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Energy level analyses of even-parity $J = 1$ and 2 Rydberg states of Sn I by multichannel quantum defect theory*

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This paper analyzes the energy levels along the even-parity $J = 1$ and 2 Rydberg series of Sn I by multichannel quantum defect theory. A good agreement between theoretical and experimental energy levels was achieved. Below 59198 cm^{-1}, a total of 85 and 23 new energy levels, respectively, in the $J = 1$ and $J = 2$ series, which cannot be measured previously by experiments, are predicted in this work. Based on the calculated admixture coefficients of each channel, interchannel interactions were discussed in detail. The results are helpful to understand the characteristics of configuration interaction among even-parity levels in Sn I.

Keywords: atom Sn, Rydberg state, multichannel quantum defect theory
PACC: 3120N, 3130, 3150

1. Introduction

Atomic Rydberg states have received considerable attention for a long time in atomic physics and laser spectroscopy.[1,2] However, most investigations concentrated mainly on the atoms which have an s-electron ion core and a highly excited nl electron in their Rydberg states.[3] The neutral atom tin, which possesses a p-electron ion core in Rydberg states, will be rather different from the former atoms. In fact, the electronic structure of Sn I has been investigated extensively. In 1958 Moore[4] compiled the early data in her book and later on, Brill[5] and Wilson[6] reported many energy levels for Sn I by analyzing the absorption spectrum and the arc spectrum, respectively. But unfortunately their results were not published. Brown *et al*[7] determined 639 odd-parity energy levels including many autoionizing levels for Sn I by investigating the high-resolution absorption spectrum between 158 and 204 nm, and the two ionization limits $^2P^\circ_{1/2}$ (59232.69 cm^{-1}) and $^2P^\circ_{3/2}$ (63484.18 cm^{-1}) were also determined by them. Using a two-step laser excitation technique, Nadeem *et al*[8,9] investigated numerous even-parity $J = 1$ and 2 Rydberg levels and they analyzed the $5pnp$ $J = 2$ and $5pnf$ $J = 2$ series by the multichannel quantum defect theory (MQDT) method in the frame of three- and two-channel models, respectively. Another systematic investigation on $5pnp$ and $5pnf$ even-parity Rydberg levels was accomplished by Jin *et al*[10,11] by using resonant multiphoton ionization and time-of-flight mass spectroscopy methods, but the detailed results of their work were not published.

On the theoretical side, many odd-parity bound and autoionizing levels, as well as the levels from a $5s5p^3$ configuration which strongly perturb odd-parity configurations, have been investigated by Dembczynski *et al*[12,13] through pseudo-relativistic Hartree–Fock (HF) *ab initio* calculations. The $J = 3$ energy levels of the odd-parity $5pnd$ and $5s5p^3$ configurations in Sn I were analyzed by Ginter *et al*[14,15] by using the perturbed coupled-channel models in the frame of MQDT. Later on, Robicheaux and Greene carried out R-matrix calculations for the properties of odd-parity $J = 0 - 3$ bound levels in Sn I.[16] Using the MQDT method, Brown *et al*[7] analyzed the interchannel mixture in the odd-parity $J = 0 - 3$ Rydberg series of Sn I in detail. To the best of our knowledge,

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however, systematic MQDT analysis for even-parity Rydberg levels of Sn I has not yet been reported in the literature since the energy level data were just published recently.[8,9] Therefore, it is necessary and interesting to investigate the even-parity Rydberg series of Sn I by means of the MQDT method in order to understand the configuration interaction characteristics and to supplement theoretical energy level data for the incomplete experimental results reported in the literature.[8,9] Based on this purpose, in the present paper we perform detailed theoretical analyses on even-parity $J = 1$ and 2 Rydberg levels of Sn I by the MQDT method in five- and six-channel models, respectively.

2. Basic theory and formulas

The detailed description of MQDT can be found in some early literature.[17−21] Here we just briefly recall some basic concepts and formulas. Between the excited electron and the ion core, the interaction is divided into two parts: (I) $\boldsymbol{r} > \boldsymbol{r}_0$, $\boldsymbol{r}_0$ is the radius of the ion core; (II) $\boldsymbol{r} < \boldsymbol{r}_0$. When the electron is in region (I), the interaction is Coulombic and described by collision channels, which is also called the i channel and usually identified in jj coupling. The interaction in region (II) is non-Coulombic and characterized by the eigenchannels which is also called the α channel or close-coupling channel. For an atom with two ionization limits, the energy E_i of the n-th discrete level can be expressed as

$$E_i = I_1 - \frac{R}{\nu_1^2} = I_2 - \frac{R}{\nu_2^2}, \tag{1}$$

where R is the mass-corrected Rydberg constant, I_j is the j-th ionization limit and ν_j is the effective quantum number relevant to I_j. To ensure correct asymptotic behavior of the wave functions of bound levels, the condition

$$\det\left|U_{i\alpha}\sin\pi\left(\nu_i+\mu_\alpha\right)\right| \equiv \det\left|F_{i\alpha}\right| = 0 \tag{2}$$

must be satisfied, where μ_α is the quantum defect of the eigenchannel α and the matrix elements $U_{i\alpha}$ describe the unitary transformation between collision channels and eigenchannels. The position of each energy level is required to simultaneously satisfy Eqs.(1) and (2). By fitting to the experimentally measured data, the best MQDT theoretical energy levels could be obtained together with a set of optimal MQDT parameters μ_α and $U_{i\alpha}$. In MQDT analyses, the Lu–Fano plot method introduced by Lu and Fano[19] is usually used to present quantum defect of all the studied levels.

In some earlier literature of MQDT, the eigenchannels are considered as near LS-coupling. Later, Lee and Lu[18] introduced intermediate bases $\bar{\alpha}$ of pure LS-coupling and defined $U_{i\alpha}$ as

$$U_{i\alpha} = \sum_{\bar{\alpha}} R_{i\bar{\alpha}} V_{\bar{\alpha}\alpha}, \tag{3}$$

where $R_{i\bar{\alpha}}$ is a matrix describing the transformation from the jj to pure LS couplings which can be analytically obtained by using 6-j symbols, the matrix $V_{\bar{\alpha}\alpha}$ can be derived by $M(M-1)/2$ successive rotations θ_{jk} where M is the number of interacting channels. In this case the angles θ_{jk} are the fitted parameters instead of $U_{i\alpha}$. Moreover, μ_α is a slowly-varying function of energy and can be expressed as $\mu_\alpha = \mu_\alpha^0 + \varepsilon\mu_\alpha^1$ with $\varepsilon = (I_1 - E_i)/R$. In contrast, the energy dependence of θ_{jk} is so small that it can be neglected.

The wave functions of the n-th discrete level can be expressed by the linear combination of the wave functions of collision channels, i.e. ,

$$\Psi_n = \sum_i Z_i^{(n)} \Psi_i, \tag{4}$$

where $Z_i^{(n)}$ is the channel admixture coefficient with the form

$$\begin{aligned} Z_i^{(n)} = {} & (-1)^{l_i+1}\left(\nu_i^{(n)}\right)^{3/2} \sum_\alpha A_\alpha^{(n)} U_{i\alpha} \\ & \times \cos\pi\left(\nu_i^{(n)} + \mu_\alpha\right)/N_n, \end{aligned} \tag{5}$$

where l_i is the angular momentum quantum number of the excited electron in the i channel, N_n is the normalization factor and $A_\alpha^{(n)}$ is the eigenchannel expansion coefficient having a form

$$A_\alpha^{(n)} = \frac{C_{i\alpha}(v_i)}{\sqrt{\sum_\alpha C_{i\alpha}^2(v_i)}}, \tag{6}$$

where $C_{i\alpha}$ is the cofactor of the element $F_{i\alpha}$.

3. Results and discussion

3.1. $J = 1$ series

Experimental energy levels in the $J = 1$ Rydberg series ranging from 42342.3 cm^{-1} to 59090.7 cm^{-1} used in calculations were taken from the published data: the levels lower than 56485.5 cm^{-1} from Moore's table[4] and the others from Nadeem's results.[8,9] The experimental values measured by Jin *et al*[11] are

rather different from the results given by Nadeem *et al*,[8,9] and the biggest energy level difference between the two groups is more than 10 cm^{-1}. In the present paper, we prefer to use the published data compiled by Moore[4] and measured by Nadeem *et al*.[8,9] It should be pointed out that in our MQDT analyses the positions of the experimental levels $5p16p$ $(1/2,\ 3/2)_1$ and $(1/2,\ 3/2)_2$ have been interchanged based on the Landé factors measured by Xu *et al*.[22] The even-parity $J = 1$ levels under investigation involve five collision channels which can be labeled as $5pnp$ $(1/2,1/2)_1$, $(1/2,3/2)_1$, $(3/2,1/2)_1$, $(3/2,3/2)_1$ and $5pnf$ $(3/2,5/2)_1$. The first two channels converge to the first ionization limit and the others to the second one.

Using the MQDT model of five channels and two ionization limits, we obtain the optimal MQDT parameters by fitting theoretical levels to the experimental ones using the nonlinear minimization method,[23]; the results are listed in Table 1. The Lu–Fano plot for the $J = 1$ Rydberg series is shown in Fig.1, from which it is seen that the fitted results are rather good, i.e., no experimental level lies far from the fitted curve. Therefore our MQDT analyses could well predict unmeasured levels along the $5pnp$ $(1/2,3/2)_1$ and $(1/2,1/2)_1$ Rydberg series.

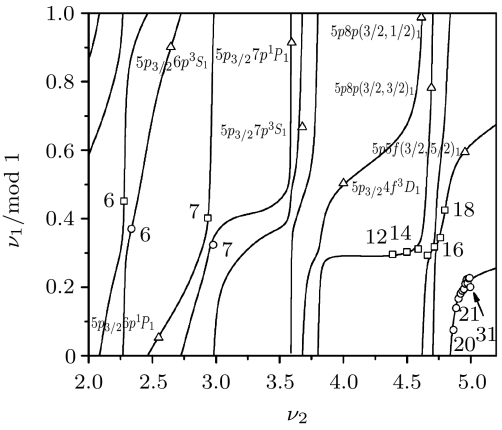


Fig.1. Lu–Fano plot for even-parity $J = 1$ levels of Sn I. Circle: $5pnp$ $(1/2,1/2)_1$; square: $5pnp$ $(1/2,3/2)_1$; triangle: the perturbers.

Table 1. MQDT parameters for even-parity $J = 1$ levels of Sn I.

i, $\bar{\alpha}$,α	1	2	3	4	5
$\|i\rangle$	nf $(3/2,5/2)_1$	np $(3/2,1/2)_1$	np $(1/2,1/2)_1$	np $(3/2,3/2)_1$	np $(1/2,3/2)_1$
I_i	63484.18	63484.18	59232.69	63484.18	59232.69
$\|\bar{\alpha}\rangle$	nf $^3D_1$	np $^3S_1$	np $^3P_1$	np $^1P_1$	np $^3D_1$
μ_α^0	0.1001	0.3612	0.3191	0.3030	0.6864
μ_α^1	7.5231	1.5591	−1.8944	−3.9243	−5.2514
$U_{i\alpha}$	0.4594	−0.4783	−0.4223	−0.0785	−0.6129
	0.2671	−0.1432	−0.5796	0.3604	0.6651
	0.2808	0.1907	0.3105	0.8487	−0.2610
	−0.4937	−0.7915	0.2156	0.2818	0.0630
	0.6285	−0.2965	0.5856	−0.2536	0.3315

The theoretical energy levels up to $n = 59$ for $5pnp$ $(1/2,3/2)_1$ and $(1/2,1/2)_1$ levels together with all the experimental levels in the $J = 1$ Rydberg series are listed in Table 2. Below 59198 cm^{-1}, a total of 85 new levels of $5pnp$ $(1/2,3/2)_1$ and $5pnp$ $(1/2,3/2)_1$ are predicted which have not been measured previously. It is seen that most calculated and experimental levels agree with each other quite well. Considering all 31 experimental data, we find that the root-mean-square (rms) deviation between theory and experiment is 28.6 cm^{-1}. In fact, the low-lying levels are influenced much more by the core-polarization effect and the MQDT analysis cannot reproduce them well. So if the eight lowest levels below 55373.8 cm^{-1} ($5p_{3/2}7p^3S_1$) are excluded, the rms deviation will reduce to 2.53 cm^{-1}.

Table 2. MQDT theoretical energy levels and comparison with experimental values for even-parity $J = 1$ series of Sn I. Units: cm^{-1}.

term[a]	$E_{\rm MQDT}$	$E_{\rm exp}$	$E_{\rm MQDT} - E_{\rm exp}$
$5p_{1/2}6p$ $^3P_1$	42330.3	42342.3[b]	−12.0
$5p_{1/2}6p$ $^3D_1$	43366.5	43368.5[b]	−2.0

Table 2 *Continued*

term[a]	E_{MQDT}	E_{exp}	$E_{\mathrm{MQDT}} - E_{\mathrm{exp}}$
$5p_{3/2}6p\ ^1P_1$	46581.2	46603.4[b]	−22.2
$5p_{3/2}6p\ ^3S_1$	47809.6	47805.7[b]	3.9
$5p_{1/2}7p\ ^3P_1$	50761.3	50755.8[b]	5.5
$5p_{1/2}7p\ ^3D_1$	51058.6	51113.3[b]	−54.7
$8p\ (1/2,3/2)_1$	51651.5		
$8p\ (1/2,1/2)_1$	53980.4		
$9p\ (1/2,3/2)_1$	54139.1		
$5p_{3/2}7p\ ^1P_1$	54960.1	54990.0[b]	−29.9
$5p_{3/2}7p\ ^3S_1$	55281.6	55373.8[b]	−92.2
$9p\ (1/2,1/2)_1$	55583.7		
$10p\ (1/2,1/2)_1$	55858.0		
$4f\ (3/2,5/2)_1$	56636.0	56632.9[b]	3.1
$10p\ (1/2,3/2)_1$	56794.3		
$11p\ (1/2,1/2)_1$	57251.3		
$11p\ (1/2,3/2)_1$	57386.4		
$12p\ (1/2,1/2)_1$	57676.2		
$12p\ (1/2,3/2)_1$	57785.2	57784.3[c]	0.9
$13p\ (1/2,1/2)_1$	57976.7		
$13p\ (1/2,3/2)_1$	58066.2	58065.7[c]	0.5
$14p\ (1/2,1/2)_1$	58191.64		
$14p\ (1/2,3/2)_1$	58270.0	58272.1[c]	−2.1
$8p\ (3/2,1/2)_1$	58331.8	58327.8[c]	4.0
$15p\ (1/2,1/2)_1$	58405.9		
$15p\ (1/2,3/2)_1$	58435.5	58432.0[c]	3.5
$8p\ (3/2,3/2)_1$	58497.1	58497.6[c]	−0.5
$16p\ (1/2,3/2)_1$	58548.1	58550.4[c]	−2.3
$16p\ (1/2,1/2)_1$	58627.6		
$17p\ (1/2,3/2)_1$	58643.1	58644.2[c]	−1.1
$17p\ (1/2,1/2)_1$	58698.9		
$18p\ (1/2,3/2)_1$	58716.3	58716.1[c]	0.2
$18p\ (1/2,1/2)_1$	58755.0		
$19p\ (1/2,3/2)_1$	58776.7		
$19p\ (1/2,1/2)_1$	58803.3		
$20p\ (1/2,3/2)_1$	58828.3		
$20p\ (1/2,1/2)_1$	58848.3	58849.6[d]	−1.3
$21p\ (1/2,3/2)_1$	58872.3		
$21p\ (1/2,1/2)_1$	58888.4	58888.7[d]	−0.3
$22p\ (1/2,3/2)_1$	58909.8		
$22p\ (1/2,1/2)_1$	58923.2	58923.3[d]	−0.1
$23p\ (1/2,3/2)_1$	58941.8		
$23p\ (1/2,1/2)_1$	58953.2	58953.3[d]	−0.1
$24p\ (1/2,3/2)_1$	58969.4		
$24p\ (1/2,1/2)_1$	58979.2	58979.3[d]	−0.1
$25p\ (1/2,3/2)_1$	58993.3		
$25p\ (1/2,1/2)_1$	59001.8	59001.9[d]	−0.1
$5f\ (3/2,5/2)_1$	59014.0	59014.1[d]	−0.1
$26p\ (1/2,1/2)_1$	59021.5	59021.4[d]	0.1
$26p\ (1/2,3/2)_1$	59032.3		
$27p\ (1/2,1/2)_1$	59038.8	59038.6[d]	0.2

Table 2 *Continued*

term[a]	E_{MQDT}	E_{exp}	$E_{\mathrm{MQDT}} - E_{\mathrm{exp}}$
$27p\ (1/2,3/2)_1$	59048.3		
$28p\ (1/2,1/2)_1$	59054.1	59054.1[d]	0.0
$28p\ (1/2,3/2)_1$	59062.5		
$29p\ (1/2,1/2)_1$	59067.6	59067.5[d]	0.1
$29p\ (1/2,3/2)_1$	59075.1		
$30p\ (1/2,1/2)_1$	59079.7	59079.6[d]	0.1
$30p\ (1/2,3/2)_1$	59086.4		
$31p\ (1/2,1/2)_1$	59090.5	59090.7[d]	−0.2
$31p\ (1/2,3/2)_1$	59096.5		
$32p\ (1/2,1/2)_1$	59100.2		
$32p\ (1/2,3/2)_1$	59105.6		
$33p\ (1/2,1/2)_1$	59108.9		
$33p\ (1/2,3/2)_1$	59113.8		
$34p\ (1/2,1/2)_1$	59116.8		
$34p\ (1/2,3/2)_1$	59121.2		
$35p\ (1/2,1/2)_1$	59124.0		
$35p\ (1/2,3/2)_1$	59128.0		
$36p\ (1/2,1/2)_1$	59130.5		
$36p\ (1/2,3/2)_1$	59134.2		
$37p\ (1/2,1/2)_1$	59136.5		
$37p\ (1/2,3/2)_1$	59139.8		
$38p\ (1/2,1/2)_1$	59141.9		
$38p\ (1/2,3/2)_1$	59145.0		
$39p\ (1/2,1/2)_1$	59146.9		
$39p\ (1/2,3/2)_1$	59149.8		
$40p\ (1/2,1/2)_1$	59151.5		
$40p\ (1/2,3/2)_1$	59154.1		
$41p\ (1/2,1/2)_1$	59155.8		
$41p\ (1/2,3/2)_1$	59158.2		
$42p\ (1/2,1/2)_1$	59159.7		
$42p\ (1/2,3/2)_1$	59161.9		
$43p\ (1/2,1/2)_1$	59163.3		
$43p\ (1/2,3/2)_1$	59165.4		
$44p\ (1/2,1/2)_1$	59166.7		
$44p\ (1/2,3/2)_1$	59168.6		
$45p\ (1/2,1/2)_1$	59169.8		
$45p\ (1/2,3/2)_1$	59171.6		
$46p\ (1/2,1/2)_1$	59172.7		
$46p\ (1/2,3/2)_1$	59174.4		
$47p\ (1/2,1/2)_1$	59175.4		
$47p\ (1/2,3/2)_1$	59177.0		
$48p\ (1/2,1/2)_1$	59177.9		
$48p\ (1/2,3/2)_1$	59179.4		
$49p\ (1/2,1/2)_1$	59180.3		
$49p\ (1/2,3/2)_1$	59181.7		
$50p\ (1/2,1/2)_1$	59182.5		
$50p\ (1/2,3/2)_1$	59183.8		
$51p\ (1/2,1/2)_1$	59184.6		
$51p\ (1/2,3/2)_1$	59185.8		

Table 2 *Continued*

term[a]	E_{MQDT}	E_{exp}	$E_{\mathrm{MQDT}} - E_{\mathrm{exp}}$
$52p\ (1/2,1/2)_1$	59186.6		
$52p\ (1/2,3/2)_1$	59187.7		
$53p\ (1/2,1/2)_1$	59188.4		
$53p\ (1/2,3/2)_1$	59189.4		
$54p\ (1/2,1/2)_1$	59190.1		
$54p\ (1/2,3/2)_1$	59191.1		
$55p\ (1/2,1/2)_1$	59191.7		
$55p\ (1/2,3/2)_1$	59192.7		
$56p\ (1/2,1/2)_1$	59193.3		
$56p\ (1/2,3/2)_1$	59194.2		
$57p\ (1/2,1/2)_1$	59194.7		
$57p\ (1/2,3/2)_1$	59195.6		
$58p\ (1/2,1/2)_1$	59196.1		
$58p\ (1/2,3/2)_1$	59196.9		
$59p\ (1/2,1/2)_1$	59197.4		
$59p\ (1/2,3/2)_1$	59198.2		

[a]Some designations are from the references where the corresponding energy levels were reported, the others are based on the MQDT analyses.
[b]From Ref.[4].
[c]From Ref.[8].
[d]From Ref.[9].

Since the high-lying even-parity bound levels of Sn I can be suitably labeled by jj coupling,[8,9] the admixture coefficients Z_i^2 with jj coupling are shown in Fig.2. It is seen that most $5pnp\ (1/2,3/2)_1$ and $(1/2,1/2)_1$ levels are only of purities lower than 70% due to stronger interchannel interactions. Below the first ionization limit there exist 8 perturber levels in the $J = 1$ series and their positions have been previously determined in experiments.[4,8,9,11] These perturbers include $5p_{3/2}6p^1P_1$, $^3S_1$, $5p_{3/2}7p^1P_1$, $^3S_1$, $5p8p\ (3/2,3/2)_1$, $(3/2,1/2)_1$, $5p4f\ ^3D_1$ and $5p5f\ (3/2,5/2)_1$. For the corresponding relationship between LS and jj coupling schemes for these levels refer to Table 1. Their existence was reproduced in our MQDT results. Figure 2 shows that the perturber $5p_{3/2}6p^1P_1$ intensively mixes with the lowest two energy levels $5p_{1/2}6p^3P_1$ and $^3D_1$, while other levels in this perturbing channel have lesser influence on the nearby Rydberg levels. It is also found that most of the low-lying levels possess the admixture of the $5p_{3/2}6p^3S_1$ and $5p_{3/2}7p^3S_1$ levels. The perturbation of $5p_{3/2}4f^3D_1$ is so localized that only several low-lying levels have its mixture. The $5p8p$ perturbers mainly mix with the $5pnp\ (1/2,1/2)_1$ series and $5p8p$ $(3/2,1/2)_1$ components in the levels ($n = 13 - 15$) of this series are only 2%, 6% and 4%, respectively, while $5p8p\ (3/2,3/2)_1$ influences some higher levels, such as $5p16p\ (1/2,3/2)_1$ and $5p16p\ (1/2,1/2)_1$ containing 11% and 12% of $5p8p\ (3/2,3/2)_1$ character. It is worthwhile to note that based on the calculated results of the admixture coefficient the perturber $5p5f$ $(3/2,5/2)_1$ rarely disturbs the two $J = 1$ Rydberg series under investigation.

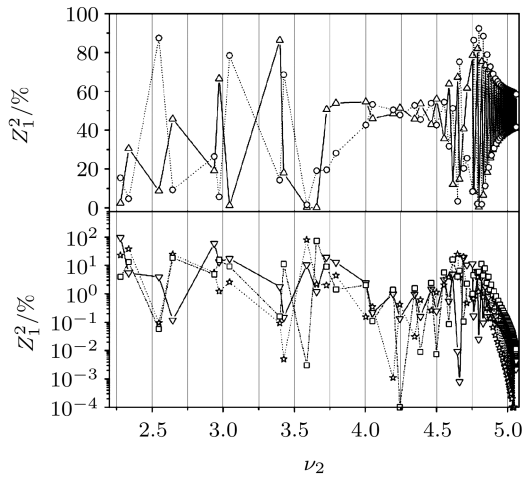


Fig.2. Admixture coefficients of even-parity $J = 1$ levels of Sn I. Sharp-up triangle: $5pnp\ (1/2,3/2)_1$; circle: $5pnp$ $(1/2,1/2)_1$; sharp-down triangle: $5pnf\ (3/2,5/2)_1$; star: $5pnp\ (3/2,3/2)_1$; square: $5pnp\ (3/2,1/2)_1$.

3.2. $J = 2$ series

Experimental level data used in the calculation for the $J = 2$ Rydberg series, covering 43238.7 to 59193.2 cm^{-1}, are also from [4], [8] and [9]. These series contain six interaction channels $5pnp\ (1/2,3/2)_2$, $(3/2,3/2)_2$, $(3/2,1/2)_2$, $5pnf\ (1/2,5/2)_2$, $(3/2,5/2)_2$ and $(3/2,7/2)_2$. Under the six-channel two-limit model, MQDT analyses for the $J = 2$ series were performed and the obtained optimal MQDT parameters are listed in Table 3. The corresponding Lu–Fano plot is shown in Fig.3. It can be seen that the MQDT analyses are satisfactory for reproducing the features of configuration interactions in the $J = 2$ series. The dispersion of the experimental points near the first ionization limit ($\nu_2 = 5.08$) is due to the sensitivity of ν_1 to the experimental errors of the measured energy levels at this place.

Table 3. MQDT parameters for even-parity $J = 2$ levels of Sn I.

i, $\bar{\alpha}$, α	1	2	3	4	5	6
$\|i\rangle$	nf (3/2,5/2)$_2$	np (3/2,1/2)$_2$	nf (3/2,7/2)$_2$	np (3/2,3/2)$_2$	np (1/2,3/2)$_2$	nf(1/2,5/2)$_2$
I_i	63484.18	63484.18	63484.18	63484.18	59232.69	59232.69
$\|\bar{\alpha}\rangle$	$5pnf\ ^3D_2$	$5pnp\ ^3P_2$	$5pnf\ ^1D_2$	$5pnp\ ^1D_2$	$5pnp\ ^3D_2$	$5pnf\ ^3F_2$
μ_α^0	1.0000	0.3589	0.0188	0.2819	0.2435	0.0678
μ_α^1	−1.7123	0.2066	1.8855	1.7560	−0.1207	−1.2642
$U_{i\alpha}$	−0.0923	0.0256	−0.4080	−0.0815	−0.2390	0.8721
	−0.0487	−0.3126	0.1145	−0.5396	−0.7461	−0.1973
	−0.3955	0.1214	0.8107	−0.1722	0.1304	0.3534
	−0.6674	−0.2118	−0.0598	0.6328	−0.3037	−0.1165
	0.5070	0.3839	0.3276	0.4684	−0.5088	0.0999
	0.3610	−0.8334	0.2287	0.2298	0.1343	0.2280

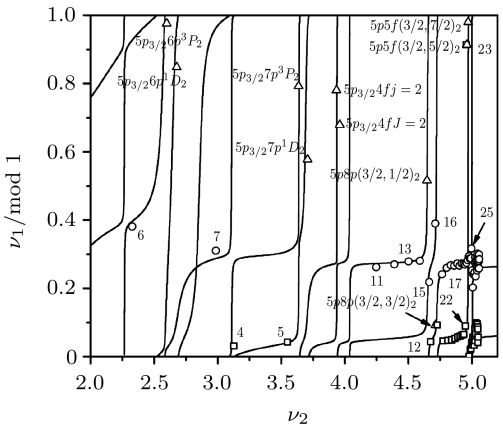


Fig.3. Lu–Fano plot for even-parity $J = 2$ levels of Sn I. Circle: $5pnp$ (1/2,3/2)$_2$; square: $5pnf$ (1/2,5/2)$_2$; triangle: the perturbers.

The MQDT theoretical energy levels up to $n = 59$ for the np series and $n = 56$ for nf series are given in Table 4 together with the experimental data known by us. Below 59198 cm^{-1}, a total of 23 new levels of $5pnp$ (1/2,3/2)$_2$ and $5pnf$ (1/2,5/2)$_2$ not measured previously are predicted. In Moore's table,[4] for some levels assignment of J values are uncertain. We have always taken these doubtful levels into account in calculations, but only the level assigned as $5p_{3/2}4f\ J = 2$ by Moore[10] is confirmed by the present MQDT analyses.

Table 4. MQDT theoretical energy levels and comparison with experimental ones for even-parity $J = 2$ series of Sn I. Units: cm^{-1}.

term[a]	$E_{\rm MQDT}$	$E_{\rm exp}$	$E_{\rm MQDT}-E_{\rm exp}$
$5p_{1/2}6p\ ^3D_2$	43077.4	43238.7[b]	−161.3
$5p_{3/2}6p\ ^3P_2$	47058.9	47235.2[b]	−176.3

Table 4 *Continued*

term[a]	$E_{\rm MQDT}$	$E_{\rm exp}$	$E_{\rm MQDT}-E_{\rm exp}$
$5p_{3/2}6p\ ^1D_2$	48017.2	48189.7[b]	−172.5
$5p_{1/2}7p\ ^3D_2$	51265.6	51170.8[b]	94.8
$4f$ (1/2,5/2)$_2$	52365.3	52263.8[b]	101.5
$8p$ (1/2,3/2)$_2$	54264.6		
$5f$ (1/2,5/2)$_2$	54770.7	54767.7[b]	3.0
$5p_{3/2}7p\ ^3P_2$	55201.8	55186.9[b]	14.9
$5p_{3/2}7p\ ^1D_2$	55421.6	55500.6[b]	−79.0
$9p$ (1/2,3/2)$_2$	55905.4		
$6f$ (1/2,5/2)$_2$	56142.8		
$4f$ (3/2,7/2)$_2$	56411.2	56396.0[b]	15.2
$4f$ (3/2,5/2)$_2$	56741.4	56486.5[b]	254.9
$10p$ (1/2,3/2)$_2$	56818.8		
$7f$ (1/2,5/2)$_2$	56964.1		
$11p$ (1/2,3/2)$_2$	57394.7	57399.9[c]	−5.2
$8f$ (1/2,5/2)$_2$	57496.2		
$12p$ (1/2,3/2)$_2$	57791.1	57792.7[c]	−1.6
$9f$ (1/2,5/2)$_2$	57861.3		
$13p$ (1/2,3/2)$_2$	58071.6	58071.5[c]	0.1
$10f$ (1/2,5/2)$_2$	58122.3		
$14p$ (1/2,3/2)$_2$	58276.5	58277.7[c]	−1.2
$11f$ (1/2,5/2)$_2$	58314.4		
$8p$ (3/2,1/2)$_2$	58403.9	58400.6[d]	3.3
$15p$ (1/2,3/2)$_2$	58438.7	58442.1[c]	−3.4
$12f$ (1/2,5/2)$_2$	58465.3	58465.1[d]	0.2
$16p$ (1/2,3/2)$_2$	58545.7	58542.6[d]	3.1
$8p$ (3/2,3/2)$_2$	58568.9	58574.0[d]	−5.1
$13f$ (1/2,5/2)$_2$	58584.5	58574.0[d]	10.5
$17p$ (1/2,3/2)$_2$	58652.5	58653.0[d]	−0.5
$14f$ (1/2,5/2)$_2$	58669.0	58669.1[d]	−0.1
$18p$ (1/2,3/2)$_2$	58727.9	58727.6[d]	0.3
$15f$ (1/2,5/2)$_2$	58741.5	58741.9[d]	−0.4
$19p$ (1/2,3/2)$_2$	58789.8	58789.3[d]	0.5
$16f$ (1/2,5/2)$_2$	58801.1	58801.4[d]	−0.3
$20p$ (1/2,3/2)$_2$	58841.0	58840.8[d]	0.2

Table 4 *Continued*

term[a]	E_{MQDT}	E_{exp}	$E_{\mathrm{MQDT}} - E_{\mathrm{exp}}$
$17f$ $(1/2,5/2)_2$	58850.4	58850.6[d]	−0.2
$21p$ $(1/2,3/2)_2$	58883.9	58883.5[d]	0.4
$18f$ $(1/2,5/2)_2$	58891.8	58891.8[d]	0.0
$22p$ $(1/2,3/2)_2$	58920.1	58920.0[d]	0.1
$19f$ $(1/2,5/2)_2$	58926.8	58926.8[d]	0.0
$23p$ $(1/2,3/2)_2$	58950.9	58950.7[d]	0.2
$20f$ $(1/2,5/2)_2$	58956.6	58956.6[d]	0.0
$24p$ $(1/2,3/2)_2$	58977.4	58977.3[d]	0.1
$21f$ $(1/2,5/2)_2$	58982.3	58982.3[d]	0.0
$25p$ $(1/2,3/2)_2$	59000.3	59000.3[d]	0.0
$22f$ $(1/2,5/2)_2$	59004.5	59004.1[d]	0.4
$26p$ $(1/2,3/2)_2$	59020.3	59020.2[d]	0.1
$23f$ $(1/2,5/2)_2$	59023.7	59026.8[d]	−3.1
$27p$ $(1/2,3/2)_2$	59037.6	59037.6[d]	0.0
$24f$ $(1/2,5/2)_2$	59038.7	59042.5[d]	−3.8
$5f$ $(3/2,7/2)_2$	59044.1	59042.5[d]	1.6
$28p$ $(1/2,3/2)_2$	59053.2	59052.9[d]	0.3
$25f$ $(1/2,5/2)_2$	59056.8	59057.1[d]	−0.3
$29p$ $(1/2,3/2)_2$	59066.8	59066.7[d]	0.1
$26f$ $(1/2,5/2)_2$	59069.9	59070.1[d]	−0.2
$30p$ $(1/2,3/2)_2$	59078.9	59078.9[d]	0.0
$27f$ $(1/2,5/2)_2$	59081.6	59081.9[d]	−0.3
$31p$ $(1/2,3/2)_2$	59089.4	59089.5[d]	−0.1
$28f$ $(1/2,5/2)_2$	59092.2	59092.3[d]	−0.1
$5f$ $(3/2,5/2)_2$	59096.1		
$32p$ $(1/2,3/2)_2$	59100.7	59099.9[d]	0.8
$29f$ $(1/2,5/2)_2$	59101.8	59101.9[d]	−0.1
$33p$ $(1/2,3/2)_2$	59109.0	59109.1[d]	−0.1
$30f$ $(1/2,5/2)_2$	59110.4	59110.3[d]	0.1
$34p$ $(1/2,3/2)_2$	59116.8	59116.7[d]	0.1
$31f$ $(1/2,5/2)_2$	59118.1	59118.2[d]	−0.1
$35p$ $(1/2,3/2)_2$	59123.9	59123.9[d]	0.0
$32f$ $(1/2,5/2)_2$	59125.2	59125.3[d]	−0.1
$36p$ $(1/2,3/2)_2$	59130.4	59130.4[d]	0.0
$33f$ $(1/2,5/2)_2$	59131.6	59131.6[d]	0.0
$37p$ $(1/2,3/2)_2$	59136.4	59136.2[d]	0.2
$34f$ $(1/2,5/2)_2$	59137.5	59137.5[d]	0.0
$38p$ $(1/2,3/2)_2$	59141.8	59141.6[d]	0.2
$35f$ $(1/2,5/2)_2$	59142.8	59142.8[d]	0.0
$39p$ $(1/2,3/2)_2$	59146.8	59146.9[d]	−0.1
$36f$ $(1/2,5/2)_2$	59147.8	59147.7[d]	0.1
$40p$ $(1/2,3/2)_2$	59151.4	59151.3[d]	0.1
$37f$ $(1/2,5/2)_2$	59152.3	59152.1[d]	0.2
$41p$ $(1/2,3/2)_2$	59155.7	59155.6[d]	0.1
$38f$ $(1/2,5/2)_2$	59156.5	59156.3[d]	0.2
$42p$ $(1/2,3/2)_2$	59159.6	59159.5[d]	0.1
$39f$ $(1/2,5/2)_2$	59160.3	59160.2[d]	0.1
$43p$ $(1/2,3/2)_2$	59163.2	59163.2[d]	0.0
$40f$ $(1/2,5/2)_2$	59163.9	59163.8[d]	0.1
$44p$ $(1/2,3/2)_2$	59166.6	59166.6[d]	0.0

Table 4 *Continued*

term[a]	E_{MQDT}	E_{exp}	$E_{\mathrm{MQDT}} - E_{\mathrm{exp}}$
$41f$ $(1/2,5/2)_2$	59167.2	59167.1[d]	0.1
$45p$ $(1/2,3/2)_2$	59169.7	59169.6$^d y$	0.1
$42f$ $(1/2,5/2)_2$	59170.3	59170.2[d]	0.1
$46p$ $(1/2,3/2)_2$	59172.6	59172.5[d]	0.1
$43f$ $(1/2,5/2)_2$	59173.2	59173.1[d]	0.1
$47p$ $(1/2,3/2)_2$	59175.4	59175.3[d]	0.1
$44f$ $(1/2,5/2)_2$	59175.9	59175.8$^d y$	0.1
$48p$ $(1/2,3/2)_2$	59177.9	59177.8[d]	0.1
$45f$ $(1/2,5/2)_2$	59178.4	59178.4[d]	0.0
$49p$ $(1/2,3/2)_2$	59180.3	59180.2[d]	0.1
$46f$ $(1/2,5/2)_2$	59180.7	59180.7[d]	0.0
$50p$ $(1/2,3/2)_2$	59182.5	59182.4$^d y$	0.1
$47f$ $(1/2,5/2)_2$	59182.9		
$51p$ $(1/2,3/2)_2$	59184.6	59184.5[d]	0.1
$48f$ $(1/2,5/2)_2$	59185.0		
$52p$ $(1/2,3/2)_2$	59186.5	59186.5[d]	0.0
$49f$ $(1/2,5/2)_2$	59186.9		
$53p$ $(1/2,3/2)_2$	59188.3	59188.3[d]	0.0
$50f$ $(1/2,5/2)_2$	59188.7		
$54p$ $(1/2,3/2)_2$	59190.1	59190.0[d]	0.1
$51f$ $(1/2,5/2)_2$	59190.4		
$55p$ $(1/2,3/2)_2$	59191.7		
$52f$ $(1/2,5/2)_2$	59192.0		
$56p$ $(1/2,3/2)_2$	59193.2		
$53f$ $(1/2,5/2)_2$	59193.5		
$57p$ $(1/2,3/2)_2$	59194.7		
$54f$ $(1/2,5/2)_2$	59195.0		
$58p$ $(1/2,3/2)_2$	59196.1		
$55f$ $(1/2,5/2)_2$	59196.3		
$59p$ $(1/2,3/2)_2$	59197.4		
$56f$ $(1/2,5/2)_2$	59197.6		

[a]Some designations are from the references where the corresponding energy levels were reported, the others are based on the MQDT analyses.
[b]From Ref.[4].
[c]From Ref.[8].
[d]From Ref.[9].

Below the first ionization limit there exist 10 perturber levels with $J = 2$ and their positions have been previously determined in experiments [4,8,9,11]. These perturbers include $5p_{3/2}6p\,^3P_2$, $^1D_2$, $5p_{3/2}7p\,^3P_2$, $^1D_2$, $5p8p$ $(3/2,3/2)_2$, $(3/2,1/2)_2$, $5p4f$ $(3/2,5/2)_2$, $(3/2,7/2)_2$, $5p5f$ $(3/2,5/2)_2$ and $(3/2,7/2)_2$. In MQDT results their existence was also reproduced. Here the perturber $5p5f$ $(3/2,5/2)_2$ needs to be discussed. Its experimental value given by Nadeem *et al*[9] is 59026.8 cm^{-1}, which is also the position of the level $5p23f$ $(1/2,5/2)_2$ determined by the same group. But the corresponding MQDT theo-

retical results are 59096.10 cm^{-1} for $5p5f$ $(3/2,5/2)_2$ and 59023.67 cm^{-1} for $5p23f$ $(1/2,5/2)_2$, respectively. Therefore, while the position of $5p23f$ $(1/2,5/2)_2$ is validated no doubt by the present MQDT analyses, the difference between the calculated and measured values for $5p5f$ $(3/2,5/2)_2$ is too large. In this case, we have to mention the experimental result 59084.64 cm^{-1} for $5p5f$ $3/2[3/2]_2$ measured by Jin *et al*,[11] who described $5pnf$ levels by using jK coupling, this measured result is somewhat close to the position of $5p5f$ $(3/2,5/2)_2$ given in this paper. Although this theoretical result cannot be proved absolutely correct, it is very possible that the measured position of $5p5f$ $(3/2,5/2)_2$ reported by Nadeem *et al*[9] is inaccurate. Consequently, the $5p5f$ $(3/2,5/2)_2$ level needs to be identified more reliably by experiment. The rms deviation for all the 94 levels except for the doubtful level $5p5f$ $(3/2,5/2)_2$ is 48.4 cm^{-1}. While the lowest ten levels with larger discrepancies were also excluded, the rms value becomes 1.86 cm^{-1}.

The admixture coefficients Z_i^2 of $J = 2$ levels are shown in Fig.4 for analyzing the interchannel interactions. It is seen that the purities of most levels in the two Rydberg series are very high and thus the identifications for these levels are reliable. The perturbers from $5p6p$ and $5p7p$ configurations only perturb several lower levels in the Rydberg series. The perturber $5p4f$ $(3/2,\ 5/2)_2$ mainly mixes with the $5p10p$ $(1/2,3/2)_2$ level with 84% purity and 8% component of this perturber. In contrast, another perturber $5p4f$ $(3/2,7/2)_2$ only slightly influences $5p10p$ $(1/2,3/2)_2$ and $5p6f$ $(1/2,5/2)_2$. The level $5p15p$ $(1/2,3/2)_2$ contains 10% component of $5p8p$ $(3/2,1/2)_2$ while the $12f$ $(1/2,5/2)_2$ level has 4% component of this perturber. It can also be seen that $5p8p$ $(3/2,3/2)_2$ mixes much with the adjacent levels $5p16p$ $(1/2,3/2)_2$ and $5p13f$ $(1/2,5/2)_2$, which possess 18% and 9% feature of this perturber, respectively. The $5p5f$ $(3/2,7/2)_2$ mixes more into the $5pnf$ $(1/2,5/2)_2$ series than into the $5pnp$ $(1/2,3/2)_2$ series while perturbations of $5p5f$ $(3/2,5/2)_2$ mainly relate to a few nearby levels in $5pnp$ $(1/2,3/2)_2$ series.

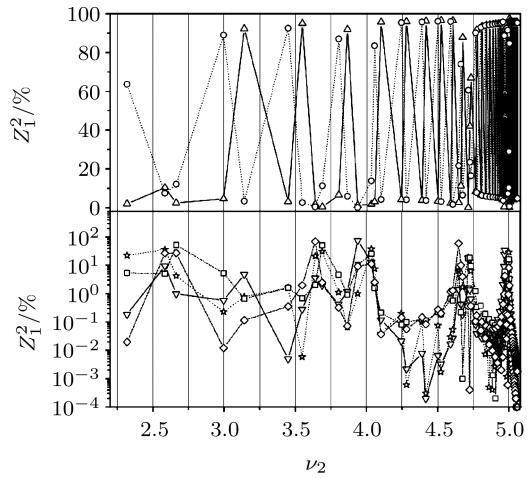


Fig.4. Admixture coefficients of even-parity $J = 2$ levels of Sn I. Sharp-up triangle: $5pnf$ $(1/2,5/2)_2$; circle: $5pnp$ $(1/2,3/2)_2$; sharp-down triangle: $5pnf$ $(3/2,7/2)_2$; star: $5pnf$ $(3/2,5/2)_2$; square: $5pnp$ $(3/2,3/2)_2$; lozenge: $5pnp$ $(3/2,1/2)_2$.

4. Conclusions

The even-parity $5pnp$ and $5pnf$ $J = 1$ and 2 Rydberg series of Sn I have been analyzed with the MQDT method in five- and six-channel models, respectively. A total of 85 new energy levels with $J = 1$ and 23 new levels with $J = 2$ below 59198 cm^{-1} were determined based on the present calculations. The admixture coefficients for the studied series were also calculated for analyses of interchannel interactions. The main perturbations from the perturbers have been discussed in detail. Moreover, it is found that there exist intense channel admixtures between the two $J = 1$ Rydberg series, which needs to be checked by other theoretical methods. The results are helpful to understand the configuration interaction characteristics of the even-parity $J = 1$ and 2 Rydberg series of Sn I. The predicted levels call for corresponding experimental verification.

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