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## Applicability of the Extended P + QQ Model in the Upper Part of the $f_{7/2}$ Shell

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The  $P_0 + P_2 + QQ$  force has been completely revised, and in its new form, it is capable of describing nuclear structure of  $N \approx Z$  nuclei well. This paper investigates the applicability of the extended P + QQ model in the upper part of the  $f_{7/2}$  shell using shell model calculations. It is shown that the extended P + QQ model can account for the collective bands of most  $52 \leq A \leq 56$  nuclei as well as the lower part of the  $f_{7/2}$  shell. However, considerable discrepancy with experiment exists for  ${}^{52}$ Fe, which suggests the limit of the applicability of this force.

## §1. Introduction

In previous papers, <sup>1), 2)</sup> we demonstrated the usefulness of an extended P + QQ (EPQQ) model in the lower part of the  $f_{7/2}$  shell. The  $P_0 + P_2 + QQ$  force has been completely revised by adding two types of interactions: (1) a strong average monopole field with T = 0 and additional monopole terms with T = 0 and T = 1 depending on orbits, and (2) T = 1 proton-neutron (*p*-*n*) pairing interactions with J = 0 and J = 2. The former interactions play essential roles in reproducing the binding energy and energy levels, which supports the claims of Zuker et al. <sup>3)-9</sup> The latter interactions contribute considerably to the moment of inertia of the ground-state band. <sup>1), 10)</sup> The exact shell model calculations within the model space  $(f_{7/2}, p_{3/2}, p_{1/2})^{1), 2}$  have shown that the EPQQ interaction describes eveneven and odd nuclei quite well (especially for  $N \approx Z$  nuclei) and odd-odd nuclei well in the A = 46 - 51 region.

The purpose of this paper is to investigate the applicability of the extended P + QQ model in the upper part of the  $f_{7/2}$  shell. For A = 52 - 56 nuclei, we have carried out the same shell model calculation in the model space  $(f_{7/2}, p_{3/2}, p_{1/2})$  as in Refs. 1) and 2). These calculations confirm that most of these nuclei are described well by the EPQQ interaction. The EPQQ model, however, fails in explaining the observed yrast band connected by large B(E2) in <sup>52</sup>Fe. This result is different from those obtained with the so-called realistic effective interactions FPD6, <sup>11</sup>) KB3<sup>10), 12</sup> and KB3G, <sup>13)</sup> and the new effective interaction GXPF1 (or GXPF2) derived by Honma et al. <sup>14)</sup> The EPQQ interaction describes the collective yrast

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bands of other even-even nuclei approximately as well as the realistic effective interactions.<sup>7), 12), 13), 15) - 17) The exceptional disagreement with experiment and the difference between the results obtained with the two types of interactions for <sup>52</sup>Fe are curious. We discuss the main cause of this significant difference in the theoretical results for <sup>52</sup>Fe.</sup>

## §2. The model

The EPQQ interaction in isospin-invariant form is written

$$H = H_{\rm sp} + V(P_0) + V(P_2) + V(QQ) + V^0 + \Delta V^{T=0} + \Delta V^{T=1}, \ (2.1)$$

$$H_{\rm sp} = \sum_{a} \varepsilon_a (\hat{n}_{a\pi} + \hat{n}_{a\nu}), \qquad (2.2)$$

$$V(P_J) = -\frac{1}{2} g_J \sum_{MK} \sum_{a \le b} \sum_{c \le d} p_J(ab) p_J(cd) A^{\dagger}_{JM1K}(ab) A_{JM1K}(cd), \qquad (2.3)$$

$$V(QQ) = -\frac{1}{2}\chi' \sum_{M} \sum_{ac\rho} \sum_{bd\rho'} q'(ac)q'(bd) : B^{\dagger}_{2M\rho}(ac)B_{2M\rho'}(bd) :, \qquad (2.4)$$

$$V^{0} = -k^{0} \sum_{a \le b} \sum_{JM} A^{\dagger}_{JM00}(ab) A_{JM00}(ab), \qquad (2.5)$$

$$\Delta V^T = -\sum_{a \le b} \Delta k^T(ab) \sum_{JM} \sum_K A^{\dagger}_{JMTK}(ab) A_{JMTK}(ab), \qquad (2.6)$$

where  $A^{\dagger}_{JMTK}(ab) = [c^{\dagger}_{a}c^{\dagger}_{b}]_{JMTK}/\sqrt{1+\delta_{ab}}$ ,  $B^{\dagger}_{JM\rho}(ac) = [c^{\dagger}_{a\rho}c_{c\rho}]_{JM}$  ( $\rho = \pm 1/2$ ),  $p_{0}(ab) = \sqrt{2j_{a}+1}\delta_{ab}$  and  $p_{2}(ac) = q'(ac) = (a \parallel r^{2}Y_{2}/b_{0}^{2} \parallel c)/\sqrt{5}$ , with  $b_{0}$  the harmonic-oscillator range parameter.

We adopt the same model space  $(f_{7/2}, p_{3/2}, p_{1/2})$  as in Ref. 2). The usefulness of this model space is discussed in Ref. 1) (also see Refs. 5) and 7)). We use the Kuo-Brown single-particle energies, <sup>18)</sup>

$$\varepsilon_{7/2} = 0.0, \quad \varepsilon_{3/2} = 2.1, \quad \varepsilon_{1/2} = 3.9 \quad \text{in MeV.}$$
 (2.7)

It is shown in Ref. 2) that the binding energy and excitation energies are affected little in the EPQQ model by altering the force strengths, even if the single-particle energies are set equal to the observed excitation energies of  $3/2^-$  and  $1/2^-$  in <sup>41</sup>Ca, which are used in the KB3 and KB3G calculations.<sup>13), 15), 16)</sup>

Previous calculations<sup>2)</sup> showed that the EPQQ interaction with the additional monopole terms  $\Delta V^T$  is better than that without  $\Delta V^T$ . We call the two sets of force parameters D and B, following Ref. 2). When improving the EPQQ interaction from B to D, we determined the force strengths so that the number of parameters is minimal. The present calculations show that the parameter set D is good also for A = 52 - 56, but that it can be improved for <sup>56</sup>Ni, as seen in §3. We therefore add the monopole parameters  $\Delta k^0(rr)$  and  $\Delta k^1(rr)$ , where  $r = p_{3/2}$  or  $p_{1/2}$ . This necessitates minor changes in  $k^0$  and  $\Delta k^1(fr)$   $(f = f_{7/2})$ . We keep the other parameters unchanged for simplicity. The new set of force parameters, which we call the set E, is as follows:

Set E :
$$g_0 = 0.48(42/A), \quad g_2 = 0.36(42/A)^{5/3},$$
  
 $\chi' = 0.31(42/A)^{5/3}, \quad k^0 = 2.13(42/A),$   
 $\Delta k^1(ff) = -0.14, \quad \Delta k^0(ff) = 0.18,$   
 $\Delta k^1(fr) = 0.07, \quad \Delta k^0(fr) = -0.07,$   
 $\Delta k^1(rr) = -0.50, \quad \Delta k^0(rr) = 0.25 \text{ in MeV.}$  (2.8)

We have carried out shell model calculations using four sets of force parameters, B, D, E and a trial set "F", specified below. We used the harmonic-oscillator range parameter  $b_0 = 1.01A^{1/6}$  and the effective charges  $e_p = 1.5e$  and  $e_n = 0.5e$  when calculating electromagnetic quantities.

# §3. Applicability in the upper part of the $f_{7/2}$ shell

Let us first consider Fig. 1, in which the level structures of <sup>56</sup>Ni found theoretically and experimentally are compared. (The experimental data considered in this paper are taken from Refs. 19) and 20).) The addition of the monopole corrections  $\Delta V^T$  from B to D causes the calculated energy levels to become much closer to the observed ones (see Ref. 2)) for discussion of this point. The correction terms  $\Delta k^T(rr)$  added to the parameter set E improve the level structure, especially for the  $6_1^+$  and  $8_1^+$  states of the yrast band. The agreement between theory and experiment is quite good, considering the simplicity of the model. The three bands obtained by the calculation correspond to the experimentally observed bands, though the calculated energies of the excited bands depend probably on the model space. It should be noted that the realistic effective interaction KB3 does not satisfactorily describe the yrast band of <sup>56</sup>Ni.<sup>13</sup>) Figure 1 indicates that the EPQQ model is applicable up to the end of the  $f_{7/2}$  shell.

The modification from the parameter set D to E also improves the predictions for the energy levels of <sup>48</sup>Ca. We see in Fig. 2 that using set E, the order of the calculated energy levels is corrected for the lowest six excited states. Although we do not give the results for other nuclei, the modified parameter set E gives predictions for the binding energy, excitation energies and B(E2) for the A = 46 - 51 nuclei that are approximately as good as those found in Refs. 1) and 2). Note that for the parameter set E, we do not manipulate individual interaction matrix elements apart from the monopole corrections  $\Delta V^T$ , which have been extensively discussed by Zuker et al. <sup>3)-9</sup>

As shown in Refs. 1) and 2), the EPQQ model works well for even-even and odd-A nuclei and succeeds in describing the collective excitations in odd-odd nuclei. However, the QQ force, which plays a leading role in nuclear collective motion, seems to give interaction matrix elements that are too simple if we compare them with those of the realistic effective interactions. The matrix elements  $\langle (f_{7/2})^2 JT | V(QQ) | (f_{7/2})^2 JT \rangle$ , to which the  $f_{7/2}$  shell nuclei are sensitive, depend only on the Racah coefficient, apart from the force strength  $\chi'$ . For instance, the





Fig. 1. Level structure of  $^{56}$ Ni. The results calculated using the EPQQ model with the parameter sets B, D and E are compared with the experimentally observed energy levels.

Fig. 2. Energy levels of <sup>48</sup>Ca calculated using the EPQQ model with the parameter sets B, D and E compared with the experimentally observed energy levels.

EPQQ interaction gives the same value for J = 4, T = 1 and J = 6, T = 1. This flaw appears in the low-lying states of odd-odd nuclei that have the structure of the last *p*-*n* pair coupled to a collective even-even system, because their energies are directly affected by individual *p*-*n* interaction matrix elements. A typical example is <sup>54</sup>Co, in which the low-lying states of the main configuration  $(f_{7/2})^{-2}$  are not sufficiently collective. The energy levels of <sup>54</sup>Co calculated with the parameter sets D and E are compared with the experimentally observed energy levels<sup>21</sup> in Fig. 3. The present model does not reproduce the order of the experimentally observed energy levels, but there is one-to-one correspondence between the calculated and observed levels, and the disagreement in energy does not exceed 0.9 MeV.

To improve the agreement between the theoretical predictions and the experimental results, and to prepare for the investigation given in the next section, let us add correction terms to  $\langle (f_{7/2})^2 JT | V | (f_{7/2})^2 JT \rangle$ , which we denote by  $\Delta V(ffJT)$ . We have tried to determine the corrections  $\Delta V(ffJT)$  so that the predictions for the energy level structure and binding energy are improved in the most sensitive nucleus, <sup>54</sup>Co. It is, however, known that arbitrary changes in these matrix elements cause a large disturbance in the binding energies and level structures of other nuclei. We therefore determine the values of  $\Delta V(ffJT)$  so as to obtain overall agreement with experiment in the  $f_{7/2}$  shell nuclei. The values are

$$\begin{aligned} \Delta V(ff, J = 4, T = 1) &= -0.12, \quad \Delta V(ff, J = 6, T = 1) = 0.09, \\ \Delta V(ff, J, T = 0) &= 0.15 \quad \text{for } J = 1, 3, 5, \\ \Delta V(ff, J = 7, T = 0) &= -0.21 \quad \text{in MeV.} \end{aligned}$$
(3.1)

We call this modified parameter set "F". The results for <sup>54</sup>Co are shown in the column labeled "F" in Fig. 3. It is found that with this parameter set, the order of  $7_1^+$  and  $1_1^+$  and the energies of the T = 1 states  $4_1^+$  and  $6_1^+$  are improved. In Fig. 3, the T = 1 states are reproduced better than the T = 0 states, which suggests that the T = 1 states analogous to those of <sup>54</sup>Fe are collective. The task of improving the T = 0 interaction matrix elements is left for the EPQQ interaction, which involves the non-collective features of odd-odd nuclei.

Still, it is confirmed that the EPQQ model describes even-even nuclei well, especially the yrast-state band connected by large B(E2). The calculated



Fig. 3. Energy levels of <sup>54</sup>Co calculated using the EPQQ model with the parameter sets D, E and F compared with the experimentally observed energy levels.

results for  ${}^{52}Cr$  and  ${}^{54}Fe$  are shown in Fig. 4. The agreement with experiment for  ${}^{52}Cr$  is excellent and is comparable to that obtained using the realistic effective interactions KB3 and KB3G in Ref. 13). The EPQQ interaction predicts the energy



Fig. 4. Energy levels of (a) <sup>52</sup>Cr and (b) <sup>54</sup>Fe calculated using the EPQQ model with the parameter sets D, E and F compared with the experimentally observed energy levels.



Fig. 5. Energy levels of (a) <sup>53</sup>Mn and (b) <sup>53</sup>Fe calculated using the EPQQ model with the parameter sets D, E and F compared with the experimentally observed energy levels.

levels of the single-closed shell nucleus  ${}^{54}$ Fe well. It reproduces the yrast states of  ${}^{52}$ Cr,  ${}^{54}$ Fe and  ${}^{56}$ Ni better than the FPD6 interaction (as is seen by comparing our results with those reported in Ref. 22)).



Fig. 6. Energy levels of <sup>52</sup>Mn calculated using the EPQQ model with the parameter sets D, E and F compared with the experimentally observed energy levels.

The EPQQ model also describes odd-A nuclei well. The calculated energy levels for <sup>53</sup>Mn and <sup>53</sup>Fe are compared with the experimentally observed ones in Fig. 5. The agreement between theory and experiment is satisfactorily good. The collective band for the ground state  $7/2^{-}$  is reproduced, except that the order of  $13/2^-$  and  $15/2^$ in  ${}^{53}$ Mn and that of  $13/2^-$  and  $19/2^$ in <sup>53</sup>Fe are reversed. Energies of states outside the collective bands are also reproduced well, except for a few states, such as the  $5/2^{-}_{1}$  state of <sup>53</sup>Fe. As shown in Fig. 6, the EPQQ model can explain the observed energy levels of the oddodd nucleus <sup>52</sup>Mn, except the fact that the  $2^+_1$  state has the lowest energy.

Does the EPQQ model describe the wavefunctions of the  $A \approx 52$  nuclei well?

We attempted to answer this question by calculating electromagnetic quantities. Tables I and II list the quadrupole moment Q, magnetic moment  $\mu$ , B(E2) and B(M1)for <sup>51</sup>Mn, <sup>52</sup>Cr, <sup>52</sup>Mn and <sup>53</sup>Fe. The results of the EPQQ model obtained with the parameter sets E and F are compared with the experimentally observed values and

| $^{51}{ m Mn}$                |                              |                   |          |   |         |   |       |
|-------------------------------|------------------------------|-------------------|----------|---|---------|---|-------|
|                               | exp                          |                   | EPQQ(E)  |   | EPQQ(F) |   | KB3G  |
| $Q(5/2^{-}) { m efm}^2$       | $42 \pm 7$                   |                   | 35       |   | 35      |   | 35    |
| $B(E2) \ e^2 fm^4$            |                              |                   |          |   |         |   |       |
| $7/2^- \rightarrow 5/2^-$     | $528 \pm 146$                |                   | 312      |   | 316     |   | 305   |
| $9/2^- \rightarrow 5/2^-$     | $169 {\pm} 67$               |                   | 89       |   | 88      |   | 84    |
| $\rightarrow 7/2^{-}$         | $303 \pm 112$                |                   | 246      |   | 245     |   | 204   |
| $11/2^- \rightarrow 7/2^-$    | $236 {\pm} 67$               |                   | 149      |   | 150     |   | 154   |
| $\rightarrow 9/2^{-}$         | $4.2 \pm 1.4$                |                   | 198      |   | 200     |   | 190   |
| $17/2^- \rightarrow 13/2^-$   | $1.2 {\pm} 0.3$              |                   | 0.99     |   | 0.98    |   | 2.215 |
| $3/2^- \rightarrow 7/2^-$     | <1.6                         |                   | 2.4      |   | 1.5     |   |       |
| $1/2^- \rightarrow 5/2^-$     | $52 \pm 17$                  |                   | 37       |   | 36      |   |       |
| $\mu(5/2^{-}) \ \mu_N$        | $3.5683 {\pm} 0.0013$        |                   | 3.6      |   | 3.6     |   | 3.40  |
| $B(M1) \ \mu_N^2$             |                              |                   |          |   |         |   |       |
| $7/2^- \rightarrow 5/2^-$     | $0.207 \pm 0.034$            |                   | 0.09     |   | 0.10    |   | 0.177 |
| $9/2^- \rightarrow 7/2^-$     | $0.16 {\pm} 0.05$            |                   | 0.05     |   | 0.07    |   | 0.144 |
| $11/2^- \rightarrow 9/2^-$    | $0.66 {\pm} 0.21$            | $0.66 {\pm} 0.21$ |          |   | 0.43    |   | 0.423 |
| $17/2^- \to 15/2^-$           | $1.2 \pm 0.4 \times 10^{-4}$ |                   | 0.02     |   | 0.00003 |   |       |
| $19/2^- \to 17/2^-$           | > 0.57                       |                   | 1.2      |   | 1.2     |   | 0.801 |
| $3/2^- \rightarrow 5/2^-$     | < 0.0091                     |                   | 0.012    |   | 0.016   |   |       |
|                               |                              | 527               | n        |   |         |   |       |
|                               | r                            | . (               | Jr       | _ |         |   |       |
|                               | exp                          | Ŀ                 | EPQQ (E) | Ŀ | PQQ(F)  | ŀ | KB3G  |
| $Q(2^+) \text{ efm}^2$        | $-8.2\pm1.6^{23}$            |                   | -19.0    |   | -19.3   |   | -9.4  |
| - ( - ) 2- 4                  | $-14\pm8^{24}$               |                   |          |   |         |   |       |
| $B(E2) e^2 fm^4$              |                              |                   |          |   |         |   |       |
| $2^+ \rightarrow 0^+$         | $131 \pm 6$                  |                   | 162      |   | 165     |   | 132   |
| $4^+ \rightarrow 2^+$         | $761 \pm 265$                |                   | 162      |   | 155     |   | 107   |
| $6^+ \rightarrow 4^+$         | $59 \pm 2.1$                 |                   | 92       |   | 77      |   | 68    |
| $8^+ \rightarrow 6^+$         | $75\pm 24$                   |                   | 84       |   | 89      |   | 84    |
| $9^+ \rightarrow 8^+$         | $0.5^{+1.6}_{-0.5}$          |                   | 0.2      |   | 0.3     |   | 0.2   |
| $4^+_2 \rightarrow 2^+_2$     | $69{\pm}18$                  |                   | 0.2      |   | 9.1     |   |       |
| $2^+_2 \rightarrow 0^+$       | $0.06 \pm 0.05$              |                   | 9.8      |   | 1.1     |   |       |
| $2^+_2 \rightarrow 2^+_2$     | $150 \pm 35$                 |                   | 0.3      |   | 9.4     |   |       |
| $6^+ \rightarrow 4^+_2$       | $29.7 \pm 1.0$               |                   | 11       |   | 27      |   |       |
| $3^{+} \rightarrow 4^{+}_{2}$ | $7^{-5}_{-5}$                |                   | 2.3      |   | 3.3     |   |       |
| $6_2^+ \rightarrow 5^+$       | 69±58                        |                   | 18       |   | 24      |   |       |
| $7' \rightarrow 6'_2$         | $3500\pm3500$                |                   | 202      |   | 240     |   |       |
| $8_2 \rightarrow 7^+$         | $35_{-35}^{+104}$            |                   | 11       |   | 4.5     |   | 0.50  |
| $\mu(2^{+}) \mu_N$            | $3.0 \pm 0.5$                |                   | 2.84     |   | 2.77    |   | 2.50  |
| $B(M1) \mu^2$                 |                              |                   |          |   |         |   |       |
| $D(M1) \mu_N$                 | 0.05710.000                  |                   | 0.000    |   | 0.002   |   | 0.040 |

Table I. Electromagnetic properties of  ${}^{51}$ Mn and  ${}^{52}$ Cr. The results for the EPQQ interaction are listed for the parameter sets E and F.

| <sup>52</sup> Mn              |                              |                      |                    |         |       |        |       |
|-------------------------------|------------------------------|----------------------|--------------------|---------|-------|--------|-------|
|                               |                              | exp                  | EP                 | QQ(E)   | EP    | QQ(F)  | KB3G  |
| $Q(2^+) \text{ efm}^2$        | Î                            | $50\pm7$             |                    | 50      |       | 51     | 50    |
| $B(E2) e^2 fm^4$              |                              |                      |                    |         |       |        |       |
| $7^+ \rightarrow 6^+$         | ę                            | $92^{+484}_{-81}$    |                    | 126     |       | 131    | 126   |
| $8^+ \rightarrow 6^+$         |                              | >1.2                 |                    | 37      |       | 35     | 35    |
| $8^+ \rightarrow 7^+$         |                              | >4.2                 | 160                |         | 166   |        | 126   |
| $9^+ \rightarrow 7^+$         | 1                            | $04^{+300}_{-46}$    |                    | 63      |       | 63     | 66    |
| $11^+ \rightarrow 9^+$        | H)                           | $54 \pm 6.9$         | 37                 |         | 38    |        | 53    |
| $4^+ \rightarrow 2^+$         | $2248 \pm 876$               |                      | 136                |         | 137   |        |       |
| $4^+ \rightarrow 6^+$         | $692 \pm 277$                |                      |                    | 23      |       | 21     |       |
| $\mu(6^+) \ \mu_N$            | 3.06                         | $53 \pm 0.001$       |                    | 3.07    |       | 2.98   | 2.95  |
| $\mu(2^+)$ $\mu_N$            | $0.00768 {\pm} 0.00008$      |                      | 0.08               |         | 0.003 |        |       |
| $B(M1) \mu_N^2$               |                              |                      |                    |         |       |        |       |
| $7^+ \rightarrow 6^+$         | $0.50 {\pm} 0.25$            |                      |                    | 1.22    |       | 1.16   | 0.667 |
| $8^+ \rightarrow 7^+$         | >0.016                       |                      | 0.38               |         | 0.41  |        | 0.405 |
| $9^+ \rightarrow 8^+$         | $1.1^{+3}_{-0.5}$            |                      |                    | 1.62    |       | 1.46   | 0.757 |
| $^{53}$ Fe                    |                              |                      |                    |         |       |        |       |
|                               |                              | exp                  |                    | EPQQ    | (E)   | EPQQ   | (F)   |
| B(E2) e                       | $^{2}$ fm <sup>4</sup>       |                      |                    |         |       |        |       |
| $9/2^- \rightarrow 7/2^-$     |                              | $95 \pm 71$          |                    | 256     |       | 256    |       |
| $11/2^- \to 9/2^-$            |                              | $106 \pm 47$         |                    | 186     |       | 189    |       |
| $3/2^- \rightarrow 7/2^-$     |                              | $0.0399 {\pm} 0.001$ |                    | 0.03    |       | 0.09   |       |
| $5/2^- \rightarrow 1/2^-$     |                              | $367 \pm 95$         |                    | 11      |       | 19     |       |
| $5/2^- \rightarrow 3/2^-$     |                              | $130 \pm 35$         |                    | 0.05    |       | 0.2    |       |
| $7/2^2 \to 3/2^-$             |                              | $473^{+590}_{-470}$  |                    | 267     |       | 267    |       |
| $3/2^2 \to 7/2^-$             |                              | $66 \pm 14$          | $66{\pm}14$        |         | 72    |        |       |
| $\mu(3/2^{-}) \mu_{N}$        |                              | $-0.386\pm0.$        | $-0.386 \pm 0.015$ |         | -1.31 |        | 9     |
| B(M1)                         | $\mu_N^2$                    |                      |                    |         |       |        |       |
| $9/2^- \to 7/2^- \qquad 0.93$ |                              | $0.98 \pm 0.4$       | 1                  | 0.7     |       | 0.8    |       |
| $11/2^- \rightarrow$          | $11/2^- \to 9/2^ 0.63 \pm 0$ |                      | .4 1.3             |         |       | 1.4    |       |
| $13/2^- \rightarrow$          | $11/2^{-}$                   | >0.50                | 1.2                |         |       | 1.3    |       |
| $5/2^- \rightarrow 3/2^-$     |                              | $0.030 {\pm} 0.011$  |                    | 0.00003 |       | 0.0002 |       |

Table II. Electromagnetic properties of  ${}^{52}$ Mn and  ${}^{53}$ Fe. The results for the EPQQ interaction are listed for the parameter sets E and F.

with those calculated using the KB3G.<sup>13)</sup> It is found that modification of the  $f_{7/2}$  interaction matrix elements from E to F changes the electromagnetic quantities only slightly, except for the non-yrast states  $2^+_2$  and  $4^+_2$  of  ${}^{52}$ Cr. The predictions of the EPQQ model exhibit some deviations from the experimental values, for instance, for B(E2) and B(M1) (and also the excitation energy) of the  $5/2^-_1$  state of  ${}^{53}$ Fe, which suggests a defect of the model space excluding the  $f_{5/2}$  orbit. Our interaction including the QQ force yields B(E2) values for collective states that are larger than those obtained using the KB3G interaction, and yields B(M1) values that are somewhat different from the experimental values. Our results, however, are similar to those found with the KB3G interaction, and are qualitatively consistent with the experimental quantities for the ground-state bands.

We do not consider nuclei with N > 28, because our truncated model space excluding  $f_{5/2}$  may be incapable of treating the case in which nucleons always occupy orbits above  $f_{7/2}$ . Although the nuclei  ${}^{52}$ Cr,  ${}^{52}$ Mn,  ${}^{53}$ Mn,  ${}^{53}$ Fe,  ${}^{54}$ Fe and  ${}^{56}$ Ni possess a main structure that consists of only a few holes in  $f_{7/2}$  or are quasi-single- or quasi-double-closed-shell nuclei, the satisfactory results given above indicate that the collectivity is sufficiently strong that the EPQQ model is applicable in the region around  ${}^{52}$ Fe, except for some states of odd-odd nuclei in which the *p*-*n* interactions appear directly.

The results of this section reveal that the EPQQ model is useful to investigate the structure of the upper  $f_{7/2}$  shell nuclei. With respect to the energy levels, the applicability of the EPQQ model decreases in the order even-even nuclei, odd-Anuclei and odd-odd nuclei. In particular, the EPQQ model describes the energy levels of even-even nuclei very well. The electromagnetic quantities obtained using the EPQQ model effectively account for at least the collective ground-state bands of the even-even, odd-A and odd-odd nuclei.

## §4. Discrepancy in ${}^{52}$ Fe

The above results lead us to expect the success of the EPQQ model in describing the even-even nucleus  ${}^{52}$ Fe as well. Figure 7 displays the  ${}^{52}$ Fe energy levels obtained using the EPQQ model. These are compared with the experimental results<sup>25</sup>) and with those obtained using the realistic effective interaction KB3.<sup>25)</sup> The columns labeled "D", "E" and "F" correspond to the sets of force parameters D, E and F. If we assign the states connected by large values of B(E2) to the collective groundstate band, which are denoted by the thick lines in the figure, the EPQQ interaction appears to reproduce the observed ground-state band. The EPQQ interaction, however, predicts that the  $6_1^+$ ,  $8_1^+$  and  $10_1^+$  states lie below the collective band. This has not been observed experimentally. This prediction is contradicted by the effective interaction GXPF1 (or GXPF2) recently proposed by Honma et al.<sup>14)</sup> The agreement of the predictions obtained with this new interaction with experiment indicates that the calculated yrast states  $(0_1^+, 2_1^+, \dots, 10_1^+)$  should correspond to the observed ground-state band connected by large B(E2). In contrast, for the EPQQ model calculations, the  $6_1^+$  level is much lower than the observed level, and  $B(E2:6_1^+ \rightarrow 4_1^+)$ is smaller than 12% of  $B(E2:6_2^+ \to 4_1^+)$ . The present EPQQ model encounters the strange problem that the yrast states with even-J in the even-even nucleus <sup>52</sup>Fe do not compose a collective band connected by large B(E2). Such a strange situation does not exist in even-even nuclei with usual interactions, nor does it exist in other even-even nuclei from A=44 to A=54 in the EPQQ model. It is curious that the energy levels of  ${}^{52}$ Fe are reproduced less accurately than those of  ${}^{52}$ Cr and  ${}^{54}$ Fe by the EPQQ interaction, since  ${}^{52}$ Fe probably has stronger collectivity than  ${}^{52}$ Cr and  $^{54}$ Fe. This unique behavior is probably related to the unique structure of  $^{52}$ Fe, whose main configuration has four holes of 2p-2n with T=0. A strange level scheme similar to Fig. 7 is found also in <sup>96</sup>Cd using a shell model calculation with the effective interaction given in Ref. 26), though we do not give the calculated result here.





Fig. 7. Energy levels of  ${}^{52}$ Fe calculated with the EPQQ model using the parameter sets D, E and F compared with the experimentally observed levels. The result of Ur et al.  ${}^{25)}$  obtained using the full fp shell model calculation with the KB3 interaction is also shown.

Fig. 8. Energy levels of  ${}^{52}$ Fe calculated with the EPQQ model in the space  $\Sigma_t(f_{7/2})^{12-t}(p_{3/2}, p_{1/2}, f_{5/2})^t$  compared with the experimentally observed levels.

One may question the applicability of the model space  $(f_{7/2}, p_{3/2}, p_{1/2})$ . We have also carried out calculations with the space  $\Sigma_t(f_{7/2})^{12-t}(p_{3/2}, p_{1/2}, f_{5/2})^t$ . Although we are forced to employ the restriction  $t \leq 5$  to keep the computation time from becoming too long, the convergence of the energies is sufficient for the results to be considered. We have readjusted the force parameters for  ${}^{48}$ Cr in the full fp shell calculation, using the Kuo-Brown single-particle energy also for the  $f_{5/2}$  orbit,  $\varepsilon_{5/2} =$ 6.5 MeV. Their values are  $g_0 = 0.45(42/A), \chi' = 0.285(42/A)^{5/3}, k^0 = 2.18(42/A),$  $\Delta k^{1}(ff) = -0.13, \ \Delta k^{0}(ff) = 0.21, \ \Delta k^{1}(rr) = -0.30 \text{ in MeV} (r \text{ includes } f_{5/2}).$ The other parameters are not changed from the parameter set E in Eq. (2.8). These parameters yield accurate predictions of the binding energy, excitation energies and backbending for <sup>48</sup>Cr and <sup>50</sup>Cr. They are expected to also work well for <sup>52</sup>Fe, given our experience with the  $(f_{7/2}, p_{3/2}, p_{1/2})$  calculations, from which we have found that force parameters reproducing  ${}^{48}$ Cr are good for all the  $f_{7/2}$  shell nuclei. The  ${}^{52}$ Fe energy levels obtained are compared with the experimental levels in Fig. 8, where  $2^{+}_{3}$ ,  $6_3^+$  and  $8_3^+$  were not calculated to shorten the computation time. This calculation including  $f_{5/2}$  gives results that differ little from the level structure given in Fig. 7, and the strange feature of B(E2) found in the  $(f_{7/2}, p_{3/2}, p_{1/2})$  calculations also remains. It is rather difficult to drastically change the level structure and B(E2)between the collective states predicted by the EPQQ model by varying the force strength parameters within a model space. This suggests an origin other than the effect of  $f_{5/2}$  for the discrepancy with experiment for <sup>52</sup>Fe.

There remains another possibility that the EPQQ interaction misses important correlations that strongly admix the  $6_1^+$ ,  $8_1^+$  and  $10_1^+$  states with others. We can see in the t = 0 column of Fig. 8 that the main configuration  $(f_{7/2})^{12}$  of <sup>52</sup>Fe produces a level structure that is far from rotational in the EPQQ model. The Q moments of the  $2_1^+$ ,  $4_1^+$ ,  $6_1^+$  and  $6_2^+$  states are, respectively, -12.7, -6.9, 19.4 and -2.4 efm<sup>2</sup> (which suggests that  $6_1^+$  has a different structure from  $2_1^+$  and  $4_1^+$ ). The correlations among orbits (configuration mixing) give the energy gain 4.5 MeV to the ground state and change the Q moments of the  $6_1^+$  and  $6_2^+$  states to 41.7 and -24.6 efm<sup>2</sup>. In contrast with this, the KB3G interaction produces a rotation-like band up to  $8^+_1$ already in the configuration  $(f_{7/2})^{12}$ , where the  $2_1^+$ ,  $4_1^+$  and  $6_1^+$  states have negative Q moments, -14.3, -13.7, -4.7 efm<sup>2</sup>, respectively. The correlations among orbits cause a larger energy gain of 6 MeV for the ground state and change the sign of the Q moment of  $6_1^+$  to 6.4 efm<sup>2</sup>. The FPD6 interaction yields a result similar to that for KB3G. Thus, the interaction matrix elements for  $f_{7/2}$  are significantly different for the EPQQ and Kuo-Brown-type interactions, and the correlations among orbits are weaker for the EPQQ interactions than for the KB3G and FPD6 interactions.

We showed in Ref. 1) that the main difference between the EPQQ and Kuo-Brown-type effective interactions is in the T = 0 interaction matrix elements. In the EPQQ interaction, the major part of the T = 0 interactions is represented by the average monopole field  $V^0$ , and residual T = 0 interactions come from the QQ force. The QQ force plays a decisive role in widening spaces between high-spin levels so as to look like a rotational band. This is consistent with the findings of Ref. 27), which investigates the effects of setting all the T = 0 interaction matrix elements equal to zero. The strength of the QQ force is very relevant to the spread of the T = 0 levels  $(1^+ - 7^+)$  of  ${}^{42}$ Sc, as well as the spread of the high-spin levels in the all  $f_{7/2}$  shell nuclei. We determined the QQ force strength so as to obtain overall agreement. We compare residual T = 0 interaction matrix elements  $\langle (f_{7/2})^2 JT | V V^0|(f_{7/2})^2 JT = 0$  for the EPQQ interaction and Kuo-Brown-type interactions in Table III. We can see in Table III that the EPQQ magnitudes are much smaller than the corresponding ones of the Kuo-Brown-type effective interactions. It should be noted that the reductions of the force strengths  $g_0$  and  $\chi'$  are less than 10% when the model space is extended from  $(f_{7/2}, p_{3/2}, p_{1/2})$  to the full fp.

To see the effects of the different interaction matrix elements, we have carried out trial calculations within the  $(f_{7/2}, p_{3/2}, p_{1/2})$  space, obtaining the following results. Even if we replace the residual T = 0 matrix elements  $\langle (f_{7/2})^2 JT | V - V^0 | (f_{7/2})^2 JT = 0 \rangle$  with the KB3 ones,  $B(E2:6_2^+ \to 4_1^+)$  is still larger than  $B(E2:6_1^+ \to 4_1^+)$ . Only

Table III. Residual T = 0 interaction matrix elements  $\langle (f_{7/2})^2 JT | V - V^0 | (f_{7/2})^2 JT = 0 \rangle$  for <sup>52</sup>Fe, where  $\langle V^0 \rangle = -1.761$  (in MeV). The EPQQ values are for the full fp space.

| J | Т | EPQQ   | KB     | FPD6   | KB3    |
|---|---|--------|--------|--------|--------|
| 1 | 0 | -0.100 | 1.236  | 1.596  | 0.586  |
| 3 | 0 | 0.192  | 1.553  | 1.297  | 0.903  |
| 5 | 0 | 0.411  | 1.259  | 0.790  | 0.909  |
| 7 | 0 | 0.031  | -0.438 | -0.535 | -0.788 |

when we substitute the KB3 values for  $\langle (f_{7/2})^2 JT | V - \delta_{T0} V^0 | (f_{7/2})^2 JT \rangle$  with both T = 0 and T = 1 can the yrast states  $6_1^+$  and  $8_1^+$  be assigned to the collective groundstate band connected by large B(E2). This replacement, however, suppresses the high-spin yrast levels and hence requires stronger correlations among orbits so as to restore the appropriate positions of the high-spin yrast levels by lowering the lowspin yrast states. The outline of how the KB3 interaction differs from the EPQQ interaction is explained in this way. This is consistent with the above discussion regarding the Q moment and the correlations among orbits.

The above considerations have shown that the considerable difference between the EPQQ interaction matrix elements and the Kuo-Brown-type interaction matrix elements causes a discrepancy in the collective ground-state band of <sup>52</sup>Fe. In our framework, however, it is not easy to change the QQ force strength, which is relevant to the excitation energies of high-spin states. One way to change the residual T = 0interactions may be to introduce a hexadecapole-hexadecapole force, if we do not alter the individual matrix elements. As we have found, changing the interaction matrix elements from the parameter set E to F does not improve the discrepancy between the predictions and the experimental results for <sup>52</sup>Fe. A more detailed search for the monopole corrections  $\Delta k^{T}(ab)$  remains.

### §5. Conclusion

We have shown the good applicability of the EPQQ model to  $A \ge 52$  nuclei up to <sup>56</sup>Ni excluding <sup>52</sup>Fe. Combining this with the results for the A = 46 - 51 nuclei in Refs. 1) and 2), we can conclude that the EPQQ model is useful to investigate the structure of the  $f_{7/2}$  shell nuclei. The agreement with the observed energy levels is approximately the same as that of the realistic effective interactions KB3 and KB3G for even-even nuclei, and the applicability of the EPQQ model slightly decreases for odd-A nuclei. The EPQQ model can describe the ground-state bands of oddodd nuclei qualitatively. The electromagnetic properties are predicted accurately at least for the collective ground-state bands in the  $f_{7/2}$  shell nuclei. It should be noted here that the effective interaction in the  $g_{9/2}$  shell nuclei resembles the EPQQ interaction, <sup>28)</sup> and the EPQQ model provides accurate predictions of the binding energy in a wide range of nuclei. <sup>29), 30)</sup>

For <sup>52</sup>Fe, however, the present EPQQ model cannot reproduce the basic features of the collective yrast band observed in experiment. This suggests a limit of the applicability of the EPQQ interaction in some exceptional cases. The problem here is probably related to the unique structure of <sup>52</sup>Fe, whose main configuration has four holes of 2p-2n with T = 0. We have discussed the origin of the discrepancy with the results of the Kuo-Brown-type effective interactions. The difference between the results for <sup>52</sup>Fe obtained with the two types of interactions can be attributed mainly to the interaction matrix elements in the  $f_{7/2}$  orbit, and especially the magnitudes of the residual T = 0 interaction matrix elements. The correlations causing configuration mixing also seem to be too weak for the EPQQ interaction.

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