

# Deformed shell model for $T = 0, 1$ and $2$ bands in $^{52}\text{Fe}$ and $^{72}\text{Kr}$

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**Abstract.** Deformed configuration mixing shell model based on Hartree-Fock states with extension to include isospin projection (DSMT) for two- and four-particle configurations (generated by particle-hole excitations) is applied to study the structure of the low-lying  $T = 0, 1$  and  $2$  bands (or levels) in the even-even  $N = Z$  nuclei  $^{52}\text{Fe}$  and  $^{72}\text{Kr}$ . The  $pf$ -shell KB3 interaction for  $^{52}\text{Fe}$  and a modified Kuo's interaction for  $^{72}\text{Kr}$  are employed in the calculations. In this first application of DSMT with four-particle  $T$  projection, low-spin ( $J \leq 10$ ) members of the  $T = 0, 1$  and  $2$  bands in  $^{52}\text{Fe}$  are compared with experiment including the known  $E2$  transition strengths. The agreement between DSMT and experiment is reasonably good. Similarly, the low-spin members of the observed (prolate) yrast band in  $^{72}\text{Kr}$  are also well described by DSMT.

**PACS.** 21.10.Hw Spin, parity, and isobaric spin – 21.10.Re Collective levels – 21.60.Cs Shell model – 21.60.Jz Hartree-Fock and random-phase approximations

## 1 Introduction

In the last few years, with the development of radioactive ion beam facilities and large detector arrays, the study of the structure of heavy ( $A \geq 44$ )  $N = Z$  nuclei near the proton drip line has become an area of intense research as these nuclei are expected to give new insights into neutron-proton (np) correlations that are hitherto unknown and as they are important for rp-process nucleosynthesis. The initial focus being on heavy odd-odd  $N = Z$  nuclei with  $A > 60$  as they are expected to give new insights into isoscalar ( $T = 0$ ) vs. isovector ( $T = 1$ ) pairing. Recently for  $^{62}\text{Ga}$ ,  $^{66}\text{As}$ ,  $^{70}\text{Br}$  and  $^{74}\text{Rb}$  [1] many  $T = 0$  and  $T = 1$  levels have been identified. On the other hand, inspired by a large-scale shell model for  $pf$ -shell nuclei, there are experiments with new data for  $T = 0$  and  $T = 1$  bands in  $^{46}\text{V}$ ,  $^{50}\text{Mn}$  and  $^{54}\text{Co}$  [2]. Going beyond  $N = Z$  odd-odd nuclei, new experimental studies have been initiated recently for  $N = Z$  even-even nuclei with  $A > 44$  up to  $A = 88$  [3–10]. These nuclei are expected to exhibit interesting deformation characteristics, delay in angular-momentum alignments at high spins, besides the lowest  $T = 0$  band excited  $T = 1$  and  $2$  levels/bands etc. Also in many nuclear models the analysis of even-even nuclei is much easier than for odd-odd nuclei. With more data accumulating, the  $N = Z$  even-even nuclei with

$A > 60$  ( $^{68}\text{Se}$ ,  $^{72}\text{Kr}$ ,  $^{76}\text{Sr}$  and  $^{80}\text{Zr}$ ) have been analyzed recently using several models: i) the excited Vampir variational approach based on HFB with realistic interactions is used to study yrast levels [11]; ii) the projected shell model (PSM) [12] with pairing plus quadrupole-quadrupole and also quadrupole pairing is used to study ground band and quadrupole moments; iii) the Monte Carlo shell model [13] with pairing-plus-quadrupole-quadrupole interaction is used to study ground-state quadrupole moments and occupancies. Similarly, there are studies of even-even  $N = Z$  nuclei in the lower  $pf$ -shell (for  $^{48}\text{Cr}$  and  $^{52}\text{Fe}$ ) using the shell model with the so-called KB3 interaction and interpretation of some of the levels/bands in terms of the Nilsson model [8–10, 14]. On the other hand, BCS with iso-cranking including isoscalar and isovector pairing interactions is used by Wyss *et al.* to study the lowest  $T = 1$  and  $2$  levels in these nuclei [15].

Recently, in order to analyze the properties of  $A = 44$ – $100$  nuclei, the deformed configuration mixing shell model [16] based on HF single-particle states with isospin projection (hereafter called DSMT) has been developed [17]. The  $T = 0$  and  $T = 1$  levels in  $^{62}\text{Ga}$  and  $^{66}\text{As}$  [17] and the  $T = 0$  and  $T = 1$  bands in  $^{46}\text{V}$  and  $^{50}\text{Mn}$  [18] are well described by the DSMT model. In all these calculations isospin projection from two-particle configurations (generated by particle-hole excitations) is carried out in the beginning and as was shown in [18]; this is equivalent to the so-called rotor-plus-quasideuteron model [19]. However, for even-even  $N = Z$  nuclei and

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heavier  $N = Z$  odd-odd nuclei it is necessary to consider isospin projection from four- (for even-even) and six- (for odd-odd) particle configurations generated by making particle-hole excitations over the lowest intrinsic configuration based on the Hartree-Fock (HF) single-particle spectrum. The purpose of this paper is to give the method for the  $T$  projection for four-particle configurations and as a first application of this, data for the even-even  $N = Z$  nuclei  $^{52}\text{Fe}$  and  $^{72}\text{Kr}$  are analyzed using DSMT, *i.e.* one  $pf$ -shell nucleus ( $^{52}\text{Fe}$ ) and one  $A > 60$  nucleus ( $^{72}\text{Kr}$ ) are chosen. Now we will give a preview.

In sect. 2 a brief description of the DSMT model is given and then the method for  $T$  projection for four-particle configurations is described in detail. In sect. 3 spectroscopic results for  $^{52}\text{Fe}$  are described. Here the DSMT results are compared both with data and shell model calculations. Similarly, sect. 4 gives the results for  $^{72}\text{Kr}$ . Finally, sect. 5 gives concluding remarks.

## 2 Deformed shell model with isospin (DSMT): two- and four-particle isospin projection

The details of the deformed shell model (DSM) have been described in many previous publications [16]. For completeness we give here a few important steps. In this model, for a given nucleus, starting with a model space consisting of a given set of single-particle orbitals and effective two-body Hamiltonian, the lowest-energy (axially symmetric) prolate and oblate intrinsic states are obtained by solving the HF single-particle equation self-consistently. Then various excited intrinsic states are obtained by making particle-hole excitations over the lowest intrinsic state. A constrained HF calculation (tagged HF) is performed in each case. These intrinsic states do not have good angular momentum. Hence, good-angular-momentum states are projected from each of these intrinsic states. In general the good-angular-momentum states coming from different intrinsic states are not orthogonal to each other. Hence they are orthonormalized and then band mixing calculations are performed.

Let the various intrinsic states obtained by solving the axially symmetric HF equation self-consistently be denoted by  $\chi_K(\mu)$  with  $\mu$  distinguishing different intrinsic states with same  $K$ . Good-angular-momentum states are projected from each of these intrinsic states using the projection operator

$$P_{MK}^J = \frac{2J+1}{8\pi^2} \int D_{MK}^{J*}(\Omega) R(\Omega) d\Omega. \quad (1)$$

The angular-momentum projected states  $\phi_{MK}^J$  obtained from different intrinsic states have to be orthogonalized since they may not be orthogonal to each other. For this purpose, we consider the overlap matrix

$$N_{K'\mu',K\mu}^J = \langle \phi_{MK'}^J(\mu') | \phi_{MK}^J(\mu) \rangle. \quad (2)$$

For an orthonormal set of vectors, this matrix would be a unit matrix, whereas in the case of the non-orthogonal

basis, it is not diagonal. Hence the matrix  $N_{K'\mu',K\mu}^J$  is diagonalized and the resulting vectors can be written as

$$\Phi_M^J(\alpha) = \sum_{K\mu} S_{K\alpha}^J(\mu) \phi_{MK}^J(\mu), \quad (3)$$

where

$$S_{K\alpha}^J(\mu) = [n_M^J(\alpha)]^{-1/2} X_{K\alpha}^J(\mu) \quad (4)$$

with  $X_{K\alpha}^J$  corresponding to the element of the unitary transformation matrix that diagonalizes the overlap matrix  $N^J$  and  $n_M^J$  denotes the eigenvalues of  $N^J$ . The functions  $\Phi_M^J(\alpha)$  constitute an orthonormal set of vectors. The composite spectrum of a nucleus is obtained by diagonalizing the Hamiltonian matrix in the basis of these orthonormalized projected states. The overlap

$$B_K^J(\eta, \alpha) = \langle \phi_{MK}^J(\eta) | \Phi_M^J(\alpha) \rangle = \sum_{K_1\eta_1} S_{K_1\eta_1}^J(\alpha) N_{K\eta, K_1\eta_1}^J \quad (5)$$

gives the measure of the state  $\phi_{MK}^J(\eta)$  projected from a given intrinsic state  $\chi_K(\eta)$  that the eigenstate  $\Phi_M^J(\alpha)$  contains. The larger the amplitude  $|B_K^J(\eta, \alpha)|^2$ , the more pronounced will be the characteristic of that parent intrinsic state in the state  $\Phi_M^J(\alpha)$ . The calculations of electric and magnetic transition probabilities between the states  $\Phi_M^J(\alpha)$  involve the evaluation of the matrix elements of the appropriate transition operators  $O_m^l$  of rank  $l$  between these states.

Recently DSM has been extended to include isospin projection so that the band structures in  $N = Z$  odd-odd nuclei can be analyzed. This extended model is called DSMT with  $T$  denoting isospin projection [17]. Alternatively one can consider a large enough number of intrinsic states and perform band mixing calculations as described above. Then, as the Hamiltonian respects isospin, the states will carry good isospin. In the selection of the basis, it is important to ensure that whenever a particular state is present, also the one in which protons and neutrons are interchanged, is present. Finally one has to calculate the expectation value of the  $T^2$  operator in the final states to identify the isospin of these states. This approach is not complicated. However, in the present paper, DSMT is employed where isospin projection is carried out in the beginning.

In its elementary version DSMT is developed for  $T$  projection from quasideuteron configurations. As a simple example for this let us consider  $N = Z$  odd-odd nuclei. For these, the lowest prolate and oblate HF intrinsic states the unpaired proton and neutron occupy the same HF single-particle orbits and hence these are symmetric in space co-ordinates. Therefore, these intrinsic states will have  $T = 0$  (protons and neutrons in the other occupied orbits will have  $\alpha$ -particle-like structure with  $T = 0$ ). If in an excited intrinsic state (say  $\phi_{k_1}^p \phi_{k_2}^n$ ), the unpaired proton occupies the single-particle orbit specified by the azimuthal quantum number  $k_1$  and the unpaired neutron occupies the state  $k_2$  ( $k_1 \neq k_2$ ), then one can also consider an intrinsic state where the occupancies of the unpaired nucleons are reversed. By taking a linear combination of

these intrinsic states, one can construct intrinsic states which are symmetric (or antisymmetric) in space coordinates. Symmetric combination will have isospin  $T = 0$  and the antisymmetric combination gives  $T = 1$ . Thus,

$$\begin{aligned} \frac{1}{\sqrt{2}} [\phi_{k_1}^p \phi_{k_2}^n + \phi_{k_2}^p \phi_{k_1}^n] &\Leftrightarrow T = 0, \\ \frac{1}{\sqrt{2}} [\phi_{k_1}^p \phi_{k_2}^n - \phi_{k_2}^p \phi_{k_1}^n] &\Leftrightarrow T = 1. \end{aligned} \quad (6)$$

## 2.1 Four-particle isospin projection in DSMT

For even-even  $N = Z$  nuclei one has to go beyond the simple  $T$  projection for quasideuteron configurations and consider  $T$  projection for a  $(2p, 2n)$  system in four  $k$  orbits. Towards this end, let us consider four distinct orbits  $A, B, C$  and  $D$  in which two protons and two neutrons are distributed. Then there are six  $(2p, 2n)$  states and they can be written as

$$\begin{aligned} \Phi_1 &= \phi_A^p \phi_B^p \phi_C^n \phi_D^n, & \Phi_2 &= \phi_A^p \phi_C^p \phi_B^n \phi_D^n, \\ \Phi_3 &= \phi_A^p \phi_D^p \phi_B^n \phi_C^n, & \Phi_4 &= \phi_B^p \phi_C^p \phi_A^n \phi_D^n, \\ \Phi_5 &= \phi_B^p \phi_D^p \phi_A^n \phi_C^n, & \Phi_6 &= \phi_C^p \phi_D^p \phi_A^n \phi_B^n. \end{aligned} \quad (7)$$

In order to construct  $(2p, 2n)$  states with good isospin the  $T^2$ -matrix in the basis defined by the six states in (7) is constructed and diagonalized. For four particles the allowed isospin values are  $(2, 1, 0)$  with  $T^2$  eigenvalues 6, 2 and 0. As the Young tableaux corresponding to  $T = 2, 1$  and  $0$  are  $\{4\}$ ,  $\{3, 1\}$  and  $\{2, 2\}$ , from the symmetry group  $S_4$  properties, it is easily seen that there must be one  $T = 2$ , three  $T = 1$  and two  $T = 0$  states. The  $T^2$ -matrix is constructed using

$$\begin{aligned} T^2 &= \left( \sum_i t_i \right) \cdot \left( \sum_i t_i \right) \\ &= \sum_i t_i^2 + \sum_{i \neq j} t_i \cdot t_j \\ &= \sum_i (3/4) + 2 \sum_{i < j} t_i \cdot t_j \\ &= \sum_i (3/4) + 2 \sum_{i < j} \left\{ t_0^{i:1} t_0^{j:1} - t_1^{i:1} t_{-1}^{j:1} - t_{-1}^{i:1} t_1^{j:1} \right\}. \end{aligned} \quad (8)$$

In (8)  $i$  is the particle index and  $t$  is the single-particle isospin operator. In the last form in (8) the isospin operator is written in tensorial form. It should be noted that  $t_1^1 = -\frac{1}{\sqrt{2}} t_+$  and  $t_{-1}^1 = \frac{1}{\sqrt{2}} t_-$ . With  $|p\rangle = |\frac{1}{2} \frac{1}{2}\rangle$  and  $|n\rangle = |\frac{1}{2} -\frac{1}{2}\rangle$ ,  $t_+$  will change  $n \rightarrow p$  and similarly  $t_-$  will change  $p \rightarrow n$ . Using this property and (8) the matrix for the  $T^2$  operator in the basis defined by (7) is

$$T^2 = \begin{pmatrix} 2 & -1 & 1 & 1 & -1 & 0 \\ -1 & 2 & -1 & -1 & 0 & -1 \\ 1 & -1 & 2 & 0 & -1 & 1 \\ 1 & -1 & 0 & 2 & -1 & 1 \\ -1 & 0 & -1 & -1 & 2 & -1 \\ 0 & -1 & 1 & 1 & -1 & 2 \end{pmatrix}. \quad (9)$$

Diagonalizing matrix (9) gives the following six orthonormalized states with good isospin:

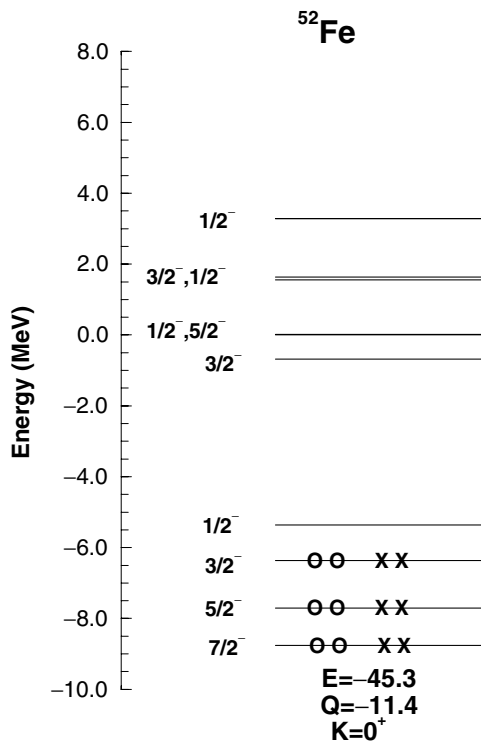
$$\begin{aligned} \Psi_1(T=0) &= \frac{1}{2} [\Phi_1 - \Phi_3 - \Phi_4 + \Phi_6], \\ \Psi_2(T=0) &= \frac{1}{2\sqrt{3}} [\Phi_1 + 2\Phi_2 + \Phi_3 + \Phi_4 + 2\Phi_5 + \Phi_6], \\ \Psi_1(T=1) &= \frac{1}{\sqrt{2}} [-\Phi_1 + \Phi_6], \\ \Psi_2(T=1) &= \frac{1}{\sqrt{2}} [-\Phi_2 + \Phi_5], \\ \Psi_3(T=1) &= \frac{1}{\sqrt{2}} [-\Phi_3 + \Phi_4], \\ \Psi(T=2) &= \frac{1}{\sqrt{6}} [\Phi_1 - \Phi_2 + \Phi_3 + \Phi_4 - \Phi_5 + \Phi_6]. \end{aligned} \quad (10)$$

Equation (10) is applied in sects. 3 and 4 in constructing good  $T$  states, within the DSM, for the even-even nuclei  $^{52}\text{Fe}$  and  $^{72}\text{Kr}$ . For completeness let us add that the construction of good  $T$  states for the  $(2p, 2n)$  systems is simple when there are only two or three orbits. As we can put only one proton or one neutron in a given orbit, for the  $(2p, 2n)$  system we need a minimum of two orbits (in this discussion, orbits with  $k$  and  $-k$  are treated as different orbits). With only two orbits (say  $A$  and  $B$ ), only a  $T = 0$  state is possible and it is  $[\phi_A^p \phi_A^n \phi_B^p \phi_B^n]^{T=0}$ . With three orbits (say  $A, B$  and  $C$ ) two states are possible and they are  $\phi_A^p \phi_A^n \phi_B^p \phi_C^n$  and  $\phi_A^p \phi_A^n \phi_C^p \phi_B^n$ . Using them one can construct easily (see eq. (6)) one  $T = 0$  state and one  $T = 1$  state.

## 3 Results for $^{52}\text{Fe}$

In order to apply DSMT with four-particle isospin projection, *i.e.* the results with eq. (10), we have first analyzed the  $pf$ -shell nucleus  $^{52}\text{Fe}$  for which  $T = 1, 2$  levels, in addition to the  $T = 0$  levels, have been identified (recent experiments are due to Lenzi *et al.* [7, 10]). For the spectroscopy of the low-lying states in this nucleus,  $^{40}\text{Ca}$  is taken as the inert core with the  $pf$ -shell orbitals  $1f_{7/2}, 2p_{3/2}, 2p_{1/2}$  and  $1f_{5/2}$  as active orbits. The well-known KB3 interaction with single-particle energies 0.0, 2.0, 4.0 and 6.5 MeV, respectively [20], is employed in the calculations as in our previous study of  $^{46}\text{V}$  and  $^{50}\text{Mn}$  [18]. For this nucleus, we have used the effective charges of proton and neutron to be  $1.5e$  and  $0.5e$  for calculating  $B(E2)$ 's and quadrupole moments. These effective charges and the KB3 interaction are also used in the shell model analysis reported in [10].

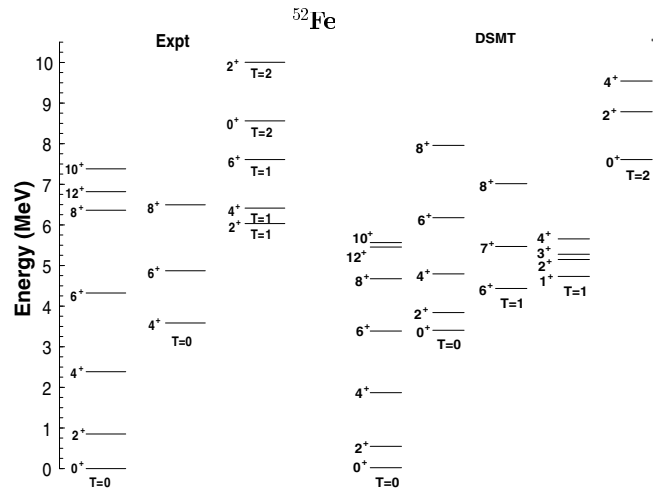
The HF single-particle (sp) spectrum, (the states are labeled  $|k_i\rangle$ , where the  $i$  label distinguishes different states with the same  $k$  value) for the lowest HF intrinsic state, which is oblate, is given in fig. 1. Besides the lowest oblate configuration, we have considered 16 excited oblate configurations and they are: i)  $(7/2^-)^{2p2n}(5/2^-)^{2p2n}(3/2^-)^{-\nu}(1/2^-)^\nu$  configurations giving  $K = 1, 2$  with  $\nu = p$  or  $n$  and they decompose into  $T = 0, 1$ ; ii)  $(7/2^-)^{2p2n}(5/2^-)^{2p2n}$  core plus 2 protons and 2 neutrons with two nucleons in the  $3/2^-$  and two nucleons in the  $1/2^-$  orbits giving six  $K = 0$ , two



**Fig. 1.** Spectrum of single-particle states for the lowest-energy HF intrinsic state for  $^{52}\text{Fe}$ . The circles represent protons and the crosses represent neutrons. All the single-particle states are of negative parity. The Hartree-Fock energy ( $E$ ) is in MeV and the mass quadrupole moment ( $Q$ ) is in units of the square of the oscillator length parameter. The total  $K$  quantum number of the intrinsic state in the figure is  $K = \sum k_i = 0$ , where the sum is over the occupied states and the parity  $\pi = +1$ .

$K = 1$ , one  $K = 2$ , two  $K = 3$  and one  $K = 4$  configurations. The  $K = 4, 1$  states are pure  $T = 0$  and the  $K = 2, 3$  states can be decomposed into  $T = 0, 1$  states. Similarly, the six  $K = 0$  states decompose into  $T = 0, 1, 2$  states as given by eq. (5). For the lowest prolate configuration the HF sp spectrum is given by  $1/2_1^-$  ( $-10.9$  MeV),  $3/2_1^-$  ( $-8.89$  MeV),  $1/2_2^-$  ( $-5.15$  MeV),  $5/2_1^-$  ( $-4.34$  MeV) etc. with the lowest three being occupied and the third being empty. For the prolate excited configurations i) and ii) above are used for the orbits  $1/2_2^-$  and  $5/2_1^-$  and they produce 16 excited configurations: i) gives  $K = 3, 2$  each with  $T = 0, 1$  and ii) gives six  $K = 0$  (decomposing into two  $T = 0$ , three  $T = 1$  and one  $T = 2$ ), two  $K = 1$  (decomposing into  $T = 0, 1$ ), one  $K = 4$  (with  $T = 0$ ), two  $K = 5$  (decomposing into  $T = 0, 1$ ) and one  $K = 6$  (with  $T = 0$ ) states. For each  $T$  separately, band mixing calculations are performed using the  $J$  projected (from the 34 intrinsic states described above) states.

The calculated spectrum, using DSMT, is compared with data [10,21] in fig. 2. The ground  $T = 0$  band is somewhat compressed with respect to data but otherwise the agreement between the two is reasonably good. DSMT produces the observed  $12^+, 10^+$  inversion. The  $B(E2)$ 's along this band, as given in table 1, are well described (they indicate a change in collectivity above  $8^+$  and this

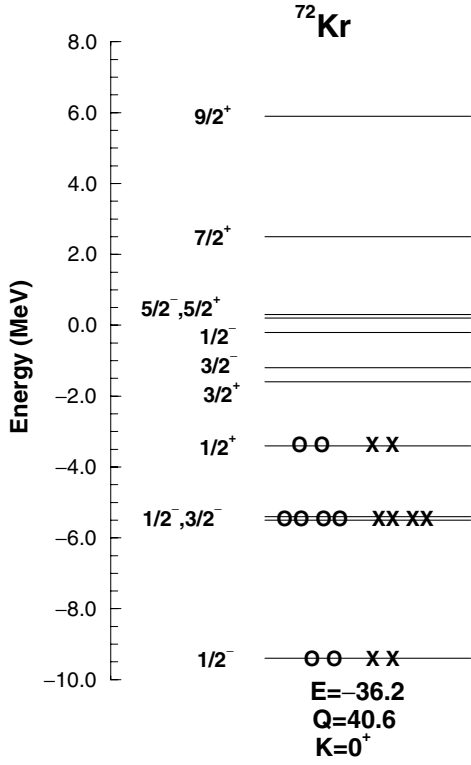


**Fig. 2.**  $T = 0$ ,  $T = 1$  and  $T = 2$  bands in  $^{52}\text{Fe}$  obtained from the deformed shell model with isospin projection (DSMT) are compared with experimental data [10,21]. See text for further details.

**Table 1.** DSMT model predictions for  $B(E2; K_i J_i T_i \rightarrow K_f J_f T_f)$  in  $e^2 \text{fm}^4$  for  $^{52}\text{Fe}$  are compared with experimental data and shell model (SM) results given in [10].

$B(E2)$ 's for $^{52}\text{Fe}$				
$K_i J_i T_i$	$K_f J_f T_f$	DSMT	Expt.	SM
$0 2^+ 0$	$0 0^+ 0$	129	$< 1844$	155
$0 4^+ 0$	$0 2^+ 0$	289	$300 \pm 69$	224
$0 6^+ 0$	$0 4^+ 0$	226	$124 \pm 40$	118
$0 8^+ 0$	$0 6^+ 0$	67	$74 \pm 25$	86
$0 10^+ 0$	$0 8^+ 0$	27		
$0 6_2^+ 0$	$0 4_1^+ 0$	23	$29 \pm 14$	83
$0 8_2^+ 0$	$0 6_1^+ 0$	2	$43 \pm 15$	11
$6 7^+ 1$	$6 6^+ 1$	38		
$6 8^+ 1$	$6 6^+ 1$	17		
$6 8^+ 1$	$6 7^+ 1$	22		
$1 2^+ 1$	$1 1^+ 1$	114		
$1 3^+ 1$	$1 2^+ 1$	53		
$1 3^+ 1$	$1 1^+ 1$	188		
$1 4^+ 1$	$1 3^+ 1$	37		
$1 4^+ 1$	$1 2^+ 1$	33		

is also seen in static quadrupole moments of these levels). There are also excited  $4^+$ ,  $6^+$  and  $8^+$  levels in the data given in [10]. It is plausible that these levels are members of the excited  $T = 0$  band given by DSMT (see fig. 2).  $B(E2)$ 's for the decay of the  $6_2^+$  and  $8_2^+$  to the ground  $4_1^+$  and  $6_1^+$  levels, respectively, provide a good justification for this interpretation; see table 1 for the comparison between data and DSMT for these transitions. Going beyond this, it is seen that the DSMT results for the two  $T = 0$  bands are similar to the results obtained by Ur *et al.* [10] within the framework of the spherical shell model in the full  $pf$ -shell. Shell model energies are close to data for the lowest  $T = 0$  band up to  $8^+$  and for the observed  $4^+$ ,  $6^+$  and  $8^+$  levels of the excited  $T = 0$  band the deviations are similar



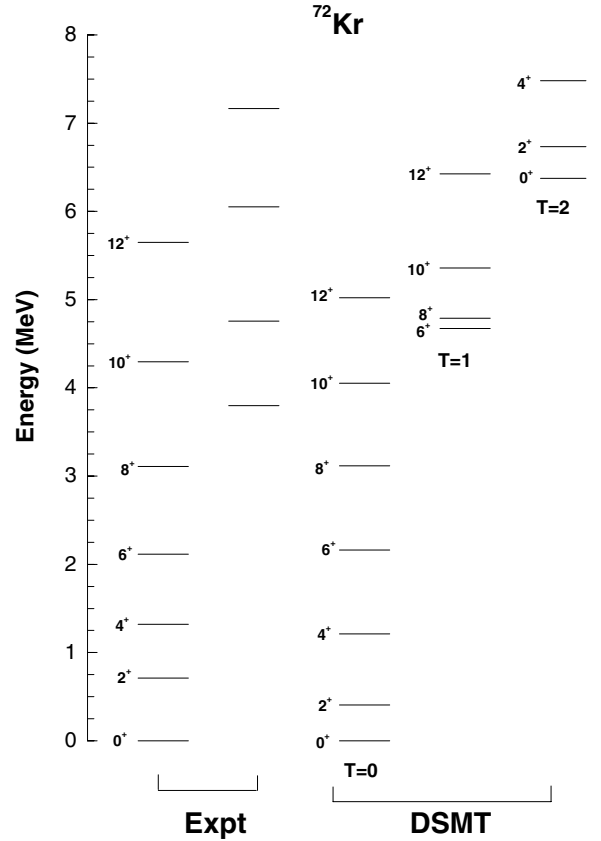
**Fig. 3.** Spectrum of single-particle states for the lowest-energy prolate HF intrinsic state for  $^{72}\text{Kr}$ . See fig. 1 and the text for other details; note that here both positive- and negative-parity levels are possible.

to those shown in fig. 1 for the DSMT calculations; fig. 5 of ref. [10] gives the shell model spectrum. The shell model  $B(E2)$ 's shown in table 1, being close to DSMT values, further confirm that the basis (*i.e.* the intrinsic states) chosen for the DSMT calculations is adequate.

In addition to the  $T = 0$  bands, DSMT gives low-lying  $T = 1$  bands with  $K = 6$  and  $K = 1$  and also a  $T = 2$  band with  $K = 0$ . The observed [21]  $T = 1$  levels with  $2^+$  and  $4^+$  could be the members of the  $K = 1$  band and the  $6^+$  may be the member of the  $K = 6$  band. The position of the first  $0^+$  level with  $T = 2$  is close to the DSMT value. Thus, DSMT gives a reasonably good account of not only the  $T = 0$  bands/levels but also of the observed  $T = 1, 2$  levels. Table 1 gives  $B(E2)$ 's predicted by DSMT for some of the  $T = 1$  levels. Further experiments on  $T = 1, 2$  bands in  $^{52}\text{Fe}$  will provide additional tests of DSMT.

## 4 Results for $^{72}\text{Kr}$

Fischer *et al.* [4] recently generated data for the yrast and near-yrast bands (for spins up to  $26^+$ ) in  $^{72}\text{Kr}$ . Besides the ground  $K = 0^+$  band, there is a side band starting from 3799 keV but the spins of this band are not established. However, the 3799 keV level is found to decay to the yrast  $6^+$  level and the next 4758 keV level to the yrast  $8^+$  level. Similarly, there is a band starting from 8747 keV with  $16^+$  decaying to the yrast  $14^+$  level. There is also another



**Fig. 4.**  $T = 0$ ,  $T = 1$  and  $T = 2$  bands in  $^{72}\text{Kr}$  obtained from the deformed shell model with isospin projection (DSMT) are compared with experimental data [4]. In ref. [23] a low-lying isomeric  $0^+$  state at 671 keV excitation, presumably the prolate band head (with the ground state  $0^+$  being essentially oblate), was reported and this level is not included in the figure. See the text for further details.

$16^+$  level in the same place. Unfortunately no  $T = 1$  or  $T = 2$  levels are identified by the experiments. We will see ahead that the band starting from 3799 keV could be a  $T = 1$  band. Before proceeding further, let us add that the PSM calculations for the ground  $K = 0^+$  band reported in [12] also include two- and four-quasiparticle configurations similar to the present calculations but no isospin projection is carried out unlike in the present work.

For  $^{72}\text{Kr}$  the interaction used is a modified Kuo's interaction in the  $2p_{3/2}$ ,  $1f_{5/2}$ ,  $2p_{1/2}$  and  $1g_{9/2}$  space with single-particle energies (in MeV) 0.0, 0.78, 1.08 and 4.25, respectively, as in the earlier DSM studies of  $^{74,76,78}\text{Kr}$  [22]. The HF sp spectrum for the lowest prolate configuration is shown in fig. 3. The oblate configurations which lie very low in energy (compared to prolate states) are neglected just as in the earlier studies of mass-80 nuclei [16,22]. As has been discussed above, one should include both the prolate and oblate intrinsic states in the band mixing calculation. But the effective interaction does not produce correct prolate-oblate separation. To test whether our assumption regarding the neglect of the oblate states is correct, we carried out a parallel calculation taking only the oblate intrinsic states. The energy

**Table 2.** DSMT model predictions for  $B(E2; K_i J_i T_i \rightarrow K_f J_f T_f)$  in  $e^2 \text{fm}^4$  for  $^{72}\text{Kr}$ .

$B(E2)$ 's for $^{72}\text{Kr}$		
$K_i J_i T_i$	$K_f J_f T_f$	DSMT
0 2 <sup>+</sup> 0	0 0 <sup>+</sup> 0	1190
0 4 <sup>+</sup> 0	0 2 <sup>+</sup> 0	1619
0 6 <sup>+</sup> 0	0 4 <sup>+</sup> 0	1833
0 8 <sup>+</sup> 0	0 6 <sup>+</sup> 0	2193
0 10 <sup>+</sup> 0	0 8 <sup>+</sup> 0	3086
6 8 <sup>+</sup> 1	6 6 <sup>+</sup> 1	2061
6 10 <sup>+</sup> 1	6 8 <sup>+</sup> 1	1713

spectra for  $J = 0^+, 2^+, 4^+, 6^+, 8^+$  and  $10^+$  taking only the oblate intrinsic states are 0.0, 0.766, 2.405, 4.709, 7.431 and 9.831 MeV, respectively. Comparing with fig. 4 ahead, we see that unlike the prolate states, the oblate intrinsic states fail to reproduce the observed energy spectrum. It is appropriate to add here that recently Bouchez *et al.* [23] reported a new excited  $0^+$  state at 671 keV above the ground  $0^+$  and interpreted this to be the band head for the yrast prolate band while the ground  $0^+$  is oblate. DSMT calculations with Kuo's interaction produce much larger spacing between the lowest prolate and oblate  $0^+$  states. Therefore the oblate  $0^+$  ground state is not considered in this paper and only the prolate states are described. It should be mentioned that the PSM calculations in [12] also use only prolate configurations.

Besides the lowest prolate configuration we have considered 20 excited prolate configurations and they are: i)  $(1/2_1^-)^{2p2n}(1/2_2^-)^{2p2n}(3/2^-)^{2p2n}(1/2^+)^{-\nu}(3/2^+)^{\nu}$  configurations giving  $K = 1, 2$  with  $\nu = p$  or  $n$  and they decompose into  $T = 0, 1$ ; ii) 2 protons and 2 neutrons in  $1/2^+$  and  $3/2^+$  orbits giving six  $K = 0$ , two  $K = 1$ , one  $K = 2$ , two  $K = 3$  and one  $K = 4$  configurations; iii) 2 protons and 2 neutrons in  $1/2^+$  and  $3/2_2^-$  orbits giving six  $K = 0$ , two  $K = 1$ , one  $K = 2$ , two  $K = 3$  and one  $K = 4$  configurations. In ii) and iii) the  $K = 2, 4$  states are pure  $T = 0$  and the  $K = 1, 3$  states can be decomposed into  $T = 0, 1$  states. Similarly, the six  $K = 0$  states decompose into two  $T = 0$ , three  $T = 1$  and one  $T = 2$  states as given by eq. (5). DSMT calculations are performed using these 28 configurations and the results are compared with data in fig. 4. Except for the position of the  $2^+$  level, the ground  $K = 0^+, T = 0$  band is reasonably well described up to  $12^+$ . All the levels of this band come mainly from the lowest prolate intrinsic state. However, the mixing with other configurations increases with spin. The DSMT gives a quasi- $\gamma$   $K = 2^+, T = 0$  band starting from 2.075 MeV and it is not shown in the figure (the energies of  $3^+, 4^+, 5^+, 6^+, 7^+$  and  $8^+$  members of this band are (in MeV) 2.380, 2.905, 3.249, 4.225, 4.326 and 5.151, respectively). Experimentally there is a band of states starting from 3.799 MeV and the decay of its lowest member to the yrast  $6^+$  indicates that it could be a  $6^+$  or  $8^+$  (assuming  $E2$  decay). This is consistent with the observation that the next member of the band is found to decay to the yrast  $8^+$  level. DSMT gives a band-like structure with  $6^+, 8^+, 10^+, 12^+$  etc. with  $T = 1$  starting

from 4.672 MeV excitation (the  $6^+$  and  $8^+$  are very close) and below this band there is no  $T = 0$  band with  $6^+$  or  $8^+$  as band head. Thus, comparing with the data it is plausible that the observed side band is the DSMT predicted  $T = 1$  band. In addition to the  $T = 1$  band, the model gives a  $0^+, T = 2$  band starting from 6.374 MeV. So far no  $T = 2$  levels are identified in  $^{72}\text{Kr}$  and a search for them is clearly called for. Finally, the DSMT predicted  $B(E2)$ 's are given in table 2 (the effective charges used are  $e_p = 1.6$  and  $e_n = 1.0$  as in [16, 22]) and no data are available yet for comparison. However, they compare well with the results (see table 2 in the first reference of [11]) from the much more complicated "excited-Vampir variational approach".

## 5 Conclusions

In this paper is given the method for four-particle isospin projection in DSMT and its first applications to the analysis of data for  $^{52}\text{Fe}$  and  $^{72}\text{Kr}$  with predictions for  $T = 1, 2$  states/bands in these nuclei. The DSMT model with the mixing of small number of bands (therefore the basis space is very small compared to the full shell model) is able to capture the essential structure of the observed levels in these two nuclei and therefore, combined with the results in [17, 18], proves to be a useful tool in nuclear-structure studies of  $N = Z$  nuclei. Future studies should include: i) expansion of the single-particle space for  $A > 70$  nuclei so that high-spin states in these nuclei can be studied; ii) good effective interactions in  $(f_{5/2} p g_{9/2})$  space should be generated (the interaction, due to the Madrid-Strasbourg group, used in [17] gives close-to-spherical configurations for  $A > 66$  nuclei and the modified Kuo's interaction used for  $^{72}\text{Kr}$  gives very low-lying oblate configurations); iii) six-particle (in six states) isospin projection results are needed for odd-odd  $N = Z$  nuclei with  $A > 70$  and this problem is being solved. We are addressing i) and iii) and see [24] for a recent attempt towards ii).

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