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INFLUENCE OF PAIRING CORRELATIONS ON E1 TRANSITION PROBABILITIES IN ODD-MASS DEFORMED, RARE-EARTH NUCLEI

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Abstract: Theoretical calculations of E1 and E3 transition rates for deformed rare-earth nuclei are made, taking into account the retarding effect of pairing correlations. It is found that pairing correlation correction factors R improve the general agreement with experiment for one class of transition, viz. E1 with $\Delta K = \pm 1$. However, the factors R generally cause poorer agreement for E1 with $\Delta K = 0$ and for E3 than results from simple use of Nilsson single-particle wave functions with no pairing corrections. The importance of taking into account wave function components admixed by the Coriolis coupling is illustrated by a calculation fitting the many E1 transition rates between two bands in Hf^{177}. It is further suggested that effects due to three-quasi-particle components (or, in other language, octopole phonon or "effective charge" effects) are probably of great importance and deserve further study.

1. Introduction

The retardation of E1 transitions in deformed nuclei has been the subject of several papers [1–7]) in the past few years. The reduction factor F of a transition is defined as equal to the ratio of the theoretical to the experimental transition probabilities. The theoretical transition probability has been computed by using the spherical shell model (transition probability P_W, reduction factor F_W) and the Nilsson model (transition probability P_N, reduction factor F_N). The reduction factors F_N have been found to be much smaller than the reduction factors F_W, and it has therefore been concluded that the Nilsson model represents a large improvement over the spherical shell model when computing the transition probabilities in deformed nuclei. Nevertheless, the agreement between the Nilsson model predictions and the experimental results is still unsatisfactory, some F_N factors being of the order of several hundreds. It has often been concluded that a part at least of this disagreement is due to the fact that the Nilsson model does not take into account a retarding effect of the pairing correlations between the nucleons.

It can be shown [8]) that the theoretical probability for an electric transition between one quasi-particle states may be written as the product of the ordinary particle transi-

tion probability (for example P_N if the Nilsson model is used) by a reduction factor R. It is therefore possible to take into account the influence of the pairing correlations by defining a new reduction factor $F'_N = F_N R$.

The pairing reduction factor can be written as

$$R \approx (UU' \pm VV')^2,$$

the U^2 and V^2 are the respective probabilities to find the initial level empty or occupied by a pair of particles. The primed quantities correspond to the final level.

The terms UU' and VV' appear with opposite signs for electric transitions and the same sign for magnetic transitions. The two terms arise when there is a distribution of pairs in available orbitals because there are two classes of contributions to the electromagnetic transition matrix elements. From components of the initial wave function where the final state odd-particle orbital is unoccupied initially we get one class, and from components where it is occupied initially by a pair, we get the second class. One class is essentially an odd-particle transition, and the other class may be thought of as a hole transition or a particle transition in the opposite direction. Where initial and final odd-particle orbitals are on opposite sides of the Fermi surface by energies comparable to the energy gap 2Δ, the factor R approaches unity. In other cases, such as where both orbitals lie on the same side of the Fermi surface or (as is often encountered in the computations here) where they both lie close to the Fermi surface, R may become quite small and rather sensitive to the position of the orbitals with respect to the chemical potential.

The quantities U and V can be computed by choosing energies for the single particle Nilsson orbitals, a reasonable value for the pairing force, and solving the BCS equations. Several computations of this kind have been performed [9-11]) for the deformed nuclei but the values of U and V are not tabulated. When this work was undertaken, only one attempt had been made [8]) to compute the new reduction factor F'_N, and this work concerned only two transitions. For these two transitions the reduction factor F'_N, was close to one. This result was considered as promising and a general computation of the factor F'_N for the electric transitions in the odd-mass, rare-earth nuclei was undertaken.

2. Methods of Computation

A programme already written for the IBM 7090 in Berkeley was used to solve the BCS equations with a constant value of the pairing force. Reasonable values for this force were obtained from refs. [9-11]) on the inertial parameters and on the deformations of the rare earth nuclei.

The G values of 0.022 for the neutrons and 0.025 for the protons, in units of $\hbar\omega_0$, were used in the computations. For protons, as well as for neutrons, twenty-eight single-particle levels were used. The energies of these levels were obtained by successive approximations. It was estimated that a good criterion for the single-particle model

was to predict correctly the experimentally known spins and parities of the ground state levels. For a given value of the number of odd particles (Z or N) the theoretical ground state level corresponds to the minimum value of the quasi-particle energy, and this quantity was computed by the programme.

For protons we first took the Nilsson energies with some modifications; the levels belonging to the $N = 6$ shell shifted to $+\infty$ and the levels belonging to the $N = 3$ shell were shifted by -0.29, in units of $\hbar\mathring{\omega}_0$. Between $Z = 63$ and $Z = 71$, this model (model A) predicted correctly four ground state levels out of five. By shifting by $+0.19$ all the levels coming from the $h_{\frac{9}{2}}$ orbital, it was possible to reach a complete agreement (model B).

For neutrons we also tried the Nilsson energies, with slight modifications; the levels belonging to the $N = 7$ shell were shifted to $+\infty$ and the levels belonging to the $N = 4$ shell were shifted by -0.37. This model (model A) predicted correctly only two ground states out of ten between $N = 89$ and $N = 107$. A complete agreement was reached only after several successive approximations (model B). All the levels coming from the $g_{\frac{9}{2}}$ and $i_{\frac{11}{2}}$ orbitals were shifted by $+0.25$; the other modifications from model A to model B are listed in table 1.

TABLE 1

Energy shifts to Nilsson orbital energies for model B (in units of $\hbar\mathring{\omega}_0$)

Level	$\frac{11}{2}^-(505)$	$\frac{5}{2}^+(642)$	$\frac{3}{2}^-(521)$	$\frac{5}{2}^-(523)$	$\frac{1}{2}^-(521)$	$\frac{7}{2}^+(633)$
Shift	+0.079	+0.112	+0.06	+0.10	+0.088	+0.038

The values of the pairing reduction factor R were computed using model A and model B energy levels for all the electric transitions in the odd-mass, rare-earth nuclei.

The values of the Nilsson probability P_N had been previously computed [1]) by hand for the E1 transitions. In order to obtain more precise values and also to compute the probability P_N for E2 and E3 transitions, the formula [12]) giving P_N was programmed for the IBM 7090. Using this programme, values of P_N were calculated for all the electric transitions in the rare-earth nuclei. The results corresponding to E1 transitions were generally in fair agreement with the ones previously computed [7]).

3. Discussion

The values of the reduction factors F_W, F_N and F'_N for the E1 transitions are given in table 2. A value of unity would denote complete agreement with experiment. The experimental probabilities have been taken from table 1 of ref. [7]) and corrected when new data were available [13]). Two new transitions have been included: a transition of 217 keV in Hf^{179} (ref. [14])) and a transition of 30.7 keV in Ta^{179} (ref. [15])). The transitions have been separated into two classes [7]) according to the value of ΔK.

It is clear from table 2 that the mere inclusion of the pairing correlations does not solve the problem of the E1 transition rates. For the transitions with $\Delta K = 0$, the reduction factor F_N is already close to one, which means a relatively good agreement between the experimental and the Nilsson theoretical transition probabilities. This agreement tends to be destroyed as a result of the inclusion of the pairing force. On the other hand, for the transitions with $\Delta K = 1$, the reduction factor F_N is generally large, and the agreement with the experimental results is evidently improved for most of the transitions by the introduction of the pairing reduction factor.

TABLE 2

E1 transitions in rare-earth nuclei

Orbitals: Initial	Orbitals: Final	Final nucleus	E_γ (keV)	F_W	F_N	F'_N Model A	F'_N Model B	δ
$\Delta K = 0$ transitions								
$\frac{3}{2}^+(651)$,	$\frac{3}{2}^-(521)$	Gd^{155}	86	2.2×10^4	2.7	5.4×10^{-2}	$3.\times10^{-1}$	0.3
$\frac{5}{2}^-(523)$,	$\frac{5}{2}^+(642)$	Dy^{161}	25.6	$8.\times10^3$	1.0	4.8×10^{-2}	$8.\times10^{-4}$	0.3
$\frac{7}{2}^-(523)$,	$\frac{7}{2}^+(404)$	Tm^{169}	63	6.5×10^4	9.4×10^{-1}	6.7×10^{-2}	2.3×10^{-2}	0.28
$\frac{7}{2}^-(514)$,	$\frac{7}{2}^+(633)$	Yb^{173}	286	$7.\times10^4$	2.6	$1.\times10^{-2}$	8.2×10^{-2}	0.28
$\Delta K = 1$ transitions								
$\frac{3}{2}^+(411)$,	$\frac{5}{2}^-(532)$	Eu^{153}	75	$5.\times10^4$	5.6×10^{-1}	3.4×10^{-4}	2.8×10^{-3}	0.3
$\frac{5}{2}^+(642)$,	$\frac{3}{2}^-(521)$	Gd^{155}	106	$1.\times10^5$	4.3	5.2×10^{-1}	1.5	0.3
$\frac{3}{2}^+(411)$,	$\frac{5}{2}^-(532)$	Eu^{155}	141	7.5×10^4	2.1	1.3×10^{-3}	1.1×10^{-2}	0.3
$\frac{5}{2}^-(532)$,	$\frac{3}{2}^+(411)$	Tb^{159}	362	3.3×10^4	9.1×10^{-1}	1.6×10^{-1}	1.7×10^{-1}	0.3
$\frac{3}{2}^-(521)$,	$\frac{5}{2}^+(642)$	Dy^{161}	74.5	$4.\times10^4$	1.6×10^1	2.2	1.5	0.3
$\frac{7}{2}^+(633)$,	$\frac{5}{2}^-(512)$	Yb^{173}	351	$3.\times10^6$	$5.\times10^2$	7.5	5.6×10^1	0.28
$\frac{9}{2}^-(514)$,	$\frac{7}{2}^+(404)$	Lu^{175}	396	$2.\times10^6$	1.9×10^2	5.7×10^1	4.3×10^1	0.28
$\frac{9}{2}^+(624)$,	$\frac{7}{2}^-(514)$	Hf^{177}	320	$7.\times10^6$	1.3×10^3	1.7×10^2	2.2	0.27
$\frac{9}{2}^-(514)$,	$\frac{7}{2}^+(404)$	Lu^{177}	148	$3.\times10^6$	2.3×10^2	4.4×10^1	3.5×10^1	0.26
$\frac{9}{2}^+(624)$,	$\frac{7}{2}^-(514)$	Hf^{179}	217	$1.\times10^5$	1.4×10^1	3.5×10^{-1}	1.4	0.26
$\frac{9}{2}^-(514)$,	$\frac{7}{2}^+(404)$	Ta^{179}	30.7	$1.\times10^6$	7.4×10^1	1.2	1.8	0.26
$\frac{9}{2}^-(514)$,	$\frac{7}{2}^+(404)$	Ta^{181}	6.2	3.5×10^5	2.4×10^1	3.9×10^{-1}	$6.\times10^{-1}$	0.23

The E1 transition probabilities being very small, it is evident that the theoretical value predicted by the Nilsson model results from the near cancellation of several terms in the matrix elements. The probabilities P_N are, therefore, very sensitive to the details of the wave function.

The cancellation of terms in the matrix elements is much less pronounced for electric multipoles of order higher than one, the reduction factor F_W being already quite small for these multipoles. The E2 and E3 transitions should, therefore, permit a better trial of the pairing reduction factor than the E1 transitions. The number of experimentally known E2 transitions between intrinsic states is too small, and four well-known E3 transitions will be used to try to decide whether or not the inclusion

of the pairing force results in an improvement of the agreement between the experimental results and the theoretical predictions.

The values of the reduction factors F_W, F_N and F'_N for the E3 transitions are given in table 3. The experimental probabilities have been computed using the data of ref. [14]) and for the conversion coefficient of the 24 keV transition in Yb^{169}, using an extrapolated theoretical value.

It is clear from table 3 that the reduction factor F_N is already close to one, as it was for the E1 transitions with $\Delta K = 0$. This relatively good agreement tends to be destroyed as a result of the inclusion of the pairing force.

TABLE 3

E3 transitions in rare-earth nuclei

Orbitals: initial	final	Final nucleus	E_γ (keV)	F_W	F_N	F'_N model A	F'_N model B	δ
$\frac{1}{2}^+(411)$,	$\frac{7}{2}^-(523)$	Ho^{163}	305	1.4×10^2	6.3×10^{-1}	6.3×10^{-2}	6.3×10^{-2}	0.3
$\frac{1}{2}^-(521)$,	$\frac{7}{2}^+(633)$	Dy^{165}	108	$1.\ \times10^2$	2.1	5.9×10^{-2}	9.2×10^{-2}	0.3
$\frac{1}{2}^-(521)$,	$\frac{7}{2}^+(633)$	Er^{167}	208	$2.\ \times10^2$	4.7	1.3×10^{-1}	2.1×10^{-1}	0.29
$\frac{1}{2}^-(521)$,	$\frac{7}{2}^+(633)$	Yb^{169}	24	7.2×10^1	1.8	$5.\ \times10^{-2}$	$8.\ \times10^{-2}$	0.28

The accuracy and sensitivity of our pairing reduction factors to the hypotheses made in their calculation could evidently be questioned. However, since the completion of this work, we have received two preprints [16,17]) dealing with the computation of the pairing reduction factor and compared their results with ours. It can be concluded that, when the pairing reduction factor is not too small, the different methods of computation give results which are in reasonable agreement. When the reduction factor is very small, which corresponds to near cancellation of the two terms in R (25.6 keV transition in Dy^{161} and 320 keV transition in Hf^{177}) such is not the case, but it seems normal for the cancellation to be very sensitive to small differences in the methods of computation or in the single-particle levels used. The further refinement carried out by Monsonego and Piepenbring [17]) of projecting only the BCS component with correct particle number does not in itself seem to reduce materially the remaining discrepancies found by all of us.

From the preceding discussion, we can conclude that the simple inclusion of a pairing reduction factor R multiplying the Nilsson single-particle transition probability P_N does not yield a satisfactory rate theory for the E1 transitions in deformed nuclei.

The E1 transitions with $\Delta K = 0$ and the E3 transitions are in better agreement with the Nilsson model before introducing the extra retardation due to the pairing correlations.

The E1 transitions with $\Delta K = 1$ are improved in general agreement in comparison with the pure Nilsson model without pairing. However, the agreement is still far from good, and the hindrance of these transitions does not seem to be clearly correlated with the reductions produced by the pairing force.

There are two other considerations that merit attention. First, are there significant contributions to E1 transition probabilities from Coriolis-admixed components in the nuclear wave functions? Second, are there important effects due to admixed components of collective odd-parity excitations of the even nucleon structure?

TABLE 4

Ratios of relative E1 reduced transition probabilities compared with simple theory

Nucleus	Initial band $K_i\pi$	Final band $K_f\pi$	E_γ(keV) $\Delta I = \Delta K$	E_γ(keV) $\Delta I = \Delta K+1$	$\frac{B(\text{to } I_f = K_f+1)}{B(\text{to } I_f = K_f)}$ Theoretical $\frac{(K_i 1 K_i \Delta K \mid K_f+1 K_f)^2}{(K_i 1 K_i \Delta K \mid K_f K_f)^2}$	Experimental [a]) $\frac{\text{Int}(\Delta K+1)}{\text{Int}(\Delta K)} \times \left(\frac{E_{\Delta K}}{E_{\Delta K+1}}\right)^3$
Am^{239}	$\frac{5}{2}^+$	$\frac{5}{2}^-$	396	340		0.5
Am^{241}	$\frac{5}{2}^+$	$\frac{5}{2}^-$	206	164	$\frac{2}{5} = 0.40$	~0.5
Am^{243}	$\frac{5}{2}^-$	$\frac{5}{2}^-$	84	42		~0.4
Np^{239}	$\frac{5}{2}^+$	$\frac{5}{2}^+$	74.7	43.5		0.3
Np^{237}	$\frac{5}{2}^-$	$\frac{5}{2}^+$	59.62	26.38		1.1
Th^{231}	$\frac{5}{2}^-$	$\frac{5}{2}^+$	185	143		0.47
Cm^{245}	$\frac{9}{2}^-$	$\frac{7}{2}^+$	394	340	$\frac{5}{22} = 0.23$	0.32, 0.42
Hf^{177}	$\frac{9}{2}^-$	$\frac{7}{2}^+$	321.36	208.36		175
Lu^{175}	$\frac{9}{2}^-$	$\frac{7}{2}^+$	396	283		1.4
Yb^{173}	$\frac{7}{2}^+$	$\frac{5}{2}^-$	351.2	272.4	$\frac{8}{27} = 0.30$	79
Gd^{155}	$\frac{5}{2}^+$	$\frac{3}{2}^-$	105.3	45.3		0.45
Tb^{159}	$\frac{5}{2}^-$	$\frac{3}{2}^+$	364	300	$\frac{3}{7} = 0.43$	~0.02

[a]) Data mainly selected from ref. [23]).

With regard to the first question we may look to nuclei for which two or more E1 transition intensities between the same pair of rotational bands are known. According to basic geometrical considerations [18]) the statistical factor η multiplying the transition rates should be simply the square of a Clebsch-Gordan coefficient $(I_i 1 K_i K_f - K_i | I_f K_f)^2$, provided the K values (projection of I on the nuclear symmetry axis) are good quantum numbers. An examination of table 4 shows generally poor agreement with the rule. For the most striking disagreement we are fortunate in having a large number of B(E1) values between the bands, thanks mainly to the detailed decay scheme study on Lu^{177m} by Alexander, Boehm and Kankeleit [19]). Deviations from the branching rule can only mean that there are contributions from wave function components differing in K quantum number from the principal component. A Coriolis coupling term (U_1 of Bohr [20])), the rotation-particle coupling "RPC" of Kerman [21]) in the Hamiltonian for an odd-mass deformed nucleus is the best understood mechanism for admixing K values. The admixture into the base state of a component with K one less than the principal K value is especially large for Nilsson bands

with high j values. We shall show that the simple assumption of RPC admixture of a $K = \frac{7}{2}^+$ component into the predominant $K_i = \frac{9}{2}^+$ band of Hf^{177} affords a semi-quantitative explanation of nine E1 transition probabilities in table 8 of ref. [19]). Only two adjustable parameters will be used, first the E1 matrix element μ_9 for the dominant $K_i = \frac{9}{2}^+$ component and the product $\mathscr{P}_7$ of the RPC matrix element and the E1 matrix element from the $K_i = \frac{7}{2}^+$ component. It is not difficult to derive that the E1 reduced transition probabilities from the admixed band should be proportional to

$$B \propto |\mu_9(I_i 1 \tfrac{9}{2} - 1 | I_f \tfrac{7}{2}) + \mathscr{P}_7 \sqrt{I_i(I_i+1) - (\tfrac{7}{2})(\tfrac{9}{2})}(I_i 1 \tfrac{7}{2} 0 | I_f \tfrac{7}{2})|^2. \quad (1)$$

We use the first two transition probabilities of table 8 of ref. [19]) to fix μ_9 and $\mathscr{P}_7$ and calculate the remaining values as a test of the theory. Actually, because of the quadratic nature of eq. (1) two sets of μ_9 and $\mathscr{P}_7$ values would satisfy any two B(E1) values. For this rough calculation we adjusted the $\mathscr{P}_7/\mu_9$ ratio to give complete cancellation for the highly retarded first transition. Our table 5 summarizes the results.

TABLE 5

Reduced E1 rates between $K = \frac{9}{2}^+$ and $\frac{7}{2}^-$ bands in Hf^{177} with account of Coriolis mixing

I_i	I_f	E_γ (keV)	$T(E1)/T(E1)_W$ Experimental Ref. [19]) ($\times 10^5$)	Theory Eq. (1)
$\frac{9}{2}$	$\frac{7}{2}$	321.4	0.013	0 [a])
$\frac{9}{2}$	$\frac{9}{2}$	208.4	3	3 [a])
$\frac{9}{2}$	$\frac{11}{2}$	71.6	1.2	1.5
$\frac{11}{2}$	$\frac{9}{2}$	313.5	0.5	0.44
$\frac{11}{2}$	$\frac{11}{2}$	177.0	7	4.6
$\frac{13}{2}$	$\frac{11}{2}$	306.0	0.9	2.0
$\frac{13}{2}$	$\frac{13}{2}$	145.6	7	5.6
$\frac{15}{2}$	$\frac{13}{2}$	299.1	0.6	4.0
$\frac{15}{2}$	$\frac{15}{2}$	117.0	12	7.4

[a]) Values assumed to fix the two matrix elements of eq. (1).

The qualitative features of low transition probabilities for $\Delta I = -1$ and high for $\Delta I = 0$ or $+1$ follow directly from the fact that the Clebsch-Gordan coefficients of eq. (1) always have opposite signs in the first case and the same signs in the last two. Clearly, Coriolis mixing can play a large role in determining E1 rates, and any comprehensive theoretical treatment should not ignore its effects. Coriolis mixing effects can cause especially high hindrance, as in the first transition of table 5, but they do not offer an explanation for the puzzling fact that the experimental rates for E3 and $\Delta K = 0$, E1, transitions are generally two orders of magnitude faster than the theoretical including the pairing R factor. The E3 rates are especially revealing in this regard, since three of the four are odd-neutron transitions but calculated with charge

unity, as for the proton caes. There is no significant difference between proton and neutron cases, and they are all too fast relative to our theory. Such behaviour strongly suggests the important influence of coupling of collective octopole excitations of the even structure. In terms of "effective charge" the results suggest an effective charge of around 10 for protons and neutrons. A more sophisticated theory might express the wave functions inclusing odd-particle plus one-octopole-phonon components, and the dominant contributions to the E3 transition rate would involve a change of one in phonon number between initial and final states. An equivalent but still more sophisticated approach would be to express the wave functions in terms of admixtures of three-quasi-particle states (through the H_{31} interaction term of Belyaev [22])).

Similar remarks about a large effective charge might apply to E1 transitions of the $\Delta K = 0$ class. It is remarkable that the collective excitation of the even structure should be important for $\Delta K = 0$, whereas the simple theory with normal effective charges ($\approx e(1-Z/A)$ and $-eZ/A$ for odd proton and neutron, respectively) works for $\Delta K = 1$. However, the lowest collective octopole bands with different K values in even deformed nuclei may be quite different in energy; the $K = 0^-$ is known to come quite low in some regions. These lowest collective octopole phonons with $K = 0$ would mainly influence the $\Delta K = 0$, E1 transitions in odd nuclei.

It is clear that much work remains to be done to provide a quantitative theory of E1 transition rates.

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