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Peculiarities of the Microscopic Description of Multipole Excitations:

Doubly-Open Shell Spherical Nuclei

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The microscopic description of the first 2^+ and 3^- levels of spherical nuclei ($90 \leqq A \leqq 150$ and $186 \leqq A \leqq 206$) is examined, both in the Tamm-Dancoff and the Random Phase Approximations. Peculiar effects of the schematic model are discussed. The consistency of the theory is investigated.

1. Introduction

The microscopic description of vibrational states, either in the particle-hole subspace (Tamm-Dancoff Approximation, RPA) or in the two quasi-particle one (QTDA, QRPA), has become very usual in nuclear spectroscopy.

Undoubtedly, one of the factors that have contributed to encourage the practical application of these theoretical approaches resides in the fact that, even with simple, separable forces, remarkably good results are obtained. Moreover, such kind of interactions permit the solution of the corresponding equations by recourse to the schematic treatment (s.t.) proposed by Brown and Bolsterli [1], in which all the numerical effort involved is that of looking for the roots of a very simple secular equation [2].

In order to employ the schematic approach in superconducting nuclei, drastic approximations must be made, i.e., one must discard all particle-particle and exchange particle-hole terms [3]. The effect of these approximations has been recently investigated [3–6], and found to be intimately related to a much deeper and fundamental problem: that of the consistency of the QRPA [3]. A strong relationship has been established between collectivity, ground state correlations and the effects of the schematic treatment [3–6], and this association has been encountered both in the microscopic description of gamma [3], beta and octupole [4] vibrations (Rare Earth and Transuranic regions), and that of quadrupole excitations in single-closed shell nuclei [5, 6].

The latter exhibit low collectivity, and are due to the coherent motion of a relatively small number of either protons or neutrons around an equilibrium situation characterized by spherical symmetry. On the contrary, the former are strongly collective excitations in which many protons *and* neutrons participate, the corresponding ground state having acquired a stable deformation. There remains a large number of nuclides whose low-lying collective excitations have not yet been investigated in the sense referred to above. The corresponding excited states (2^+ and 3^- ones) share properties with both of the types just mentioned. On the one hand, the equilibrium shape of the nucleus is spherical. On the other hand, both protons and neutrons contribute coherently to the vibrations of the nuclear surface, and both the degree of collectivity, and the number of particles involved in the process, lie roughly in between the corresponding figures for deformed heavy and single-closed shell nuclei. We are, of course, talking about those (spherical) nuclei with proton- and neutron open shells, found in the regions $90 \leqq A \leqq 150$ and $186 \leqq A \leqq 206$. For the sake of brev-

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ity these nuclides shall be called, in what follows, doubly-open shell (D.O.S.) ones. Their low-lying excited states have not received much attention from the microscopic point of view. The only comprehensive work in this respect is that of Lombard [7], who described 2_1^+ and 3_1^- levels, paying special attention to the excitation energies and transition rates to the ground state. The detailed calculations of [7] were performed with the Pairing plus Quadrupole (or Octupole) force, within the framework of the schematic treatment of both the QTDA and the QRPA.

Since no effort has been reported concerning a non-schematic treatment (n.s.t.) of these two approaches (that is, a treatment in which none of the interaction terms mentioned above is discarded), as applied to the description of 2_1^+ and 3_1^- states in D.O.S. nuclides, it seems appropriate to investigate whether the findings of [3–6] are also corroborated here. Notice that one shall be dealing with about 80 nuclei, so that the gap that exists in the literature in this respect is a non negligible one. To fill it is the purpose of the present work.

Due to the fact that the necessary formalism has been abundantly described elsewhere [3–5] no repetition is needed. It must be pointed out, however, that a considerable amount of computing time can be saved by extending the algorithm of [8] (spherical case) to that situation in which both protons and neutrons must be simultaneously dealt with. (This algorithm becomes applicable since, in order to study properties of the schematic model, separable forces must be used.) The corresponding procedure avoids the diagonalization of large, non-symmetric matrices and is thoroughly discussed in [9].

In Section 2 details of the calculations are given. The corresponding results are presented in Section 3, while the conclusions extracted from them are put forward in Section 4.

2. Details of the Calculations

As usual, the spherical shell model Hamiltonian constitutes the starting point. The surface Delta Interaction [10] is employed as the residual interaction (the method of [8, 9] can not be used non schematically in conjunction with the Pairing plus Quadrupole force). Short range correlations are taken into account by means of the Bogoliubov-Valatin transformation, the corresponding gap equations being solved for protons and neutrons separately. The ground state of even-even nuclei is thus assumed to be the product of two BCS states. Neglect of the proton-neutron short range correlations is justified since in most cases protons and neutrons fill different shells.

The single particle states for the different regions studied in this work have been taken from [7], while the pairing constants have been adjusted so as to fit the even-odd mass differences. They are found to be of the order of $26/A$ MeV (protons) and $23/A$ MeV (neutrons), as expected [11].

Only valence particles are assumed to be active. Calculations have been performed with four methods: schematic (QRPA and QTDA) and non schematic (QRPA and QTDA) [5]. For the coupling constant of the Surface Delta Interaction the standard Triplet-Singulet mixture [12] $V_T = V_S/0.6$ has been adopted. As a consequence, the interaction is characterized by the Singulet strength V_S, which, in principle, should adopt those values that result from the even-odd mass fit. As it is often the case [10], however, in view of the simplifications introduced in the calculation (neglect of core excitations, or radial effects [10], etc.), some degree of renormalization is unavoidable [13].

3. Results

We follow the usual procedure in this kind of calculation and adjust the strength V_S to the form K/A, K being constant for each isotopic group [10, 11, 13]. This constant is, of course, different for each of the four methods used here and depends also upon the type of excitation to be described [11, 13]. For quadrupole vibrations, the corresponding values agree reasonably well, for three of the theoretical approaches employed, with the figures arising from the even-odd mass fit, the schematic QRPA case being the exception. As for octuple excitations, larger coupling constants are, as expected [13], required, due to the fact that there are less 2 q.p. states available for a 3^- state than for a 2^+ one.

It is of interest to our present purposes to discuss the *mutual* relationship of the K-values corresponding to the different theoretical approximations. The information displayed in Table 1, where the ratio between nonschematic and schematic coupling constants is given, is quite significant. It is seen that in the quadrupole case the neglect of particle-particle and exchange particle-hole interaction terms implies greater collectivity, since lower strengths are needed in order to lower the 2_1^+ into the energy gap. Since a similar effect is not found in connection with the QTDA, where no ground state correlations are included [2], one is forced to conclude that this enhancement of quadrupole collectivity, associated with the schematic QRPA approach, is to be attributed solely to the way

Table 1. Non-schematic to schematic ratio of the coupling constants that, in each isotopic zone, yield the best fit to 2_1^+ and 3_1^- energies, when adjusted to the form K/A (MeV)

Zone	Coupling Constant (n.s.t.)/ Coupling Constant (s.t.)			
	QRPA		QTDA	
	2_1^+	3_1^-	2_1^+	3_1^-
Zr	1.23	1.65	0.90	1.71
Mo	1.51	1.49	0.94	1.47
Ru	1.54	1.32	1.00	1.26
Pd	1.54	1.40	1.14	1.34
Cd	1.51	1.58	1.12	1.52
Te	1.42	1.03	0.98	0.92
Xe	1.34	1.16	0.98	1.06
Ba	1.41	0.97	1.02	0.86
Nd	1.37	1.11	1.00	0.97
Sm	1.38	1.20	1.00	1.03
Os	1.48	0.91	1.16	0.74
Pt	1.44	1.83	1.13	0.57
Hg	1.35	–	1.06	–

in which ground state correlations are handled within the s.t. framework. For the octupole case, the numbers exhibited in the third and fifth column display similar trends, which should imply, as we shall confirm later, that the associated ground state correlations are of small magnitude.

Having determined the values of V_S in the different isotopic regions, the next step is to compare theoretical trends with experimental ones, for excitation energies and transition rates, as is done in [7] for the schematic model. The *new* results here would be the non-schematic ones. However, it is seen that they do not sensibly differ from those obtained keeping only the direct particle-hole interaction term. The quality of the agreement with experiment is similar in both cases, so that we do not explicitly display it here, in view of the large amount of space that would be required (see [7] to appreciate how much space is saved!). We must make it clear, however, that the corresponding pictures *exist* and are available upon request. See also [9].

Important differences between the QRPA schematic and non-schematic approaches arise as one considers the stability of the solutions of the corresponding secular equations. We deem it worthwhile to illustrate this point (see Table 2) since it has not been dealt with in [3–6]. It is well known [2] that, for large values of the coupling constant, the schematic model yields imaginary solutions. This may also happen with the non-schematic treatment, but here the range of possible strength values is *much* larger. Table 2 exhibits, for the case of ^{114}Cd, the effect that small changes in V_S have upon excitation energies, $B(E\lambda)$ values and average quasi-particle population

Table 2. Effect of small changes in the interaction strength upon excitation energies, transition rates, and average q.p. population in the correlated ground state, for the case of ^{114}Cd

Deviation	−5%	0.0	+2%	+4%	+6%	+8%	+10%
2_1^+ Energy (MeV)							
n.s.t	0.667	0.558	0.508	0.453	0.394	0.317	0.221
s.t.	0.734	0.558	0.462	0.339	0.118	Imaginary	
3_1^- Energy (MeV)							
n.s.t.	2.062	1.945	1.896	1.846	1.795	1.743	1.689
s.t.	2.057	1.945	1.898	1.851	1.802	1.752	1.701
$B(E2, 2_1^+ \to 0_1^+)$ (s.p.u)							
n.s.t.	27.5	32.9	36.1	40.5	46.9	57.7	82.5
s.t.	39.1	53.8	65.8	90.9	265.7	–	–
$B(E3, 3_1^- \to 0_1^+)$ (s.p.u)							
n.s.t.	19.0	20.0	20.5	21.0	21.6	22.2	22.8
s.t.	18.1	19.1	19.6	20.1	20.6	21.2	21.9
Average q.p. population in ground state							
n.s.t. (2_1^+)	0.199	0.295	0.356	0.442	0.571	0.797	1.335
s.t. (2_1^+)	0.507	0.888	1.213	1.910	6.837	–	–
n.s.t. (3_1^-)	0.132	0.162	0.176	0.191	0.208	0.227	0.249
s.t. (3_1^-)	0.127	0.156	0.169	0.183	0.199	0.217	0.237

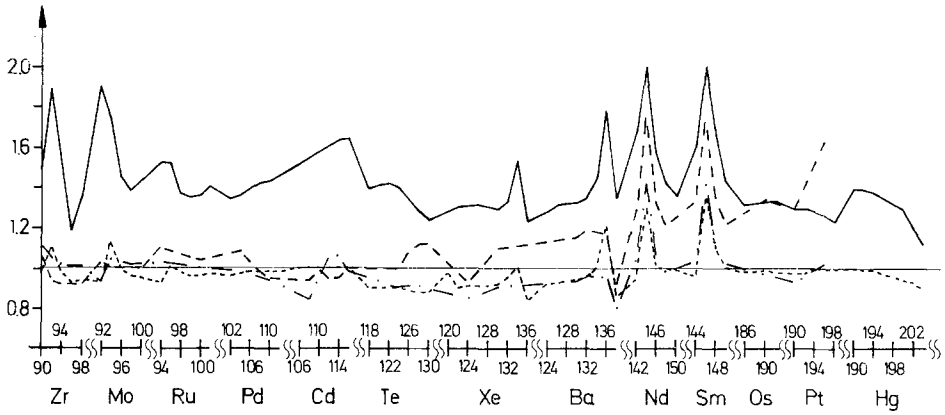

Fig. 1. Relative transition rates (see Eq. (1)). The solid line corresponds to $R_1(2)$, the long-dashed one to $R_1(3)$, the short-dashed curve to $R_2(2)$ and the dotted-dashed one to $R_2(3)$

(induced by the collective excitation [5]) of the correlated ground state. The strength is adjusted so as to reproduce the experimental excitation energy, and is then varied around that value. The consequences of the variation acquire a dramatic character in the quadrupole case. The relationship between collectivity and ground state correlations is apparent.

This relationship can also be discerned from inspection of Figure 1, which depicts the ratio

$$R_i(\lambda) = B(E\lambda, \text{s.t.})/B(E\lambda, \text{n.s.t.}), \quad (1)$$

with $i=1$ for the QRPA and $i=2$ for the QTDA. λ is the multipole order and the transitions referred to are those from the collective excitation to the ground state. The values shown in Figure 1 have been computed in each instance with that value of V_S which reproduces the experimental excitation energy. The fact that $R_1(2)$ is always greater than unity while $R_2(2)$ is close to, and oscillates around it, indicates again that the schematic treatment overestimates the 2_1^+ collectivity, and that this is an effect associated with the behaviour of the corresponding ground state correlations. As those of Tables 1 and 2, the results of Figure 1 show that the ground state correlations induced by the octuple states are small.

Next, we explicitly compute figures that are directly related to the behaviour of ground state correlations, in order to confirm, on the one hand, what has been deduced above and, on the other one, to discuss the consistency of the QRPA. Let us denote with $n_i(J)$ the average quasiparticle population, in the correlated ground state (c.g.s.), of the orbital $|i\rangle$, as induced by the collective state of angular momentum J [5]. Further, let $n_{\max}(J)$ denote the largest $n_i(J)$ among the different orbital occupancies. The method employed to evaluate the n_i has been described in [3, 5]. It is well known that in order for the QRPA to be

Table 3. Maximum orbital occupancy in the correlated ground state, associated with the 2_1^+ state $n_{\max}(2_1^+)$

Nucleus	s.t.	n.s.t.	Nucleus	s.t.	n.s.t.
^{90}Zr	0.074	0.022	^{128}Xe	0.290	0.192
^{92}Zr	0.296	0.080	^{130}Xe	0.205	0.118
^{94}Zr	0.224	0.109	^{132}Xe	0.139	0.062
^{96}Zr	0.029	0.015	^{134}Xe	0.089	0.023
^{98}Zr	0.090	0.060	^{136}Xe	0.145	0.001
^{92}Mo	0.409	0.035	^{124}Ba	1.440	0.811
^{94}Mo	0.131	0.037	^{126}Ba	1.100	0.625
^{96}Mo	0.164	0.059	^{128}Ba	0.736	0.438
^{98}Mo	0.161	0.056	^{130}Ba	0.391	0.246
^{100}Mo	0.289	0.151	^{132}Ba	0.261	0.143
^{94}Ru	0.315	0.010	^{134}Ba	0.172	0.073
^{96}Ru	0.141	0.045	^{136}Ba	0.105	0.025
^{98}Ru	0.189	0.097	^{138}Ba	0.178	0.003
^{100}Ru	0.243	0.159	^{142}Nd	0.208	0.009
^{102}Ru	0.283	0.210	^{144}Nd	0.167	0.057
^{104}Ru	0.425	0.343	^{146}Nd	0.280	0.168
^{102}Pd	0.205	0.141	^{148}Nd	0.523	0.321
^{104}Pd	0.201	0.146	^{150}Nd	1.350	0.851
^{106}Pd	0.226	0.173	^{144}Sm	0.152	0.007
^{108}Pd	0.311	0.235	^{146}Sm	0.156	0.048
^{110}Pd	0.479	0.299	^{148}Sm	0.221	0.119
^{112}Pd	0.572	0.323	^{150}Sm	0.445	0.281
^{106}Cd	0.175	0.089	^{186}Os	1.550	0.642
^{108}Cd	0.183	0.089	^{188}Os	1.330	0.608
^{110}Cd	0.199	0.078	^{190}Os	1.010	0.515
^{112}Cd	0.253	0.088	^{192}Os	0.806	0.443
^{114}Cd	0.329	0.107	^{190}Pt	0.570	0.380
^{116}Cd	0.368	0.122	^{192}Pt	0.489	0.318
^{118}Te	0.444	0.135	^{194}Pt	0.418	0.271
^{120}Te	0.479	0.144	^{196}Pt	0.315	0.205
^{122}Te	0.410	0.131	^{198}Pt	0.235	0.130
^{124}Te	0.280	0.106	^{190}Hg	0.238	0.135
^{126}Te	0.159	0.075	^{192}Hg	0.223	0.123
^{128}Te	0.098	0.049	^{194}Hg	0.205	0.110
^{130}Te	0.063	0.027	^{196}Hg	0.190	0.104
^{120}Xe	0.970	0.464	^{198}Hg	0.183	0.105
^{122}Xe	0.917	0.433	^{200}Hg	0.207	0.130
^{124}Xe	0.736	0.352	^{202}Hg	0.171	0.070
^{126}Xe	0.490	0.261	^{204}Hg	0.157	0.075

Table 4. Quasi-particle occupation numbers for ^{126}Xe and ^{128}Xe, according to different QRPA treatments

Approximation	Nucleus	Level	$s_{1/2}$	$d_{3/2}$	$d_{5/2}$	$g_{7/2}$	$h_{11/2}$
n.s.t.	^{126}Xe	Proton	0.035	0.087	0.071	0.260	0.009
		Neutron	0.203	0.243	0.028	0.040	0.097
QRPA	^{128}Xe	Proton	0.025	0.064	0.051	0.192	0.007
		Neutron	0.117	0.144	0.015	0.023	0.095
s.t.	^{126}Xe	Proton	0.030	0.096	0.076	0.361	0.008
		Neutron	0.404	0.490	0.050	0.075	0.242
QRPA	^{128}Xe	Proton	0.024	0.077	0.061	0.290	0.006
		Neutron	0.221	0.276	0.026	0.040	0.231
Ref. 14	^{126}Xe	Proton	0.024	0.043	0.078	0.230	0.007
		Neutron	0.273	0.299	0.046	0.052	0.236
	^{128}Xe	Proton	0.016	0.030	0.051	0.169	0.004
		Neutron	0.180	0.210	0.023	0.027	0.190

consistent these quantities must be small in relation to unity [3–6].

Table 3 lists the $n_{\max}(2)$ values for the 80 nuclides studied in the present work. Both schematic and non-schematic figures are given, and a glance at them allow us to quickly determine in which instances is the consistency of the QRPA to be doubted. Schematic values are, as expected, larger than non-schematic ones. Table 4 compares, for ^{126}Xe and ^{128}Xe, our $n_i(2)$ with those of Ikeda, Udagawa and Yamaura [14], (evaluated within the schematic framework with the Pairing plus Quadrupole force) who have developed an interesting method [14] to treat violations of the Pauli principle, which are the origin of the consistency problem discussed here. We see that their approach constitutes an improvement upon the s.t., but is still inferior as compared to a complete treatment (the n.s.t. one) of the QRPA equations.

As for the $n_i(3)$ figures, they are, as expected, always small, with an average value located within the (0.001–0.01) interval. The largest $n_i(3)$ found, among the 13 isotopic regions that concern us, does not exceed 0.1. As a result, ground state correlations do not sensibly affect the structure of octupole states, which is then described in a similar fashion either by the QRPA or by the QTDA, as evidenced in Tables 1–2 and in Figure 1.

4. Conclusions

The main results of the present study can be summarized as follows:

i) Lombard has shown [7] that a rough agreement with experiment is obtained, for 2_1^+ and 3_1^- states in even-even D.O.S. nuclei, if one attempts a schematic description in the two quasi-particle space. In the present work, it has been found that the quality of the microscopic picture is not affected by the inclusion (or, more properly, the neglect) of exchange particle-hole and both direct and exchange particle-particle terms.

ii) As is also the case for deformed heavy nuclei [3, 4] and single-closed shell ones [5, 6], it is seen also for D.O.S. nuclides that the schematic treatment *exaggerates* the collective character of quadrupole vibrations. Agreement with experiment is unimpaired, however, because one simply renormalizes the strength of the interaction (Table 1).

iii) This overestimation is due to differences in the ground state correlations that the 2_1^+ induces, according to which of the two treatments, the schematic, or the nonschematic one, is employed.

iv) Non-schematic solutions of the QRPA equations are more stable, more consistent and display a smoother behaviour than the corresponding schematic ones.

v) In both approaches one encounters instances in which the consistency of the QRPA could be questioned. Non-schematic $n_i(2)$ values larger than, say, 0.35 are found for the following nuclides: Xe (120–122), Ba (124–128), ^{150}Nd, Os (186–192). The same happens, within a schematic context, in a larger number of cases, i.e., ^{104}Ru, Pd (110–112), Te (118–122), Xe (120–126), Ba (124–130), Nd (146–150), ^{150}Sm, Os (186–192), Pt (190–194). Some of these nuclei may more properly be treated as deformed ones (Nd, Sm, Os). In others (Te, Xe, Ba), the neglect of short range proton-neutron correlations is not justified (protons and neutrons fill the same shells). In any case, however, there would remain inconsistencies in the s.t. of

^{104}Ru, Pd (110–112) and Pt (190–194), where schematic $n_i(2)$ exceed 0.4.

Consequently, it is not safe to take for granted the consistency of the QRPA in every application. Violations thereof give us clues concerning possible inadequacies of the theoretical treatment. Let us in this connection mention that large $n_i(2)$ may indicate that four quasi-particle components must be included. The larger the number of valence particles (holes), the greater the likelihood that four, or more, q.p. states may become necessary for a proper microscopic description. See, for instance, in Table 3, the Ba-sequence, which starts with 14 neutron holes ($A=124$) and ends in the single-closed nuclei ^{138}Ba. As the hole number decreases, so does $n_{max}(2)$, until eventually consistency is achieved when the valence number becomes so low that four q.p. can not be expected to contribute.

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