Shell-model studies of isomeric states in ^{51,52,53}Fe*

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Abstract The yrast bands of ^{51,52,53}Fe have been studied with a microscopical effective Hamiltonian derived from the charge-dependent Bonn NN potential. Calculations obtain satisfactory agreements with experimental data, reproducing the observed isomeric states. The possible origins of the isomers are discussed.

Key words CD-Bonn potential, shell model, Fe, isomer

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Nuclei near the center of the $0f_{7/2}$-shell are of particular interest as they have enough valence particles to form some degrees of deformation and collective motion[1]. The advent of efficient detectors has allowed the investigations of the structures of these nuclei at high spins[2—4]. Large-scale shell-model calculations[5, 6] (up to the dimension of around 10^9[7]) are now possible, giving us much more enriched understanding to the nuclear many-fermion system than heretofore possible[8].

Well-defined rotational bands in $0f_{7/2}$-nuclei (i.e., the even-even nucleus of ^{48}Cr) have been observed[9], which can be reproduced well by the nuclear shell model[10, 11]. For odd-odd $N=Z$ nuclei, the enhanced pairing correlations[12] between the odd-neutron and the odd-proton can lead to the coexistence of both $T=1$ and $T=0$ collective bands at low excitation energies[13]. The evolution patterns of energy differences (MED) for mirror nuclei along the $N=Z$ line in this shell have been successfully extended to high-spin states, providing a unique ground to study the effects of charge-independence breaking in nuclear systems[14—16].

It has been expected that the residual interaction can produce long-lived spin traps (i.e., with unusual spin sequence) in $0f_{7/2}$-nuclei[17]. Classic examples are the $J^\pi=19/2^-$ isomers in the mirror pair of ^{53}Fe and ^{53}Co. For odd-odd $N=Z$ nuclei in this shell, low-lying isomeric states can be formed with the inversion of the isovector (with $J^\pi=0^+$) and isoscalar (with odd-J) states[13]. Recently, the yrast 12^+ level of ^{52}Fe has also been confirmed as an isomeric state as a result of the inversion of the 10^+_1 and 12^+_1 states[2]. In this work, spherical shell-model calculations are done with an effective Hamiltonian derived from the charge-dependent Bonn (CD-Bonn) Nucleon-Nucleon (NN) potential[15] to study the yrast structures of the isotopes of ^{51}Fe, ^{52}Fe and ^{53}Fe. We will show that the level structures of the Fe isotopes can be reproduced well by the microscopical effective Hamiltonian. The possible origin of the isomeric states in the yrast bands will also be discussed.

The nuclear shell model restricts calculations in one or several Harmonic-Oscillator (HO) major shells[18]. The starting-point is an model-space-dependent effective Hamiltonian given as[19]

$$H_{\rm eff} \simeq PH_0P + PH_1P + PH_1\frac{Q}{E_0-H_0}H_1P, \qquad (1)$$

where H_0 (H_1) is the unperturbed (perturbed) Hamil-

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tonian and P and Q the projection operators. E_0 is the unperturbed energy. The first two terms in the equation give the single-particle Hamiltonian which can be determined from experimental single-particle energies. The last term defines the effective interaction which can be directly related to the under-lying NN interaction[8]. The diagonalzation of Eq. (1) can be done with standard shell-model codes[5, 20]. In the present work, calculations have been carried out on the 64-bit Beowulf cluster of the PKU computer center with a newly-developed parallel program[11].

In the present code, the symmetry of spin J is restored through a projection procedure by which the dimension of the matrix can be significantly reduced. Vectors with good angular momentum J are expanded in M-scheme HO bases as

$$|\Phi_i^J\rangle = \sum_{m\leqslant i} \mathcal{M}_{im} P^J |\phi_m\rangle, \tag{2}$$

where P^J is the angular momentum projection operator and $|\phi\rangle$ a set of M-scheme bases. $\mathcal{M}$ is a lower triangle matrix ensuring that the projected vectors are orthonormal. The projection operator is given as[21]

$$P^J = \prod_{J'=J_z,\ J'\neq J}^{J_M} \frac{\hat{J}^2 - J'(J'+1)}{J(J+1) - J'(J'+1)}, \tag{3}$$

where $\hat{J}^2 = J^- J^+ + J_z(J_z+1)$.

The effective interaction can be simply expressed in the form of HO two-body matrix elements as

$$V_{\text{eff}} = \sum_J \sum_{\alpha\leqslant\beta;\gamma\leqslant\delta} \langle \alpha\beta; J|V|\gamma\delta; J\rangle, \tag{4}$$

where the Greek letters denote HO single-particle orbits. The interaction can be determined phenomenally [20] from experimental observations or microscopically [8] from the NN potential[15].

For fp-shell, effective interactions have been proposed, like the monopole-corrected KB3 interaction[1, 22], the FPD6 analytic two-body potential[23] and the GXPF interaction[24]. Microscopical interactions calculated from NN potentials are also available[8]. In the present work we employ an effective interaction[13] derived from the CD-Bonn potential[15]. The short-range repulsive core of the NN potential is handled through the introduction of the G reaction matrix[8]. Then the G matrix is renormalized through the folded-diagram procedure[19] which can take into account the core-polarization and long-range effects.

The Hamiltonian matrix can be calculated in the j-j scheme basis as

$$\langle \Phi_i^J | H_{\text{eff}} | \Phi_j^J \rangle = \sum_{m\leqslant j} \mathcal{M}_{jm} \langle \Phi_i^J | H_{\text{eff}} | \phi_m \rangle. \tag{5}$$

The diagonalization of this matrix (usually with huge dimension) can be done iteratively through the Lanczos procedure[5, 11].

The shell model is a very efficient tool for the studies of nuclear level structures[1, 13, 16] and decay properties[25—27]. The drawbacks of the shell model lie in the painstaking handling of super-large matrices and the loss of transparency in physical interpretations. Truncation methods have been proposed[6, 28, 29] to make the model more applicable.

The isomeric state of 12^+ in ^{52}Fe was first observed in Ref. [17], with the predication of the inversion of the yrast 10^+ and 12^+ states. Calculated results for ^{52}Fe are plotted in Fig. 1. As a first approximation, the maximal number ($N_{\max}$) of particles being excited out of the $0f_{7/2}$-shell is restricted to two. Full convergence of calculated binding energies can be seen at the truncation level of $N_{\max} = 5$ in this mass region[30]. Shell-model results of the KB3 interaction[22] can be found in Ref. [2].

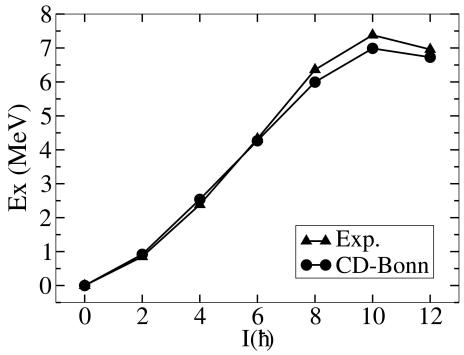

Fig. 1. Calculated and experimental[2] yrast bands of ^{52}Fe.

The inversion of the 12_1^+ isomer of ^{52}Fe with the 10_1^+ state can be reproduced in present calculations. By assuming $0f_{7/2}$-dominance, the structures of the cross-conjugate partners of ^{52}Fe and ^{44}Ti should be similar to each other. In Fig. 2, we show shell-model calculations for ^{44}Ti (a $0f_{7/2}^4$ system). The yrast 10^+ and 12^+ states of ^{44}Ti do not convert, which can be reproduced in full fp-shell calculations by all interactions shown in Fig. 2. When calculations are restricted to the pure $0f_{7/2}$-configuration, however,

all interactions give reverted results. Fig. 2 indicates that the $0f_{7/2}$-configuration can give positive contributions to the formation of the level inversion. For ^{52}Fe, both 10^+_1 and 12^+_1 states are dominated by the $0f_{7/2}$-shell, accompanied with similar contributions from upper sub-shells[2]. The dominated $0f_{7/2}$-configuration (four holes in $0f_{7/2}$) can give rise to the inversion. Since $I = 12$ is the maximal spin that can be reached in the $0f^4_{7/2}$-system, pure $0f_{7/2}$-configuration appears at the 12^+_1 state of ^{44}Ti. The energy inversion is not observed due to the existence of relatively large configuration-mixing for the yrast 10^+ state. The configuration-mixing can decrease the relative energy of the 10^+_1 state to a position lower than that of the 12^+_1 level.

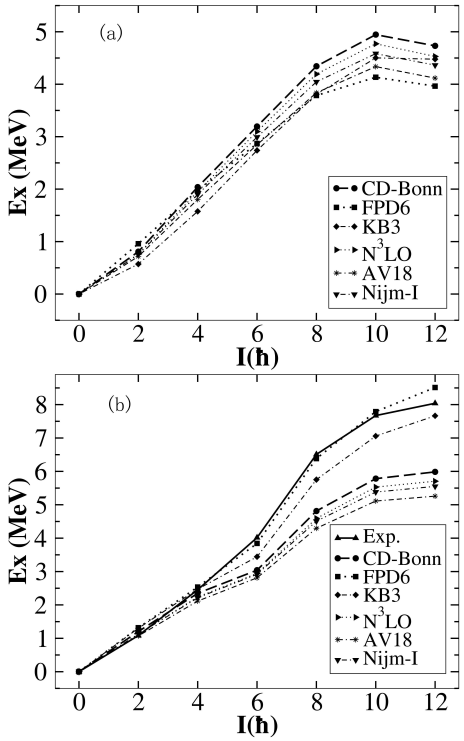

Fig. 2. Calculated yrast bands of ^{44}Ti in $0f_{7/2}$- (a) and full fp-shell (b). Experimental data are taken from Ref. [31].

For the odd-A nuclei of ^{51,53}Fe, calculations are done with the truncation of $N_{\max} = 3$. Our detailed calculations on the properties of ^{51}Fe can be found in Ref. [16]. In Fig. 3 we plotted the isoscalar band of ^{50}Mn (with one proton subtracted from ^{51}Fe). For the decay of the $17/2^-_1$ state of ^{51}Fe, shell-model calculations give rather small $E2$ and $M1$ strengths, indicating that drastic structural changes can occur around the yrast $17/2^-$ state. The $17/2^-_2$ state can belong to the $K^\pi = 5/2^-$ ground-state band of ^{51}Fe[32]. Possible reason for the lowering of the energy of the $17/2^-$ isomeric state can be due to the breaking of a proton-pair, which is also expected from the analysis of MED evolution pattern of the mirror pair ^{51}Fe and ^{51}Mn[4]. The result is consistent with Nilsson calculations[32] which show that the $17/2^-_1$ state can be the band head of a three-quasiparticle band with a high K value of $K = 17/2$.

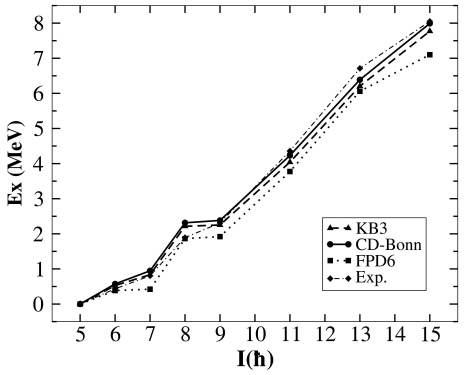

Fig. 3. Calculated and experimental[33] $T = 0$ bands of ^{50}Mn.

Calculated results for ^{53}Fe are plotted in Fig. 4. The inversion of the yrast $17/2^-$ and $19/2^-$ states occurs in ^{53}Fe. The property of this $17/2^-$ state should be different from that of the $17/2^-$ isomeric state of ^{51}Fe since a relatively strong transition of $17/2^- \to 15/2^-$ in ^{53}Fe is expected[3]. Nilsson calculations[2] suggest that the thus-formed $19/2^-$-isomer (due to spin trap) is a $K = 19/2$ intrinsic state obtained by the coupling of the odd neutron and a broken pair of proton. The alignment of particles may occur at the 6^+_1 state of ^{52}Fe[2]. The coupling of the odd proton and the 6^+ of the ^{52}Fe core may give rise to the energetically favored $19/2^-$ spin trap isomer.

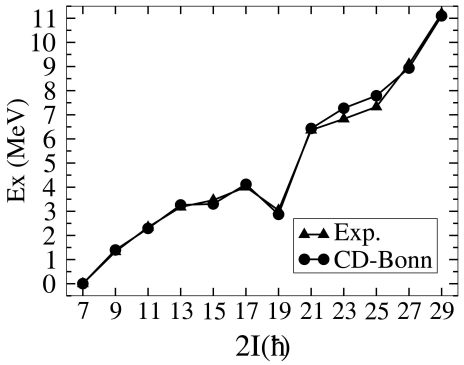

Fig. 4. Calculated and experimental[3] yrast bands of ^{53}Fe.

In summary, the yrast bands of ^{51,52,53}Fe have been studied with a microscopical effective Hamiltonian derived from the charge-dependent Bonn NN potential. Calculations obtain satisfactory agreements with experimental observations, reproducing the observed isomeric states. Shell-model calculations suggest that the $0f_{7/2}$-configuration interaction leads to the energy inversion of the 10^+ and 12^+ states of ^{52}Fe, resulting in a long-lived spin trap. The $19/2^-$spin trap in ^{52}Fe can be due to the particle-aligned coupling of the odd-proton and the band-terminated 6^+_1 state of ^{52}Fe. The formation of the $17/2^-_1$ isomer in ^{51}Fe is due to the drastic changes in configurations around the state.

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