Asymmetric-Rotator Model in the s-d Shell†

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The asymmetric-rotator model based on the non-axially-symmetric Hartree-Fock field is applied to Mg^{24}, to S^{32}, and to their odd-even neighbors. Relations between the earlier particle-bole treatment and the asymmetric-rotator model for the $K=2$ band of Mg^{24} are investigated.

I. INTRODUCTION

THE application of the asymmetric-rotator model described in this paper is strongly connected with the single-particle field deduced from the variational principle. The energy levels corresponding to rotation of the nucleus are investigated by considering the rotating core as being the self-consistent field of that nucleus.

From a solution of the Hartree-Fock (H-F) equations[1] in an extended frame (in the way summarized in Sec. II), it is expected that certain nuclei will attain a H-F ground state which is not axially symmetric. In the *s-d* shell, two regions of lack of axial symmetry have been recently found,[2] one around Mg^{24} and the other around S^{32}. The amount of asymmetry, expressed in terms of the parameter γ of the irrotational-flow model,[3] is about 30° in Mg^{24} and 35° in S^{32}. Such deviations from axial symmetry are big enough to affect the rotational spectrum of the core, and the states of total angular momentum 2, 3, 4··· which are characteristic of the asymmetric rotator come down in energy. Indications that the nuclei in the region of Mg^{24} indeed possess asymmetric intrinsic structure may be found in the experimental spectrum of Mg^{24}, and in the measured[4] electromagnetic (in particular $E2$) transition probabilities between bands with $\Delta K=2$, in Mg^{25} and in Al^{25}. These probabilities are much larger than those expected from $\Delta K=1$ Coriolis mixing, when the odd nucleon is coupled to an axially symmetric Mg^{24} core.

It is the purpose of this paper to base the investigation of the rotational spectra of the nuclei in regions of asymmetry on the appropriate self-consistent field. In Sec. III the even-even asymmetric rotator is constructed out of the nonaxially-symmetric single-particle energies and wave functions, by using the cranking model. This rotator is then used in analyzing the spectrum of Mg^{24}. It is also shown that the extra degrees of freedom added in the self-consistency problem in order to allow deviations from axial symmetry can be related to the particle-hole vibrational treatment. Such relations between the described asymmetric rotator and former particle-hole calculations[5] for the $K=2$ band in Mg^{24} are derived explicitly. In Sec. IV the odd-even nuclei are treated by coupling the odd nucleon to an asymmetric even-even core. The rotation-particle coupling (RPC) interaction is diagonalized for Mg^{25} and P^{31}.

II. NON-AXIALLY-SYMMETRIC ORBITALS

The intrinsic single-particle structure of the nucleus is derived from the many-body Hamiltonian by solving the self-consistent Hartree-Fock equations[6]

$$\langle\alpha|h|\beta\rangle=\langle\alpha|k|\beta\rangle+\sum_\lambda\langle\alpha\lambda|V_A|\beta\lambda\rangle, \tag{1}$$

$$h|\lambda\rangle=\epsilon_\lambda|\lambda\rangle. \tag{2}$$

The summation in the first equation runs over all the occupied states. The solution of these equations is achieved by the iterative method. To allow convergance of the successive iterations to possible non-axially-symmetric solutions, the trial single-particle wave functions of the occupied state $|\lambda\rangle$ are chosen as

$$|\lambda\rangle=\sum_{jm} C_{jm}{}^\lambda|jm\rangle, \tag{3}$$

where the $|jm\rangle$ are the shell-model states, and the variational parameters $C_{jm}{}^\lambda$ vanish unless $m-\frac{1}{2}$ is even. In the *s-d* shell, to which the sum is restricted, the states $d_{5/2}{}^{5/2}$, $d_{1/2}{}^{5/2}$, $d_{1/2}{}^{3/2}$, $s_{1/2}{}^{1/2}$, $d_{-3/2}{}^{5/2}$, $d_{-3/2}{}^{3/2}$ appear. This $\Delta m=2$ restriction is found to be equivalent to the assumption that the system has an ellipsoidal shape, with x, y, z being the major axes. Owing to the fourfold-degeneracy assumption, each occupied state is filled by two protons and two neutrons with spins up and down. Thus the summation on λ in Eq. (1) runs over two occupied states in Mg^{24} and over four occupied states in S^{32}. The single-body part in the Hamiltonian is of the form

$$K=(\hbar^2/2m)\Delta+\alpha_{1.s}\mathbf{l}\cdot\mathbf{s}+\alpha_{l2}\mathbf{l}^2, \tag{4}$$

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TABLE I. Single-particle self-consistent Hamiltonian for Mg^{24} and S^{22}. For each nucleus, the lowest nonaxially-symmetric and axially-symmetric cases are presented. The single-particle energies are given in MeV, and are followed by the components of the single-particle wave functions in the representation (in this order): $d_{5/2}{}^{5/2}$, $d_{-3/2}{}^{5/2}$, $d_{-3/2}{}^{3/2}$, $d_{1/2}{}^{5/2}$, $d_{1/2}{}^{3/2}$, $s_{1/2}{}^{1/2}$.

Mg^{24}	Nonax.	−20.607	−17.656	−10.243	−9.004	−6.173	−3.400
		0.118	−0.103	−0.819	−0.544	−0.094	−0.002
		0.268	−0.758	0.304	−0.418	0.260	0.139
		0.167	−0.149	0.062	−0.053	−0.262	−0.935
		0.816	−0.004	−0.390	0.379	0.189	−0.046
		−0.118	−0.522	−0.126	0.431	−0.681	0.220
		0.454	0.346	0.255	−0.445	−0.597	0.235
	Ax.	−19.499	−15.106	−12.060	−10.166	−6.187	−4.069
		0	0	0	1.000	0	0
		0	0.974	0	0	0	−0.226
		0	0.226	0	0	0	0.974
		−0.850	0	0.465	0	−0.250	0
		0.250	0	0.771	0	0.586	0
		−0.465	0	−0.436	0	0.771	0
S^{32}	Nonax.	−24.729	−23.648	21.179	−18.693	−12.024	−8.785
		0.947	0.230	0.168	0.068	0.098	0.091
		0.036	−0.581	0.674	−0.077	−0.348	0.283
		−0.001	0.095	−0.152	0.796	−0.575	0.067
		0.075	−0.598	−0.228	0.447	0.599	0.163
		−0.014	−0.053	0.420	0.264	0.146	−0.854
		−0.310	0.491	0.516	0.295	0.399	0.388
	Ax.	−22.729	−22.684	−20.547	−18.721	−13.361	−11.120
		0	1.000	0	0	0	0
		0	0	0	−0.831	0.556	0
		0	0	0	0.556	0.831	0
		−0.699	0	0.610	0	0	−0.373
		0.302	0	−0.221	0	0	−0.928
		0.648	0	0.761	0	0	0.030

and the two-body interaction is taken to be the Rosenfeld[7] mixture having the form

$$V=V_0 V_{TS} e^{-r/a}/(r/a)\,, \qquad (5)$$

where $a=1.37\times10^{-13}$ cm, and V_{TS} have the following eigenvalues:

$$V_{00}=1.8\,,\quad V_{01}=-1.0\,,\quad V_{10}=-0.6\,,\quad V_{11}=0.333\cdots.$$

By starting the iteration with different initial values for the variational parameters $C_{jm}{}^{\lambda}$, various relative minima in the energy surface are obtained, some of which belong to axially symmetric solutions (e.g., single-particle states of definite j_z), and the remainder to non-axially-symmetric solutions. For more details the reader is referred to Ref. 2.

For an oscillator radial function of range 1.65×10^{-13} cm and the values $V_0=50$ MeV, $\alpha_{l\cdot s}=2.8$ MeV, $\alpha_{l^2}=0$, the lowest self-consistent solutions for Mg^{24} and S^{32} are not axially symmetric. These solutions, together with the adjacent axially symmetric solutions, are given in Table I. The calculated rotational spectra will be based on these asymmetric solutions.

III. EVEN-EVEN NUCLEI

The even-even nucleus is described as a non-axially-symmetric rotator with an ellipsoidal shape. When the principal axes of the nucleus are taken as the body-fixed coordinate system, the Hamiltonian has the form

$$H=\sum_{\alpha=1}^{3}\frac{\hbar^2}{2\mathcal{J}_\alpha}J_\alpha{}^2. \qquad (6)$$

The principal moments of inertia are obtained from the single-particle energies and wave functions, using the Inglis cranking formula[8]

$$\mathcal{J}_\alpha=2\sum\frac{|\langle\sigma|J_\alpha|\lambda\rangle|^2}{e_\sigma-e_\lambda}\,, \qquad (7)$$

where λ stands for occupied and σ for unoccupied states. In the Davydov-Filipov asymmetric-rotator model[9] the three moments of inertia depend on two parameters, β and γ, through

$$\mathcal{J}_\alpha=4B\hbar^2\sin^2(\gamma-\tfrac{2}{3}\pi\alpha)\,, \qquad (8)$$

while in the present treatment they are independent and are directly connected to the intrinsic structure of the nucleus. The energy levels of the Hamiltonian (6) are obtained by diagonalizing it in the representation

$$\psi^I{}_{M,K}\sim\{D^I{}_{M,K}+(-1)^{I+K}D^I{}_{M,-K}\}\,. \qquad (9)$$

In the particular case of Mg^{24} the cranking formula (7) gave, for the non-axially-symmetric single-particle field of Table I, the values

$$\mathcal{J}_1=2.119\ \text{MeV}^{-1},\quad \mathcal{J}_2=2.400\ \text{MeV}^{-1},\quad \mathcal{J}_3=0.92\ \text{MeV}^{-1}.$$

[7] L. Rosenfeld, *Nuclear Forces* (North-Holland Publishing Company, Amsterdam, 1958), p. 233.

[8] D. R. Inglis, Phys. Rev. **96**, 1059 (1954).

[9] A. S. Davydov and G. F. Filippov, Nucl. Phys. **8**, 237 (1958).

The calculated rotational bands of Mg^{24} based on these moments of inertia are given in Fig. 1 and are compared with the experimental spectrum. For this special case where two of the moments of inertia are roughly equal and the third is much smaller, the spectrum gets a simple interpretation if we look at the Hamiltonian (6) written in the form

$$H=\tfrac{1}{2}(A_1+A_2)I^2+\tfrac{1}{4}(A_1-A_2)(I_+^2+I_-^2)+[A_3-\tfrac{1}{2}(A_1+A_2)]I_3^2, \quad (10)$$

where the A_α's are defined as $1/2\mathcal{I}_\alpha$. The rotational spectrum is characterized by the $K=0$ ground-state rotational band, and an excited $K=2$ band, both having the same moment of inertia $\mathcal{I}$, defined by $1/\mathcal{I}=1/2\mathcal{I}_1+1/2\mathcal{I}_2$, and the $J=2$, $K=2$ state lies at an energy $\hbar^2/\mathcal{I}+2\hbar^2/\mathcal{I}_3$ above the ground state. When we try to analyze the experimental spectrum of Mg^{24} in this manner, we obtain, approximately, $\mathcal{I}=2.2$ and $\mathcal{I}_3=0.55$ MeV^{-1}. The corresponding theoretical values are $\mathcal{I}=2.25$ and $\mathcal{I}_3=0.93$ MeV^{-1}. The agreement in $\mathcal{I}$ is pleasing, especially when we note the failure of the axially symmetric self-consistent intrinsic field to produce it.[2]

The spectrum of S^{32} does not display a rotational nature, and probably involves vibrational degrees of freedom.

A vibrational treatment, namely the one-particle one-hole theory, has also been applied[5] to the $K=2$ band in Mg^{24}. It is interesting to investigate relations between the two models, and particularly between the intrinsic state of the asymmetric core and the particle-hole state in the Tamm-Dancoff[10] approximation.

Let us denote by λ_0 the occupied, and by σ_0 the unoccupied single-particle states of the axially symmetric H-F representation. The intrinsic $K=0$ ground state is therefore

$$\Phi_0=\prod_{\lambda_0} a_{\lambda_0}^\dagger|0\rangle. \quad (11)$$

The $K=2$ excited-state band is of the form

$$\Phi_2=\sum_{\sigma_0\lambda_0} A_{\sigma_0\lambda_0}a_{\sigma_0}^\dagger a_{\lambda_0}\Phi_0 \quad (12)$$

with $k_{\sigma_0}-k_{\lambda_0}=2$; that is, Φ_2 is a linear combination of states obtained by exciting one particle out of the state Φ_0.

In the present treatment, both bands are embodied in a single determinantal asymmetric intrinsic state

$$\Phi=\prod_\lambda a_\lambda^\dagger|0\rangle. \quad (13)$$

We can expand

$$a^\dagger=\sum_{\lambda_0} B_{\lambda\lambda_0}a_{\lambda_0}^\dagger+\sum_{\sigma_0} B_{\lambda\sigma_0}a_{\sigma_0}^\dagger \quad (14)$$

with $(k_\lambda-k_{\sigma_0})$ and $(k_\lambda-k_{\lambda_0})$ assuming only even values. Substituting into (13), we have

$$\Phi=\prod_\lambda\{\sum_{\lambda_0} B_{\lambda\lambda_0}a_{\lambda_0}^\dagger+\sum_{\sigma_0} B_{\lambda\sigma_0}a_{\sigma_0}^\dagger\}|0\rangle \quad (15)$$

[10] See for example, Ref. 1.

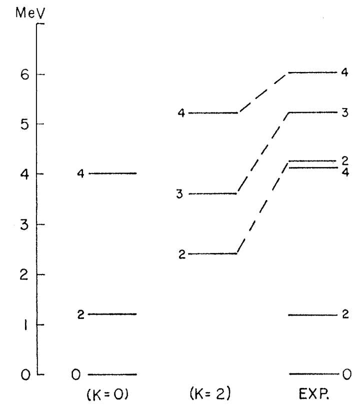

FIG. 1. A comparison between the calculated and the experimental spectrum of Mg^{24}.

from which we can project the $K=0$ and the $K=2$ components. Writing the projected states, formally, as $P^{K=0}\Phi$, and $P^{K=2}\Phi$, we immediately see that we can expand both states in terms of particle-hole excitations from Φ_0:

$$P^{K=0}\Phi=\alpha_0\Phi_0+\sum_{\sigma_0\lambda_0}\alpha_{\sigma_0\lambda_0}a_{\sigma_0}^\dagger a_{\lambda_0}\Phi_0+\sum_{\substack{\sigma_0\sigma_0',\\ \lambda_0,\lambda_0'}}\alpha_{\sigma_0\sigma_0',\lambda_0\lambda_0'}a_{\sigma_0'}^\dagger a_{\sigma_0}^\dagger a_{\lambda_0'}a_{\lambda_0}\Phi_0+\cdots, \quad (16)$$

and

$$P^{K=2}\Phi \sum_{\sigma_0\lambda_0} B_{\sigma_0\lambda_0}a_{\sigma_0}^\dagger a_{\lambda_0}\Phi_0+\sum_{\substack{\sigma_0\sigma_0',\\ \lambda_0,\lambda_0'}} B_{\sigma_0\sigma_0'\lambda_0\lambda_0'}a_{\sigma_0'}^\dagger a_{\sigma_0}^\dagger a_{\lambda_0'}a_{\lambda_0}\Phi_0+\cdots. \quad (17)$$

To check whether this is a useful expansion, we first compute the coefficients B (Table II) for the axially symmetric and nonaxially-symmetric solutions of Mg^{24} appearing in Table I. From it we get the diagonal elements of the density matrix of the state Φ, in the representation of Φ_0, which are

$$\rho_{11}=0.955,\quad \rho_{22}=0.685,\quad \rho_{33}=0.316,$$
$$\rho_{44}=0.025,\quad \rho_{55}=0.007,\quad \rho_{66}=0.011. \quad (18)$$

The domination of ρ_{11} and ρ_{22} in the trace of ρ means that $P^{K=0}\Phi$ is essentially Φ_0, and that $P^{K=2}\Phi$ may be approximated by a (normalized) state of the form

$$P^{K=2}\Phi=\sum_{\lambda_0\sigma_0} C_{\sigma_0\lambda}a_{0\sigma_0}^\dagger a_{\lambda_0}\Phi_0. \quad (19)$$

We can now calculate the overlap of Φ_2 and $P^{K=2}\Phi$,

TABLE II. The coefficients $\{B\}$. The states are labeled according to their ordering in Table I. For the axially-symmetric case, the k's of each state are also given.

$\lambda \backslash (\lambda_0,\sigma_0)$	$1\,(k=\frac{1}{2})$	$2\,(k=\frac{3}{2})$	$3\,(k=\frac{1}{2}')$	$4\,(k=\frac{5}{2})$	$5\,(k=\frac{1}{2}'')$	$6\,(k=\frac{3}{2}')$
1	−0.934	0.299	0.091	−0.118	0.077	0.102
2	−0.288	−0.772	−0.555	−0.103	−0.038	0.026

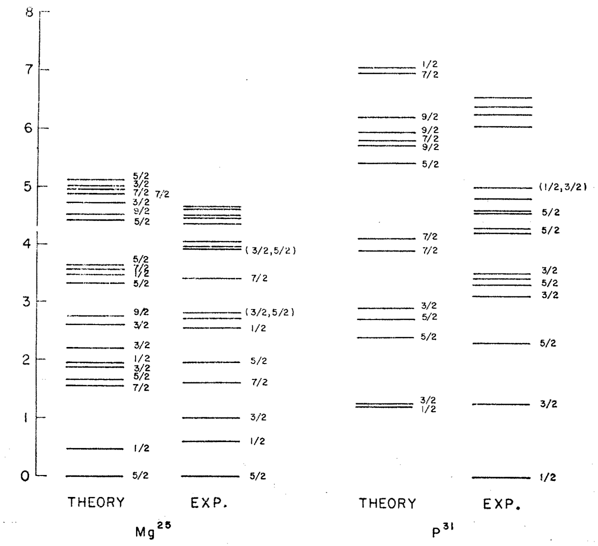

FIG. 2. The calculated rotational spectra of Mg^{25} and P^{31} achieved by rotation-particle-coupling diagonalization. The experimental spectra are also shown.

which, in the above approximation is simply

$$\langle\Phi_2|P^{K=2}\Phi\rangle=\sum_{\sigma_0\lambda_0}A_{\sigma_0\lambda_0}C_{\sigma_0\lambda_0}.$$

Inserting numerical values, we obtain for the overlap

$$\langle\Phi_2|P^{K=2}\Phi\rangle=0.94.$$

This large value is significant, since it demonstrates the close relationship between the two seemingly diverse models. The $K=2$ band, whose intrinsic state was of a vibrational nature in the limited axially symmetric treatment, attains a pure rotational character when this symmetry limitation is removed.

IV. ODD-EVEN NUCLEI

The odd-even nucleus is treated as an even-even asymmetric core with a single nucleon moving in the asymmetric H-F field coupled to it. The Hamiltonian is

$$H=\sum_{\alpha=1}^{3}\frac{\hbar^2}{2\mathcal{J}_\alpha}R_\alpha{}^2+H_{\text{asym}}, \qquad (20)$$

where R_α are the components of the angular momentum of the core. The moments of inertia $\mathcal{J}_\alpha$ are again determined by the cranking formula (7) for the same self-consistent asymmetric field which is used in coupling the extra nucleon. Since R_α are not constants of the motion, the Hamiltonian (20) is transformed in the standard manner,[11] to be expressed in terms of I_α, the total angular momentum of the nucleus, and j_α, the odd nucleon's angular momentum. It is then diagonalized in the representation

$$\Psi^I{}_{M,K,\gamma}\sim D^I{}_{M,K}\chi^\gamma+(-1)^{I+K}D^I{}_{M,-k}\bar{\chi}^\gamma, \qquad (21)$$

where χ^γ is any of the non-axially-symmetric states, available to the odd nucleon and $\bar{\chi}^\gamma$ its time-reversed state. The invariance of the intrinsic state under rotation of π radians through any of the principal axes implies[12] that the various k-components in χ^γ differ from K by an even number.

The only nuclei in the s-d shell to which this simple asymmetric treatment may be applied at all are Mg^{25} and P^{31} (and their mirror nuclei). Before proceeding with the presentation of the results, one remark is pertinent. The parameters of the force used in solving the self-consistancy problem were chosen arbitrarily, bearing only a general resemblance to a force that one might expect to be physically proper. The force and the single-particle fields derived from it were, however, used here for a qualitative description. Better fits can be achieved by extensive variations of the parameters. Figure 2 shows the rotational spectra obtained in the way described.

As expected, the agreement between the calculated spectra and the experiment is better in the case of Mg^{25}, since the region of S^{32} does not display a pure rotational nature. While the agreement in the $k=\frac{5}{2}$ ground-state band of Mg^{25} is pleasing, the states that can be related to the $k=\frac{1}{2}$ band are not in good shape. In particular the spacing between the $\frac{1}{2}$ level and the first $\frac{3}{2}$ level is too big. This deviation may come also from the fact that the decoupling parameter of the $k=\frac{1}{2}$ band is very sensitive to variations in the single-particle wave functions.

In conclusion we may say that the self-consistency approach, where deviation from axial symmetry is allowed, provides a more natural and unified basis for understanding the rotational spectra in the s-d shell. The description based on the appropriate H-F intrinsic structure seems to be in qualitative agreement in the asymmetry regions as well. It is desirable, however, to extend these methods to include the vibrational degrees of freedom, which play an important role, especially in the second half of the shell.

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[11] S. A. Moszkowski, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 39, p. 411.

[12] See, for example, A. Messiah, *Quantum Mechanics* (Interscience Publishers, Inc., New York, 1963), Vol. II, p. 1071.