $c_{\mu\nu}$ are the mixing coefficients. In (extended)-optimal-level or (E)OL calculation mode of MCDFT theory in GRASP² code, the generalized occupation number $\bar{q}(a)$ for orbital a is given by [1,12,13]

$$\bar{q}(a) = \sum_\mu d_\mu q_\mu(a), \quad (2.4)$$

where

$$d_\mu = \frac{\sum_i (2J_i + 1) c_{\nu_i\mu}^\dagger c_{\mu\nu_i}}{\sum_i (2J_i + 1)}. \quad (2.5)$$

In (extended)-average-level or (E)AL calculational mode, from the closure of the mixing coefficients, namely, $\sum_i (2J_i + 1) c_{\nu_i\mu}^\dagger c_{\mu\nu_i} = (2J_\mu + 1) \delta_{\mu\nu_i}$, Eq. (2.5) reduces to

$$d_\mu = \frac{2J_\mu + 1}{\sum_i (2J_i + 1)}. \quad (2.6)$$

In order to investigate the influence of the target states by different configuration descriptions, two calculation modes were used, namely,

(A) $2s^2, 2s2p, 2p^2, 2s3l$ ($l = s, p, d$): 12 terms or 20 levels;

(B) (A) + $2p3l$ ($l = s, p, d$) + $2s4l, 2p4l$ ($l = s, p, d, f$) + $3l3l'$ ($l, l' = s, p, d$): 133 levels.

The K -shell core is omitted for brevity.

The atomic structure code GRASP² which is based on MCDFT theory and intermediate coupling is applied to the present relativistic bound states calculations. GRASP² is based on a SCF algorithm adapted from procedures developed and extensively used by Fischer [14]. Extensive testings have revealed that great gains have been made in numerical stability, efficiency, and accuracy, when GRASP² is compared with its predecessors. All the present atomic structure data can be obtained from the GRASP² code including bound-state orbitals, angular coefficients, wavelengths, oscillator strengths or transition probabilities, and other required radial functions. All these can be transformed into the new hybrid grid using a well-tested cubic spline interpolation in order to use them for the calculation of electron impact excitation (EIE) in a contemporary paper of ours [15].

III. ATOMIC STRUCTURE CALCULATIONS AND RESULTS

A. Designations and mixing coefficients

The level designations in both LS coupling and jj coupling and mixing coefficients in the two CE modes mentioned in Sec. II are given in Table I. Here, the entries labeled ‘‘ASF index’’ are given in increasing energy order. The indices of the entries in ‘‘CSF basis set’’ are the same as those of the corresponding ASF levels for convenience. The number k in $x|k\rangle$ is the CSF basis number instead of the ASF level number. For example, in the first row containing ASF level $1\ 2s^2\ (1/2, 1/2)0$, the mixing coefficients (MC) from calculation mode (A) are given as

$$0.978|1\rangle + 0.156|10\rangle + 0.140|9\rangle. \quad (3.1)$$

Since CSF indices 10 and 9 correspond to $2p^2(3/2, 3/2)0$ and $2p^2(1/2, 1/2)0$, Eq. (3.1) is equivalent to

$$0.978|2s^2(1/2, 1/2)0\rangle + 0.156|2p^2(3/2, 3/2)0\rangle + 0.140|2p^2(1/2, 1/2)0\rangle. \quad (3.2)$$

Only the first 46 configuration state functions and their MC's are listed in the table. For each ASF level index, the entries in the first row pertain to jj coupling and in the second row to the corresponding LS -coupling quantities. Only the largest three MC's for each ASF in each calculation mode are presented provided they are greater than 1%, unless the other MC's are greater than 5%, in which case more than three MC's may be presented. The MC's change greatly from calculation mode (A) to (B), so that some new configurations appearing in mode (B) but not included in mode (A) have strong CI with those of mode (A). Therefore, to obtain accurate calculations, mode (B) is necessary. When we look into the MC in mode (B), we find that the first 46 CSF bases are the most important in catching CI correlation. However, those configurations not included in the first 46 bases also have some significant influence on the MC in calculating the first 46 ASF. Generally, MC can be changed by a few percent. For example, in ASF number 44 the MC of $2p3p(3/2, 3/2)0$ or 1S_0 is 4.4% in LS coupling and 4% in jj coupling. Generalized Breit interaction can alter the MC by perturbation theory. In some cases it is especially important to include the generalized Breit Hamiltonian in Eq. (2.2) in the CI calculation as this may cause the MC to change by a few percent. For example, when the generalized Breit Hamiltonian is not added, the ASF 30 is expanded by

$$0.690|32\rangle + 0.657|31\rangle + 0.296|30\rangle - 0.047|29\rangle. \quad (3.3)$$

In contrast, when the generalized Breit Hamiltonian is included, it is expanded by

$$0.711|32\rangle + 0.628|31\rangle + 0.309|30\rangle - 0.051|29\rangle. \quad (3.4)$$

TABLE I. Level definitions in both LS coupling and jj coupling for the lowest 46 states of Fe XXIII are given in increasing energy order. The fully occupied subshell is omitted for brevity. Mixing coefficients (>0.01) in both coupling schemes for each ASF are also presented in the two CE modes, respectively. Where there are more than three MC's greater than 1%, only the three largest MC's are presented, unless the other MC's are greater than 5%. The first-row entries of each level index are for jj coupling and the second for LS coupling. $(j_1, j_2)J$ denotes jj coupling of electrons 1 and 2 with total angular momentum J .

ASF		Mixing coefficient			CSF	
index	Level	Mode (A)	Mode (B)	basis set		
1	$2s^2$ $(1/2,1/2)0$ 1S_0	$0.978 1\rangle+0.156 10\rangle+0.140 9\rangle$ $0.978 1\rangle+0.208 10\rangle+0.024 9\rangle$	$0.978 1\rangle+0.156 10\rangle+0.139 9\rangle$ $0.978 1\rangle+0.207 10\rangle+0.024 9\rangle$	1	$2s^2$ $(1/2,1/2)0$ 1S_0	
2	$2s2p$ $(1/2,1/2)0$ 3P_0	$1.000 5\rangle$ $1.000 5\rangle$	$1.000 5\rangle-0.013 16\rangle-0.011 24\rangle$ $1.000 5\rangle-0.013 16\rangle+0.011 24\rangle$	2	$2s2p$ $(1/2,3/2)2$ 3P_2	
3	$(1/2,1/2)1$ 3P_1	$0.896 3\rangle-0.444 4\rangle$ $0.988 3\rangle+0.154 4\rangle$	$0.897 3\rangle-0.442 4\rangle-0.011 14\rangle$ $0.987 3\rangle+0.157 4\rangle-0.012 14\rangle$	3	$(1/2,1/2)1$ 3P_1	
4	$(1/2,3/2)2$ 3P_2	$1.000 2\rangle$ $1.000 2\rangle$	$1.000 2\rangle-0.012 13\rangle+0.011 21\rangle$ $1.000 2\rangle-0.012 13\rangle+0.011 21\rangle$	4	$(1/2,3/2)1$ 1P_1	
5	$(1/2,3/2)1$ 1P_1	$0.896 4\rangle+0.444 3\rangle$ $0.988 4\rangle-0.154 3\rangle$	$0.897 4\rangle+0.441 3\rangle-0.018 45\rangle$ $0.987 4\rangle-0.157 3\rangle-0.022 45\rangle$	5	$(1/2,1/2)0$ 3P_0	
6	$2p^2$ $(1/2,1/2)0$ 3P_0	$0.928 9\rangle-0.365 10\rangle-0.074 1\rangle$ $0.969 9\rangle+0.238 10\rangle-0.074 1\rangle$	$0.928 9\rangle-0.364 10\rangle-0.074 1\rangle$ $0.968 9\rangle+0.239 10\rangle-0.074 1\rangle$	6	$2p^2$ $(1/2,3/2)2$ 3P_2	
7	$(1/2,3/2)1$ 3P_1	$1.000 8\rangle$ $1.000 8\rangle$	$1.000 8\rangle-0.015 30\rangle-0.015 31\rangle$ $1.000 8\rangle-0.021 30\rangle$	7	$(3/2,3/2)2$ 1D_2	
8	$(1/2,3/2)2$ 3P_2	$0.910 6\rangle+0.415 7\rangle$ $0.864 6\rangle-0.504 7\rangle$	$0.910 6\rangle+0.413 7\rangle-0.015 26\rangle$ $0.863 6\rangle-0.505 7\rangle-0.018 27\rangle$	8	$(1/2,3/2)1$ 3P_1	
9	$(3/2,3/2)2$ 1D_2	$0.910 7\rangle-0.414 6\rangle+0.012 19\rangle$ $0.864 7\rangle+0.504 6\rangle+0.016 19\rangle$	$0.910 7\rangle-0.413 6\rangle-0.021 28\rangle$ $0.863 7\rangle+0.505 6\rangle-0.021 28\rangle$	9	$(1/2,1/2)0$ 3P_0	
10	$(3/2,3/2)0$ 1S_0	$0.918 10\rangle+0.345 9\rangle-0.196 1\rangle$ $0.949 10\rangle-0.248 9\rangle-0.196 1\rangle$	$0.918 10\rangle+0.344 9\rangle-0.195 1\rangle$ $0.948 10\rangle-0.248 9\rangle-0.195 1\rangle$	10	$(3/2,3/2)0$ 1S_0	
11	$2s3s$ $(1/2,1/2)1$ 3S_1	$1.000 11\rangle$ $1.000 11\rangle$	$0.991 11\rangle+0.079 30\rangle+0.073 32\rangle$ $-0.070 31\rangle$ $0.991 11\rangle+0.132 31\rangle-0.009 32\rangle$	11	$2s3s$ $(1/2,1/2)1$ 3S_1	
12	$(1/2,1/2)0$ 1S_0	$1.000 12\rangle+0.011 1\rangle-0.010 10\rangle$ $1.000 12\rangle-0.012 10\rangle+0.011 1\rangle$	$0.985 12\rangle+0.127 34\rangle+0.115 33\rangle$ $0.985 12\rangle+0.170 34\rangle+0.020 33\rangle$	12	$(1/2,1/2)0$ 1S_0	
13	$2s3p$ $(1/2,1/2)1$ 3P_1	$0.967 14\rangle-0.256 15\rangle$ $0.937 14\rangle+0.348 15\rangle$	$0.982 14\rangle-0.139 23\rangle+0.081 22\rangle$ $+0.067 43\rangle+0.061 44\rangle$ $0.786 14\rangle+0.590 15\rangle-0.160 23\rangle$ $+0.071 43\rangle+0.055 44\rangle$	13	$2s3p$ $(1/2,3/2)2$ 3P_2	
14	$(1/2,1/2)0$ 3P_0	$1.000 16\rangle$ $1.000 16\rangle$	$0.994 16\rangle+0.083 46\rangle+0.065 24\rangle$ $0.994 16\rangle+0.083 46\rangle-0.065 24\rangle$	14	$(1/2,1/2)1$ 3P_1	
15	$(1/2,3/2)1$ 1P_1	$0.967 15\rangle+0.256 14\rangle$ $0.937 15\rangle-0.349 14\rangle$	$0.961 15\rangle+0.210 22\rangle-0.143 23\rangle$ $-0.066 14\rangle$ $0.747 15\rangle-0.609 14\rangle-0.238 23\rangle$ $+0.089 22\rangle+0.064 45\rangle$	15	$(1/2,3/2)1$ 1P_1	
16	$(1/2,3/2)2$ 3P_2	$1.000 13\rangle$ $1.000 13\rangle$	$0.994 13\rangle+0.072 40\rangle+0.055 42\rangle$ $0.994 13\rangle+0.095 41\rangle-0.050 21\rangle$	16	$(1/2,1/2)0$ 3P_0	
17	$2s3d$ $(1/2,3/2)12$ 3D_1	$1.000 20\rangle$ $1.000 20\rangle$	$0.989 20\rangle+0.132 29\rangle+0.040 30\rangle$ $0.989 20\rangle-0.143 29\rangle-0.020 32\rangle$	17	$2s3d$ $(1/2,5/2)3$ 3D_3	
18	$(1/2,3/2)2$ 3D_2	$0.819 18\rangle-0.574 19\rangle$ $0.997 18\rangle+0.074 19\rangle$	$0.811 18\rangle-0.572 19\rangle-0.089 26\rangle$ $-0.079 27\rangle$ $0.990 18\rangle-0.119 26\rangle+0.070 19\rangle$	18	$(1/2,3/2)2$ 3D_2	
19	$(1/2,5/2)3$ 3D_3	$1.000 17\rangle$ $1.000 17\rangle$	$0.995 17\rangle-0.096 25\rangle$ $0.995 17\rangle-0.096 25\rangle$	19	$(1/2,5/2)2$ 1D_2	
20	$(1/2,5/2)2$ 1D_2	$0.819 19\rangle+0.573 18\rangle+0.015 6\rangle$ $0.997 19\rangle-0.074 18\rangle-0.018 7\rangle$	$0.808 19\rangle+0.574 18\rangle+0.094 26\rangle$ $-0.059 27\rangle-0.058 28\rangle$ $0.989 19\rangle-0.121 28\rangle-0.066 18\rangle$	20	$(1/2,3/2)1$ 3D_1	
21	$2p3s$ $(1/2,1/2)0$ 3P_0	$0.995 24\rangle-0.073 46\rangle-0.059 16\rangle$ $0.995 24\rangle+0.073 46\rangle+0.059 16\rangle$		21	$2p3s$ $(3/2,1/2)2$ 3P_2	

TABLE I. (Continued).

ASF index	Level	Mixing coefficient Mode (B)	CSF basis set
22	(1/2,1/2)1 3P_1	0.954 22> + 0.226 23> - 0.175 15> + 0.049 44> - 0.047 14> 0.909 22> - 0.366 23> - 0.170 15> + 0.075 44> + 0.063 14>	22 3P_1
23	$2p3p$ (1/2,1/2)1 3D_1	0.988 29> - 0.129 20> + 0.077 32> 0.819 29> + 0.534 32> - 0.161 31> + 0.129 20>	23 (3/2,1/2)1 1P_1
24	$2p3s$ (3/2,1/2)2 3P_2	0.990 21> + 0.117 40> + 0.057 42> 0.990 21> + 0.131 41> + 0.037 13>	24 (1/2,1/2)0 3P_0
25	(3/2,1/2)1 1P_1	0.951 23> + 0.194 15> - 0.186 22> + 0.141 14> 0.884 23> + 0.397 22> + 0.239 15>	25 $2p3p$ (3/2,3/2)3 3D_3
26	$2p3p$ (1/2,3/2)2 3D_2	0.916 26> + 0.377 27> - 0.115 19> + 0.056 18> + 0.055 28> 0.914 26> - 0.279 28> + 0.265 27> + 0.116 18> - 0.053 19>	26 (1/2,3/2)2 3D_2
27	(1/2,3/2)1 1P_1	0.945 30> - 0.238 31> - 0.200 32> - 0.076 11> - 0.055 20> 0.527 32> - 0.516 31> - 0.500 30> - 0.443 29> + 0.076 11> - 0.055 20>	27 (3/2,1/2)2 3P_2
28	(1/2,1/2)0 3P_0	0.956 33> - 0.280 34> - 0.075 12> 0.943 33> + 0.323 34> - 0.075 12>	28 (3/2,3/2)2 1D_2
29	$2p3d$ (1/2,3/2)2 3F_2	0.997 39> - 0.055 41> + 0.047 42> 0.879 39> + 0.447 42> + 0.138 40> - 0.084 41>	29 (1/2,1/2)1 3D_1
30	$2p3p$ (3/2,3/2)1 3P_1	0.711 32> + 0.628 31> + 0.309 30> - 0.051 29> 0.662 30> + 0.612 32> - 0.334 29> + 0.269 31>	30 (1/2,3/2)1 3P_1
31	$2p3p$ (3/2,3/2)3 3D_3	0.995 25> + 0.096 17> 0.995 25> + 0.096 17>	31 (3/2,1/2)1 3S_1
32	$2p3d$ (1/2,5/2)3 3F_3	0.926 36> + 0.374 37> + 0.041 38> 0.885 36> + 0.374 37> - 0.277 38>	32 (3/2,3/2)1 1P_1
33	$2p3d$ (1/2,5/2)2 1D_2	0.956 40> - 0.229 42> - 0.138 41> - 0.102 21> - 0.066 13> 0.571 42> - 0.554 41> + 0.531 40> - 0.263 38> + 0.102 21> + 0.066 13>	33 (1/2,1/2)0 3P_0
34	$2p3p$ (3/2,1/2)1 3S_1	0.737 31> - 0.665 32> + 0.098 11> + 0.051 30> 0.786 31> - 0.557 30> + 0.247 32> - 0.098 11>	34 (3/2,3/2)0 1S_0
35	(3/2,1/2)2 3P_2	0.862 27> - 0.376 28> - 0.332 26> + 0.066 18> 0.794 27> - 0.472 28> - 0.375 26> - 0.063 19>	35 $2p3d$ (3/2,5/2)4 3F_4
36	$2p3d$ (1/2,3/2)1 3D_1	0.967 43> - 0.201 45> - 0.136 44> - 0.057 14> 0.834 43> + 0.405 44> + 0.367 45>	36 (1/2,5/2)3 3F_3
37	$2p3p$ (3/2,3/2)2 1D_2	0.922 28> + 0.324 27> - 0.184 26> + 0.066 19> + 0.063 18> 0.826 28> + 0.545 27> + 0.099 26> + 0.091 19>	37 (3/2,3/2)3 3D_3
38	$2p3d$ (3/2,5/2)4 3F_4	1.000 35> 1.000 35>	38 (3/2,5/2)3 1F_3
39	(3/2,3/2)2 3D_2	0.788 41> + 0.563 42> + 0.243 40> 0.655 42> + 0.566 40> - 0.391 39> + 0.309 41>	39 (1/2,3/2)2 3F_2
40	(3/2,3/2)3 3D_3	0.696 38> - 0.676 37> + 0.242 36> 0.875 37> - 0.436 36> - 0.208 38>	40 (1/2,5/2)2 3D_2
41	(3/2,5/2)2 3P_2	0.788 42> - 0.596 41> + 0.090 40> - 0.073 21> - 0.069 13> - 0.069 39> 0.751 41> - 0.614 40> + 0.208 42> - 0.073 21> - 0.069 13> + 0.066 39>	41 (3/2,3/2)2 3P_2
42	(3/2,3/2)1 3P_1	0.959 44> - 0.252 45> + 0.076 43> - 0.068 14> 0.869 44> - 0.473 43> + 0.097 45> - 0.077 14> - 0.067 22>	42 (3/2,5/2)2 1D_2
43	(3/2,3/2)0 3P_0	0.994 46> - 0.087 16> + 0.067 24> 0.994 46> - 0.087 16> - 0.067 24>	43 (1/2,3/2)1 3D_1
44	$2p3p$ (3/2,3/2)0 1S_0	0.950 34> + 0.265 33> - 0.152 12> 0.929 34> - 0.332 33> - 0.153 12>	44 (3/2,3/2)1 3P_1
45	$2p3d$ (3/2,5/2)3 1F_3	0.717 38> + 0.634 37> - 0.287 36> 0.937 38> + 0.305 37> + 0.165 36>	45 (3/2,5/2)1 1P_1
46	(3/2,5/2)1 1P_1	0.941 45> + 0.232 44> + 0.227 43> - 0.069 15> 0.920 45> - 0.284 43> - 0.254 44> - 0.070 15>	46 (3/2,3/2)0 3P_0

TABLE II. Calculated generalized occupation numbers $\bar{q}(a)$ in the two modes from the GRASP² code. p^- means $p_{1/2}$, p means $p_{3/2}$, etc.

Mode	$1s$	$2s$	$2p^-$	$2p$	$3s$	$3p^-$	$3p$	$3d^-$	$3d$
(A)	2.0000	0.7846	0.2885	0.3885	0.1077	0.1077	0.1077	0.1077	0.1077
(B)	2.0000	0.2315	0.2321	0.3715	0.1182	0.1182	0.1755	0.1755	0.1892
	$4s$	$4p^-$	$4p$	$4d^-$	$4d$	$4f^-$	$4f$		
(B)	0.0448	0.0448	0.0597	0.0597	0.0597	0.0597	0.0597		

The level designations are assigned according to the major contribution of MC in CSF bases of a certain ASF. However, more often than not, a certain CSF basis may actually contribute dominantly to more than one ASF level, while some other SCF bases do not contribute dominantly to any energy level. For example, in jj coupling of the present calculation, CSF basis number 38 makes a major contribution to both ASF levels 40 and 45. Levels 40 and 45 are strongly mixed; hence the designations are ambiguous. Both the CI effect and the relativistic or intermediate-coupling effects can result in level crossing along the Be-like isoelectronic sequence. In our calculation, these two effects on the dominant contribution of MC are found to oppose each other. The dominant contribution of MC for $2s3p\ ^1P_1$ and $2s3p\ ^3P_1$ levels are inverted between O V and Al X from the order specified by Hund's rule, which is obeyed in Be I. The inversion is mostly the result of the CI $2s3p \times 2p3s \times 2p3d$. Also, configuration $2s2p$ partly participates in this CI. In Fe XXIII, Hund's rule is again obeyed due to the sufficiently large relativistic effect canceling the CI effect. To avoid the so-called level-crossing designation, we calculated the MC in Be-like high Z ion (e.g., $Z=92$), in which nearly pure jj coupling is expected. So we can assign the lower of levels 40 and 45 to be CSF number 37, namely, $2p3d(3/2,3/2)3$, and the higher level to be CSF number 38, namely, $2p3d(3/2,5/2)3$. Similarly, in LS coupling, CSF number 42 makes a major contribution to both ASF levels 33 and 39 and these two levels are strongly coupled together. We calculated the MC in Be-like low Z ion (e.g., $Z=6$), in which nearly pure LS coupling is expected. Then we can assign level 33 to be CSF number 42, namely, $2p3d\ ^1D_2$, and level 39 to be $2p3d\ ^3D_2$. It is interesting to note that our designations for levels 3 and 39 are the same as those of Sampson *et al.* [16] and Fawcett [17] but different from those of Bromage *et al.* [18] and Sampson *et al.* [19].

It should be noted in Table I that from the leading contribution of the CSF basis for each energy level, we cannot say whether jj coupling or LS coupling is better, and for some levels neither jj coupling nor LS coupling is appropriate since there is no nearly pure CSF contribution. So, they should be described by intermediate coupling. This indicates that both CI (correlation effect) and relativistic effect should be properly considered for Fe XXIII thus making the structure calculation of Fe XXIII very complicated.

In Table II the generalized occupation numbers for each orbital calculated from Eqs. (2.4)–(2.6) are presented, which are closely related to the MC aforementioned. These generalized occupation numbers, which are physically more reasonable than previous fictitious occupation numbers (see Ref. [13] for more detailed discussions), are to be used in

determining the distorted potentials in the RDW (relativistic distorted-wave) calculation [12,13] of electron impact excitation (EIE) in the subsequent accompanying paper [15]. They are kept fixed. Equivalently, the frozen target approximation was to be used, in the EIE calculation.

B. Energy levels and wavelengths

In Table III we compare the values of the resonance transition energies obtained by different CE modes in the present calculation and those calculated by others. Also, various observed energy levels are given for comparison, which were obtained from solar flare spectra or laboratory measurements such as tokamak spectrum. The entries labeled “MCDF” in each of the present calculational modes are obtained from the MCDF theory described in Sec. II with the effect of a finite nuclear size in a Fermi charge distribution but without the higher-order relativistic corrections. The entries labeled “MCDF*” are obtained from the same way except that higher-order relativistic effects due to retardation, relativistic generalized Breit interaction, and QED corrections from self-energy and vacuum polarization are now included. The entries labeled “BM” were obtained by Bhatia and Mason [5] using the SUPERSTRUCTURE code [20–22], in which intermediate coupling was included. The first ten entries labeled “NF” were obtained by Norrington and Grant [23] using the earlier version of the GRASP code [1] with only the configurations in the $n=2$ complex included, while the remaining 36 entries were calculated by Fawcett [17] using the well-known Cowan's code [24], which is a nonrelativistic CI atomic structure code including relativistic corrections. The entries labeled “Expt. 1” are experimental values taken from Ref. [23] and those labeled “Expt. 2” are experimental or observed values from solar-flare spectra taken from Refs. [18,25–28]. The entries labeled “Edlén” were recommended by Edlén [29] obtained by polynomials fitting according to the experimental and/or observed results. Generally, among all the theoretical values, the entries in “MCDF*” of mode (B) agree best with experimental or observed values. The discrepancies between these “MCDF*” and experimental or observed values are generally less than 1%. This indicates that in the $n=3$ and $n=4$ complexes, the CI effects, relativistic effect (using Dirac-Coulomb Hamiltonian), and higher-order relativistic corrections are all important for obtaining accurate energy levels for Fe XXIII. The results calculated by Fawcett [17] in the last 36 entries of “NF” are very irregular. Some of them agree well with the present results, while some do not, such as

TABLE III. Comparison of energy levels (in cm^{-1}) between the two modes of the present MCDF calculations and other theoretical and observed values. The meaning for each entry is explained in the text.

Level index	Mode (A)		Mode (B)		BM	NF	Expt. 1	Expt. 2	Edlén
	MCDF	MCDF*	MCDF	MCDF*					
1	0	0	0	0	0	0	0	0	0
2	348440	349628	347810	349025	348190	349400	350059		348101
3	381555	380793	380746	380020	380485	380565	381553	379100 ^a	379161
4	477075	472896	476462	472284	471927	472525	472195		471851
5	771476	768798	763869	761099	758914	766508	752791	752800 ^b	752621
6	959812	960308	960348	960967	956966	960521	956681	956200 ^c	956026
7	1032657	1030311	1033333	1031103	1027837	1031521	1029436	1027400 ^c	1027141
8	1081755	1076174	1082272	1076763	1076089	1076952	1071794	1071900 ^c	1071713
9	1218419	1211487	1218682	1211582	1209888	1213463		1204600 ^c	1204466
10	1439537	1436579	1438685	1435672	1430417	1437655		1422900 ^c	1422761
11	8925027	8918843	8912187	8905951	8920252	8900502		8891200 ^d	
12	9004048	8998327	8981279	8975389	8991251	8966092			
13	9091459	9085467	9079248	9073123	9088907	9076338		9076000 ^e	
14	9085576	9080129	9079237	9073750	9089225	9074713			
15	9144468	9137230	9112148	9104894	9118856	9109392		9107500 ^e	
16	9122707	9115624	9116023	9108931	9121415	9108578			
17	9211192	9203443	9204436	9196540	9213074	9199961		9181100 ^d	
18	9215195	9206954	9209384	9201030	9217883	9204060		9181100 ^d	
19	9222128	9213632	9217180	9208594	9225493	9210899			
20	9289514	9281377	9281561	9273523	9289548	9269536		9272900 ^d	
21			9351765	9346279		9356190			
22			9370290	9364267		9372445			
23			9462609	9456913		9462098			
24			9481972	9471735		9476946			
25			9530246	9520567		9520650			
26			9530657	9523214		9524452			
27			9531934	9525031		9526381			
28			9553713	9548349		9544992			
29			9588156	9580787		9598044			
30			9627419	9617362		9614405			
31			9634607	9623064		9621128			
32			9632304	9623946		9638137			
33			9644550	9636534		9645954			
34			9652353	9641986		9638305			
35			9654849	9644633		9638870			
36			9664082	9656035		9661659			
37			9719326	9708440		9698123			
38			9728270	9715815		9728772			
39			9738271	9726499		9733762			
40			9764164	9751733		9755728			
41			9783869	9771640		9773594			
42			9784807	9772988		9774266			
43			9787287	9776732		9776875			
44			9799367	9790190		9772804			
45			9846732	9834048		9828606			
46			9856403	9844999		9836446			

^aFrom Ref. [25].

^bFrom Ref. [26].

^cFrom Ref. [27].

^dFrom Ref. [28].

^eFrom Ref. [18].

TABLE IV. Multiplet separations between 3P_1 and 1P_1 in configurations $2s2p$, $2s3p$, $2p3s$, and $2p3d$. The meaning for each entry is the same as that in Table III.

Configuration	Mode (A)		Mode (B)		BM	NF	Expt. 1	Expt. 2	Edlén
	MCDF	MCDF*	MCDF	MCDF*					
$2s2p$	389921	388005	383123	381079	378429	385943	371238	373700	373460
$2s3p$	53009	51763	32900	31771	29949	32240		31500	
$2p3s$			159956	156300		148205			
$2p3d$			71596	72011		62180			

levels 13, 32, 33, in which the CI effects are very strong. Some designations in Ref. [17] are confusing.

Energy levels 15 and 16 are inverted in mode (A) but not so in mode (B) because it caught more correlation energy. In comparison, these levels are inverted in ‘‘NF’’ but not so in ‘‘BM.’’ So, the results of ‘‘BM’’ are better than those of

‘‘NF.’’ For the two pairs of levels, 13 and 14, 31 and 32, in ‘‘MCDF’’ and ‘‘MCDF*’’ of mode (B), it is the higher-order relativistic effects that yield the correct energy order. It is interesting to note that the energy order of levels 13 and 14 in ‘‘BM’’ and levels 31 and 32 in ‘‘NF’’ are also correct even though higher-order relativistic effects were not in-

TABLE V. Comparisons of the wavelengths (in Å) of the x-ray lines for Fe xxiii between the present calculations [by modes (A) and (B)] and various other theoretical results and/or laboratory or observed values, as explained in the text.

Transition	Present			Sampson	Experiment	
	Mode (A)	Mode (B)	BM		[18,28]	FRH
1–13	11.007	11.022	11.00	11.015	11.018	11.018
1–15	10.944	10.983	10.97	10.967	10.980	10.979
2–11	11.670	11.686	11.67			
2–17	11.295	11.303	11.28	11.293	11.298	11.298
3–11	11.712	11.729	11.71			
3–17	11.334	11.342	11.32	11.341	11.361 ^a	11.33
3–18	11.330	11.337	11.32	11.333	11.325	11.333
3–26		10.937		10.925	10.935	10.934
4–11	11.840	11.857	11.84		11.870 ^a	
4–17	11.454	11.462	11.44		11.485 ^a	
4–18	11.449	11.456	11.43	11.480		11.44
4–19	11.441	11.446	11.42	11.466	11.442	11.440
4–31		10.928		10.916	10.927	10.927
4–34		10.905		10.895		10.83
4–35		10.902		10.895	10.903	10.903
5–12	12.151	12.174	12.15			
5–20	11.747	11.748	11.72	11.769	11.737	11.737
5–37		11.177		11.164	11.166	
6–36		11.501		11.504	11.519	11.49
7–33		11.621		11.650	11.614	11.612
7–39		11.500		11.507	11.493	11.492
7–41		11.441		11.438		11.44
7–42		11.439		11.440		11.44
7–43		11.434		11.437		11.44
8–32		11.700		11.746	11.692	11.690
8–40		11.527		11.541	11.525	11.517
8–41		11.501		11.512	11.500	11.49
8–42		11.499		11.514		11.49
8–45		11.419		11.410		11.422
9–41		11.682		11.725		11.668
9–45		11.598		11.620	11.594	11.594
10–46		11.892		11.935	11.898	11.898

^aFrom Ref. [28].

TABLE VI. Electric dipole oscillator strengths (gf) and transition probabilities (A in s^{-1}) between levels in the $n=2$ complex. The various data sources are explained in the text.

Transition	gf				A				
	Present		BM	Zhang	Present		BM	NS	Glass
	Mode (A)	Mode (B)			Mode (A)	Mode (B)			
1-3	1.440[-3] ^a	1.510[-3]	1.51[-3]	1.500[-3]	4.643[+7]	4.850[+7]	4.84[+7]	5.014[+7]	5.45[+7]
5	1.562[-1]	1.553[-1]	1.56[-1]	1.567[-1]	2.053[+10]	2.000[+10]	2.00[+10]	1.974[+10]	1.984[+10]
2-7	6.420[-2]	6.345[-2]	6.39[-2]	6.440[-2]	6.614[+9]	6.563[+9]	6.56[+9]	6.432[+9]	6.617[+9]
3-6	5.537[-2]	5.474[-2]	5.50[-2]	5.550[-2]	1.240[+10]	1.232[+10]	1.22[+10]	1.225[+10]	1.234[+10]
7	4.467[-2]	4.414[-2]	4.43[-2]	4.470[-2]	4.191[+9]	4.160[+9]	4.13[+9]	4.097[+9]	4.202[+9]
8	8.370[-2]	8.310[-2]	8.36[-2]	8.490[-2]	5.400[+9]	5.382[+9]	5.39[+9]	5.206[+9]	5.392[+9]
9	5.302[-3]	5.035[-3]	4.98[-3]	4.800[-3]	4.878[+8]	4.645[+8]	4.58[+8]	4.840[+8]	
10	2.424[-4]	2.379[-4]	2.32[-4]		1.802[+8]	1.768[+8]	1.70[+8]	1.864[+8]	
4-7	6.469[-2]	6.394[-2]	6.49[-2]	6.500[-2]	4.469[+9]	4.439[+9]	4.46[+9]	4.454[+9]	4.521[+9]
8	1.577[-1]	1.555[-1]	1.59[-1]	1.580[-1]	7.659[+9]	7.580[+9]	7.75[+9]	7.502[+9]	7.567[+9]
9	6.675[-2]	6.625[-2]	6.51[-2]	6.750[-2]	4.856[+9]	4.830[+9]	4.73[+9]	4.733[+9]	
5-6	7.906[-4]	7.658[-4]	7.82[-4]	9.000[-4]	1.934[+7]	2.041[+7]	2.05[+7]	2.250[+7]	
7	4.183[-4]	4.410[-4]	4.46[-4]	3.000[-4]	6.361[+6]	7.149[+6]	7.17[+6]	7.574[+6]	
8	2.573[-2]	2.633[-2]	2.64[-2]	2.670[-2]	3.244[+8]	3.501[+8]	3.54[+8]	3.617[+8]	
9	1.615[-1]	1.632[-1]	1.67[-1]	1.677[-1]	4.220[+9]	4.419[+9]	4.54[+9]	4.353[+9]	4.56[+9]
10	1.084[-1]	1.048[-1]	1.06[-1]	1.080[-1]	3.225[+10]	3.181[+10]	3.17[+10]	3.037[+10]	3.122[+10]

^aNotation used in this and subsequent tables, e.g., $1.440[-3] = 1.440 \times 10^{-3}$.

cluded in their respective calculations. The accuracy of energy levels obtained in mode (B) provides confidence that the accurate atomic structure so obtained may be used in the following EIE calculation.

In Table IV we investigate the multiplet separations between 3P_1 and 1P_1 to illustrate the strong CI and relativistic effects in configurations $2s2p, 2s3p, 2p3s$, and $2p3d$. As expected the multiplet separations calculated by ‘‘MCDF*’’ in mode (B) agree well with the experimental or observed values.

The wavelengths of the x-ray lines for Fe XXIII are presented in Table V. The higher-order relativistic effects are included in both modes (A) and (B) in the present calculations. The entries labeled ‘‘Sampson’’ were obtained by Sampson *et al.* [19] using the CI with target ion wave functions composed of antisymmetrical sums of products of non-relativistic hydrogen-ion wave function. The entries labeled [18,28] are observed or experimental values from Refs. [18] and [28], while those of FRH are spectroscopic observations of solar flares [30]. Once again, our mode (B) values agree best with the experiment results mostly with discrepancies of less than 0.01 Å. This is more evidence indicating the high reliability of our atomic structure calculations.

C. Oscillator strengths and radiative transition probabilities

The weighted electric dipole oscillator strengths (gf) and the radiative transition probabilities (A) for the allowed transitions within the $n=2$ complex are listed in Table VI. The entries labeled ‘‘Zhang’’ are the gf values calculated by Zhang and Sampson [31] using the MCDF method in Dirac-Fock-Slater (DFS) approximation but only configurations in the $n=2$ complex were included in their procedure. The entries labeled NS and ‘‘Glass’’ as given in Refs. [32] and [33], respectively, were obtained in an elaborate CI calculation

with a few tens of configuration bases in the nonrelativistic frame. Some of the relativistic effects were perturbatively included. The codes used were a modified version of the code described in Ref. [20] and the code CIV3 [34], respectively.

Oscillator strengths are gauge-dependent in the real calculation due to the approximate wave function obtained. In the present calculation, the gf values for each transition have been calculated in two gauge forms, i.e., Coulomb gauge which in the nonrelativistic limit corresponds to the velocity form and Babushkin gauge which in the nonrelativistic limit corresponds to the length form [35]. However, it is well accepted that the inaccuracy in the velocity form for a given truncation scheme is larger than that in the length form. Hence, only gf in Babushkin gauge form are listed in the table. In general, the gf or A values for transitions within the $n=2$ complex obtained by the various theoretical results are in good agreement with discrepancies of less than a few percent. Only in very weak transitions such as 5-6 and 5-7 are the discrepancies anomalously large. So, the orbitals for configurations in the $n=2$ complex may be properly calculated by all methods mentioned above.

In Table VII, the weighted electric dipole oscillator strengths (gf) between levels in the $n=2$ and $n=3$ complexes are listed. Great differences are found among different methods. Strong CI as well as relativistic interactions may be responsible for these large differences. To show an example, we analyze the strong CI of configurations $2s2p, 2s3p, 2p3s$, and $2p3d$ with odd parity and $J=1$ in mode (B), namely, the 9 CSF bases with basis numbers 3,4,14,15,22,23,43,44,45. The corresponding 9 ASF level numbers with the largest contributions from these CSF bases are 3,5,13,15,22,25,36,42,46. The 9 CSF bases are assigned indices 1-9, respectively, in the matrix elements of H^{DC} given by

TABLE VII. Electric dipole oscillator strengths (gf) between levels in the $n=2$ and $n=3$ complexes. The various data sources are explained in the text.

Transition	Present				Transition	Mode (B)	Sampson	Transition	Mode (B)	Sampson
	Mode (A)	Mode (B)	BM	Sampson						
1-13	8.806[-2]	2.679[-1]	2.40[-1]	2.4[-1]	1-22	1.290[-2]		7-43	3.166[-1]	3.3[-1]
15	5.965[-1]	4.110[-1]	4.06[-1]	4.7[-1]	25	2.198[-2]		46	1.429[-2]	
2-11	1.826[-2]	2.649[-2]	2.13[-2]		36	5.810[-3]		8-22	8.968[-2]	
17	6.614[-1]	7.563[-1]	7.21[-1]	8.1[-1]	42	2.336[-4]		24	2.015[-1]	
3-11	5.477[-2]	7.935[-2]	6.67[-2]		46	1.932[-2]		25	7.497[-3]	
12	8.392[-4]	2.626[-4]	8.96[-5]		2-23	5.539[-2]		29	1.679[-1]	
17	4.857[-1]	5.545[-1]	5.33[-1]	5.9[-1]	27	1.734[-1]		32	9.869[-1]	9.9[-1]
18	1.486[+0]	1.664[+0]	1.60[+0]	1.77[+0]	30	2.261[-2]		33	1.633[-1]	
20	1.660[-2]	9.918[-3]	8.88[-3]		34	1.846[-3]		36	1.165[-2]	
4-11	9.872[-2]	1.378[-1]	1.30[-1]		3-23	1.134[-1]		39	2.194[-1]	
17	3.354[-2]	3.723[-2]	3.65[-2]		26	3.702[-1]	4.3[-1]	40	3.199[+0]	3.30[+0]
18	4.993[-1]	5.525[-1]	5.43[-1]	5.7[-1]	27	5.201[-2]		41	1.118[+0]	1.10[+0]
19	2.804[+0]	3.076[+0]	3.04[+0]	3.20[+0]	28	1.139[-1]		42	3.371[-1]	3.4[-1]
20	2.592[-3]	2.206[-3]	1.79[-3]		30	1.039[-1]		45	3.138[-1]	4.2[-1]
5-11	1.700[-3]	1.874[-3]	1.86[-3]		34	4.826[-3]		46	1.181[-3]	
12	4.475[-2]	3.131[-2]	2.51[-2]		35	2.399[-2]		9-22	1.231[-4]	
17	1.241[-2]	1.155[-2]	1.10[-2]		37	2.007[-2]		24	5.503[-2]	
18	7.533[-3]	1.165[-2]	1.24[-2]		44	3.406[-3]		25	1.545[-1]	
20	2.034[+0]	1.693[+0]	1.61[+0]	1.63[+0]	4-23	2.388[-5]		29	8.530[-2]	
6-13	7.448[-4]	6.049[-4]	7.37[-4]		26	1.035[-2]		32	2.997[-2]	
15	3.812[-3]	7.462[-4]	1.05[-3]		27	3.746[-3]		33	1.950[-1]	
7-13	8.687[-6]	5.951[-4]	4.99[-4]		30	2.926[-2]		36	2.406[-3]	
14	1.107[-5]	1.012[-3]	9.86[-4]		31	5.567[-1]	6.4[-1]	39	2.486[-1]	
15	1.953[-6]	7.498[-5]	9.97[-5]		34	2.991[-1]	2.9[-1]	40	2.395[-1]	
16	1.955[-5]	3.311[-3]	3.96[-3]		35	4.202[-1]	4.6[-1]	41	7.543[-1]	8.1[-1]
8-13	3.113[-5]	7.326[-3]	6.94[-3]		37	1.012[-1]		42	9.459[-2]	
15	5.950[-4]	4.254[-3]	3.87[-3]		5-23	8.703[-2]		45	4.852[+0]	5.03[+0]
16	4.553[-5]	4.767[-3]	5.65[-3]		26	3.754[-2]		46	6.330[-2]	
9-13	2.894[-4]	5.070[-3]	4.70[-3]		27	9.143[-2]		10-22	2.305[-3]	
15	1.529[-3]	1.753[-2]	1.73[-2]		28	4.757[-3]		25	6.877[+0]	
16	1.553[-5]	1.007[-3]	9.83[-4]		30	1.986[-1]		36	2.163[-2]	
10-13	4.227[-3]	9.264[-4]	9.00[-4]		34	2.746[-2]		42	1.127[-2]	
15	3.008[-2]	3.866[-4]	4.75[-4]		35	1.941[-1]		46	1.286[+0]	1.26[+0]
11-13	1.276[-1]	8.190[-2]	8.83[-2]		37	6.389[-1]	7.0[-1]	11-21	1.773[-2]	
14	4.676[-2]	4.301[-2]	4.51[-2]		44	1.129[-1]		22	4.873[-2]	
15	2.351[-2]	5.546[-2]	5.42[-2]		6-22	6.374[-2]		24	1.108[-1]	
16	2.885[-1]	2.637[-1]	2.68[-1]		25	2.159[-3]		25	1.048[-2]	
12-13	9.102[-3]	2.225[-2]	2.21[-2]		36	1.271[+0]	1.33[+0]	29	7.514[-5]	
15	1.064[-1]	4.722[-2]	4.96[-2]		42	2.245[-3]		33	1.945[-3]	
13-17	2.963[-2]	1.700[-2]	1.85[-2]		46	2.409[-2]		36	1.949[-4]	
18	9.712[-2]	6.297[-2]	6.75[-2]		7-21	5.911[-2]		39	3.328[-4]	
20	1.854[-2]	6.192[-2]	6.01[-2]		22	3.519[-2]		41	1.208[-3]	
14-17	4.710[-2]	3.816[-2]	4.04[-2]		24	1.157[-1]		42	5.322[-4]	
15-17	2.294[-3]	8.556[-3]	8.76[-3]		25	7.199[-3]		43	1.744[-4]	
18	4.365[-3]	2.218[-2]	2.19[-2]		29	2.506[-2]		46	8.842[-5]	
20	1.515[-1]	1.076[-1]	1.12[-1]		33	1.294[+0]	1.33[+0]	12-22	2.263[-2]	
16-17	1.680[-3]	1.354[-3]	1.47[-3]		36	2.753[-1]		25	1.173[-1]	
18	2.601[-2]	2.147[-2]	2.33[-2]		39	1.078[+0]	1.11[+0]	36	2.427[-4]	
19	1.579[-1]	1.340[-1]	1.44[-1]		41	1.976[-1]	2.2[-1]	42	1.976[-7]	
20	2.967[-4]	1.234[-4]	9.51[-5]		42	6.929[-1]	7.4[-1]	46	1.311[-3]	

TABLE VII. (Continued).

Transition	Mode (B)	Sampson	Transition	Mode (B)	Sampson	Transition	Mode (B)	Sampson
13-23	6.455[-2]		16-31	1.824[-1]		42	2.877[-2]	
26	3.025[-2]		34	7.983[-3]		45	7.446[-4]	
27	7.403[-3]		35	2.861[-2]		46	9.500[-3]	
28	1.517[-2]		37	3.750[-2]		19-24	5.475[-3]	
30	1.579[-2]		17-21	9.138[-4]		29	6.896[-6]	
34	1.435[-2]		22	5.587[-4]		32	4.814[-2]	
35	7.130[-2]		24	3.510[-5]		33	7.014[-2]	
37	2.665[-3]		25	1.565[-4]		38	1.166[-1]	
44	7.572[-4]		29	1.568[-2]		39	3.635[-2]	
14-23	2.110[-2]		33	1.356[-7]		40	1.091[-1]	
27	4.477[-3]		36	2.231[-2]		41	3.712[-2]	
30	2.242[-2]		39	2.732[-2]		45	2.554[-2]	
34	3.056[-2]		41	2.009[-2]		20-22	6.933[-4]	
15-23	4.325[-3]		42	7.002[-2]		24	6.823[-5]	
26	1.886[-2]		43	3.333[-2]		25	4.050[-3]	
27	3.841[-2]		46	1.100[-3]		29	1.604[-2]	
28	5.472[-3]		18-22	1.505[-3]		32	3.275[-3]	
30	3.606[-2]		24	7.880[-4]		33	3.586[-2]	
34	4.506[-2]		25	4.942[-4]		36	7.358[-3]	
35	1.099[-2]		29	1.614[-2]		39	4.963[-2]	
37	2.483[-2]		32	2.294[-2]		40	1.082[-3]	
44	1.403[-2]		33	7.514[-3]		41	8.561[-3]	
16-23	1.405[-6]		36	5.081[-2]		42	3.248[-4]	
26	5.010[-2]		39	1.239[-2]		45	7.629[-2]	
27	4.151[-2]		40	7.160[-2]		46	9.139[-2]	
30	2.454[-2]		41	9.635[-2]				

$$H_{ij}^{DC} = \langle i | H^{DC} | j \rangle \delta_{J_i J_j} \delta_{P_i P_j}, \quad (3.5)$$

where i and j are the CSF bases participating in the CI. For reasons of mathematical expediency, although all the configurations up to the $n=4$ complex are included in this CI calculation, those CSF numbers 47-133 which may also participate in this CI are excluded in the following analyses. Indeed, from our computed MC (not listed in Table I), there

were an additional 12 CSF bases out of basis numbers 47-133 which have more or less some contributions to this CI. The matrix \mathcal{H}^{DC} formed by its elements in Eq. (3.5) have $9^2=81$ matrix elements in the jj -coupled CSF bases. After diagonalizing \mathcal{H}^{DC} , we get mixing coefficients matrix \mathcal{C} for the above-mentioned 9 ASF levels from the secular equation $(\mathcal{H}^{DC} - E)\mathcal{C} = 0$, $\mathbb{1}$ being the unit matrix. The elements $c_{\mu\nu}$ of \mathcal{C} are shown in the following equation:

$$\mathcal{C} = \begin{bmatrix} 0.897 & -0.442 & -0.011 & 0.005 & 0.011 & 0.004 & -0.005 & -0.006 & 0.002 \\ 0.441 & 0.897 & -0.006 & -0.012 & 0.010 & -0.017 & -0.012 & -0.005 & -0.018 \\ 0.012 & -0.001 & 0.982 & 0.028 & 0.081 & -0.139 & 0.067 & 0.061 & 0.001 \\ -0.003 & 0.010 & -0.066 & 0.961 & 0.210 & -0.143 & 0.020 & -0.020 & 0.075 \\ -0.013 & -0.003 & -0.047 & -0.175 & 0.954 & 0.226 & 0.038 & 0.049 & -0.042 \\ 0.008 & 0.019 & 0.141 & 0.194 & -0.186 & 0.951 & 0.019 & 0.029 & -0.033 \\ 0.007 & 0.005 & -0.057 & -0.005 & -0.039 & -0.020 & 0.967 & -0.136 & -0.201 \\ 0.006 & -0.002 & -0.068 & 0.038 & -0.049 & -0.047 & 0.076 & 0.959 & -0.252 \\ 0.010 & 0.017 & -0.023 & -0.069 & -0.002 & 0.038 & 0.227 & 0.232 & 0.941 \end{bmatrix}. \quad (3.6)$$

From the elements of \mathcal{C} , we could find the reason why the gf for some transitions related to these levels are greatly changed (or even enhanced or reduced by orders of magnitude) when different computational methods are used. In MCDF theory, gf for this case is given by [1]

$$gf_{ij} \propto \left| \sum_{\mu\nu}^9 c_{i\mu}^\dagger c_{\nu j} \langle i \| \hat{O}^{(1)} \| j \rangle \right|^2, \quad (3.7)$$

where the subscripts i, j refer to ASF level indices, and μ, ν refer to CSF basis indices, and $\hat{O}^{(1)}$ is a multipole radiative field operator with rank 1. The additional CI from higher-order configurations included in mode (B) but not included in mode (A) may jointly contribute negative or additive effects to the gf value of a given transition. As illustrations, we will inspect transitions 6–15 and 9–15. In the former transition the gf value is reduced by about 20 times from mode (A) to mode (B); whereas in the latter case the gf value is enhanced by about 10 times. The CI combinations from other transitions with large gf values [such as transition 6–36 ($gf=1.271$)] jointly result in a cancellation effect on the gf of 6–15 so that its mode (B) value of 7.462×10^{-4} is much less than its mode (A) value of 3.812×10^{-3} . On the other hand, because of additive effects of other transitions with large gf the gf value of a certain transition may be immensely enhanced. An example of such transitions is 9–15 whose mode (B) gf value of 1.753×10^{-2} is an order of magnitude greater than its mode (A) gf value of 1.529×10^{-3} . Although the MC of ASF 15 from CSF number 23, 44, and 45, etc. are small, the gf values for transitions 9–25, 9–42, and 9–46 (1.545×10^{-1} , 9.459×10^{-2} , and 6.330×10^{-2} , respectively) are orders of magnitude larger than the gf value of 1.529×10^{-3} for transition 9–15. Hence these additional transitions involved have large influences on the resultant gf value of transition 9–15.

The generalized Breit Hamiltonian H^B in Eq. (2.2) results in small changes of MC *via* first-order perturbation theory which can in turn significantly influence the final gf or transition probabilities. Referring to the example mentioned in Eqs. (3.3) and (3.4), the first four major MC of ASF level numbers 30, 34, 27, 23 (corresponding to CSF bases 32, 31, 30, 29) changed by 3.0%, 4.6%, 4.4%, 8.5%, when calculated respectively from Eq. (3.3) and Eq. (3.4). While these changes of MC are all less than 10%, the resultant gf values may change several times. First, let us examine the transition 4–30. Its gf value of 2.926×10^{-2} is about an order of magnitude less than that of transition 4–34 ($gf=2.991 \times 10^{-1}$). Also, its MC value of 0.657 for CSF 31 (level 34) is nearly the same as that of 0.690 for CSF 32 (level 30). So, according to Eq. (3.7), the gf for 4–30 should change by about $10 \times 2 \times 4.6\% = 92\%$. When we recalculated the gf for this transition without H^B the result was 1.346×10^{-3} , which is smaller by 37% compared with the value 1.846×10^{-3} calculated with H^B , thus demonstrating the importance of including H^B . The situation is the same for the transition 13–30, whose gf values were 1.579×10^{-2} and 2.470×10^{-2} when calculated with and without H^B . However, when we inspect transition 2–30, according to the same analysis, the gf values should change by about $7.7 \times 2 \times 4.4\% = 67\%$ (the gf value of transition 2–27 is 7.7 times that of 2–30 in Table

VII) if H^B was not added, but the resultant gf was 2.124×10^{-2} , representing a change of less than 10% from the value of 2.261×10^{-2} when H^B was added. This may be mainly due to cancellation effects, as mentioned earlier. In addition, other factors in Eq. (3.7) may also contribute to this result.

IV. SUMMARY

The MCDF theory has been used to obtain the atomic structure for Fe xxiii. Large scale CSF bases including configurations in the $n=2-4$ complexes have been performed in configuration expansion to accurately calculate the first 46 energy levels, and the wavelengths and oscillator strengths for transitions between them. These accurate data are needed for the identifications of solar-flare spectra and the modeling of high-temperature plasmas such as those in x-ray laser and astrophysical research. Also, these data together with the calculated orbital wave functions, angular coefficients, and the theoretical generalized occupation numbers are needed for the calculation of electron impact excitation for Fe xxiii in a contemporary paper of ours.

The mixing coefficients for the first 46 levels are comprehensively investigated in 133-level CE of the MCDF frame. A typical example of the strong mixing for levels with $J=1$ and odd parity in configurations $2s2p, 2s3p, 2p3s, 2p3d$ is analyzed and insight knowledge has been acquired. Both the configuration interaction described by MCDF and the fully relativistic effect have large influences on the atomic structure of Fe xxiii. Indeed, these two effects are coupled together and cannot be clearly separated. The influences of these two effects on energy levels, wavelengths, and oscillator strengths are analyzed in detail. Mixing coefficients are key quantities needed for the related analyses. In addition to orbital wave function, both the relativistic and correlation effects and higher-order relativistic corrections are reflected in the MC values. Small MC changes due to the CI effect and/or relativistic effect of the configurations in the $n=3$ and $n=4$ complexes may have great influence on the atomic structure especially in relation to their transition probabilities. Furthermore, we have demonstrated that the generalized Breit Hamiltonian has significant influence on the oscillator strengths even though its influence on the MC may be minor. So, to obtain accurate atomic structure, generalized Breit Hamiltonian cannot be disregarded.

Our results reveal some significant differences compared with those from previous nonrelativistic and relativistic calculations. Considering the present elaborate and accurate calculations, these new atomic data should enable a more objective reexamination of the Fe xxiii lines expected in laboratory experiments and solar-flare spectra.

ACKNOWLEDGMENTS

The authors are indebted to Professor I. P. Grant and Dr. P. Marketos for providing us with the GRASP² code. We are also grateful to the Singapore National Supercomputing Research Center (NSRC) for their facilities and valuable advice on the Cray T94 supercomputer. One of the authors (C.G.X.) acknowledges financial support from the National University of Singapore.

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