

symmetry axis because the nuclei can be treated as mass points and because the electrons do not rotate collectively in the axially symmetric binding field.)

The restriction on the rotational degrees of freedom resulting from axial symmetry corresponds to the constraint

$$I_3 = J_3 \quad (4-10)$$

where  $J_3$  is the operator representing the component of intrinsic angular momentum. The condition (4-10) implies that the operations associated with rotations about the symmetry axis, which are generated by  $I_3$ , have prescribed values determined by the intrinsic structure.

Since the axial symmetry makes it impossible to distinguish orientations differing only in the value of the third Euler angle  $\psi$ , this variable is redundant. The constraint (4-10) ensures that the total nuclear wave function, which is a product of intrinsic and rotational wave functions (see Eq. (4-4)), is independent of the value of  $\psi$ . In fact, a rotation of the intrinsic frame through an angle  $\Delta\psi$  about the 3 axis multiplies the intrinsic wave function by the factor  $\exp\{-iJ_3\Delta\psi\}$  and the rotational wave function by  $\exp\{iI_3\Delta\psi\}$ ; the total wave function is therefore invariant, for  $J_3 = I_3 (=K)$ . Instead of treating the Euler angle  $\psi$  as a redundant variable, one may constrain  $\psi$  to have a definite value, such as  $\psi=0$  or  $\psi=-\phi$ ; see the comment on the helicity wave function in Appendix 3A, Vol. I, p. 361. If  $\psi$  were fixed, the normalization constants in Eqs. (4-7) and (4-8) would be multiplied by  $(2\pi)^{1/2}$ .

#### 4-2c $\mathcal{R}$ Invariance

A further reduction in the rotational degrees of freedom follows if the intrinsic Hamiltonian is invariant with respect to a rotation of  $180^\circ$  about an axis perpendicular to the symmetry axis. Rotations about different axes perpendicular to the symmetry axis are equivalent; for definiteness, we choose a rotation  $\mathcal{R} \equiv \mathcal{R}_2(\pi)$  with respect to the 2 axis. (For systems with axial symmetry but not spherical symmetry,  $\mathcal{R}$  invariance is the only possible additional rotational invariance; in fact, invariance with respect to any other rotation would imply an infinity of symmetry axes and hence spherical symmetry.)

The  $\mathcal{R}$  invariance implies that the rotation  $\mathcal{R}$  is part of the intrinsic degrees of freedom, and is therefore not to be included in the rotational degrees of freedom. We can express this constraint by requiring that the operator  $\mathcal{R}_e$ , which performs the rotation  $\mathcal{R}$  by acting on the collective orientation angles (external variables), is identical to the operator  $\mathcal{R}_i$ , which

performs the same rotation by acting on the intrinsic variables

$$\mathcal{R}_e = \mathcal{R}_i \quad (4-11)$$

The condition (4-11) is analogous to the constraint (4-10) associated with the invariance under infinitesimal rotations about the symmetry axis.

Intrinsic states with  $K=0$  can be labeled by the eigenvalue  $r$  of  $\mathcal{R}_i$ ,

$$\begin{aligned} \mathcal{R}_i \Phi_{r,K=0}(q) &= r \Phi_{r,K=0}(q) \\ r &= \pm 1 \end{aligned} \quad (4-12)$$

The eigenvalues of  $\mathcal{R}_i$  are  $\pm 1$  because  $\mathcal{R}^2 = \mathcal{R}_2(2\pi) = +1$  for a system with integer angular momentum.

The operation  $\mathcal{R}_e$  acting on the rotational wave function (4-8) inverts the direction of the symmetry axis ( $\theta \rightarrow \pi - \theta$ ,  $\phi \rightarrow \phi + \pi$ ), and we obtain

$$\mathcal{R}_e Y_{IM}(\theta, \phi) = (-1)^I Y_{IM}(\theta, \phi) \quad (4-13)$$

The constraint  $\mathcal{R}_i = \mathcal{R}_e$  therefore implies

$$(-1)^I = r \quad (4-14)$$

and the rotational spectrum contains states with only even values or only odd values of  $I$ ,

$$\begin{aligned} \Psi_{r,K=0,IM} &= (2\pi)^{-1/2} \Phi_{r,K=0}(q) Y_{IM}(\theta, \phi) \\ I=0, 2, 4, \dots & \quad r = +1 \\ I=1, 3, 5, \dots & \quad r = -1 \end{aligned} \quad (4-15)$$

The constraint  $\mathcal{R}_e = r$  halves the domain of independent orientation angles and removes every other  $I$  value from the rotational spectrum.

The intrinsic states with  $K \neq 0$  are twofold degenerate, as a consequence of the  $\mathcal{R}$  invariance. We shall use a notation such that  $K$  is taken to be positive, and the rotated states with negative eigenvalues of  $J_3$  are denoted by  $\bar{K}$ ,

$$\Phi_{\bar{K}}(q) \equiv \mathcal{R}_i^{-1} \Phi_K(q) \quad (4-16)$$

If the intrinsic states are expanded in components of total angular momen-

tum  $J$ , the phase convention (4-16) implies (see Eq. (1A-47))

$$\Phi_K = \sum_J c_J \Phi_{JK} \quad (4-17)$$

$$\Phi_{\bar{K}} = \exp\{i\pi J_2\} \Phi_K = \sum_J (-1)^{J+K} c_J \Phi_{J, -K}$$

where  $\Phi_{J, \pm K}$  are components of a  $J$  multiplet with  $J_3 = \pm K$ .

The effect of  $\mathcal{R}_e$  on the rotational wave function is given by

$$\begin{aligned} \mathcal{R}_e \mathcal{D}_{MK}^I(\omega) &= \exp\{-i\pi I_2\} \mathcal{D}_{MK}^I(\omega) \\ &= (-1)^{I+K} \mathcal{D}_{M-K}^I(\omega) \end{aligned} \quad (4-18)$$

In the derivation of Eq. (4-18), we have employed the relation (1A-47) and the fact that the matrix elements of  $I_2$  have the opposite sign from those of  $I_y$  (see Eqs. (1A-93)). In order to fulfill the condition (4-11), the nuclear wave functions must therefore have the form

$$\begin{aligned} \Psi_{KIM} &= 2^{-1/2} (1 + \mathcal{R}_i^{-1} \mathcal{R}_e) \left( \frac{2I+1}{8\pi^2} \right)^{1/2} \Phi_K(q) \mathcal{D}_{MK}^I(\omega) \\ &= \left( \frac{2I+1}{16\pi^2} \right)^{1/2} \{ \Phi_K(q) \mathcal{D}_{MK}^I(\omega) + (-1)^{I+K} \Phi_{\bar{K}}(q) \mathcal{D}_{M-K}^I(\omega) \} \\ & \quad I = K, K+1, \dots \quad (K > 0) \end{aligned} \quad (4-19)$$

(Note that  $\mathcal{R}_i^2 = \mathcal{R}_e^2 = (-1)^{2I}$ .) From the two intrinsic states  $\Phi_K$  and  $\Phi_{\bar{K}}$ , we can thus form only a single rotational state for each value of  $I$ , as a consequence of the restrictions in the rotational degrees of freedom imposed by the  $\mathcal{R}$  invariance of the deformation.

The wave function (4-19) is not of the simple product form (4-4), but involves a sum of two such terms, associated with the degenerate intrinsic states. The superposition of the two components represents an interweaving of intrinsic and rotational degrees of freedom, which gives rise to interference effects with no counterpart in a classical system. The matrix elements of an operator  $F$  between symmetrized states of the type (4-19) can be written

$$\begin{aligned} &\langle K_2 I_2 M_2 | F | K_1 I_1 M_1 \rangle \\ &= \langle K_2 I_2 M_2 | F | K_1 I_1 M_1 \rangle_{\text{unsym}} + (-1)^{I_1+K_1} \langle K_2 I_2 M_2 | F | \bar{K}_1 I_1 M_1 \rangle_{\text{unsym}} \quad (4-20) \\ & \quad (K_1 > 0, K_2 > 0) \end{aligned}$$

in terms of matrix elements for unsymmetrized states

$$(\Psi_{KIM})_{\text{unsym}} = \left( \frac{2I+1}{8\pi^2} \right)^{1/2} \Phi_K(q) \mathcal{D}_{MK}^I(\omega)$$

$$(\Psi_{KIM})_{\text{unsym}} = \left( \frac{2I+1}{8\pi^2} \right)^{1/2} \Phi_K(q) \mathcal{D}_{M-K}^I(\omega)$$
(4-21)

In deriving the result (4-20), we have used the relation

$$\mathcal{R}_i^{-1} \mathcal{R}_e F \mathcal{R}_e^{-1} \mathcal{R}_i = F \quad (4-22)$$

expressing the condition that any physical operator must transform in the same manner under the equivalent operations  $\mathcal{R}_e$  and  $\mathcal{R}_i$ .

The second term in Eq. (4-20) involves the phase factor

$$\sigma \equiv (-1)^{I+K} \quad (4-23)$$

which is referred to as the signature (following the terminology applied to Regge trajectories). The contribution of this term to the matrix element alternates in sign for successive values of  $I$  (if we assume the operator  $F$  itself to be a smooth function of orientation angles and angular momenta). The signature-dependent term in the matrix elements implies that the rotational bands with  $K \neq 0$ , in a system with axial symmetry and  $\mathcal{R}$  invariance, tend to separate into two families distinguished from each other by the quantum number  $\sigma$ .

The occurrence of two interfering terms in the matrix element (4-20) is a specific quantal effect. For matrix elements between two states in the same band, the signature-dependent term contributes if the operator  $F$  can invert the sign of  $I_3$  and thereby produce effects equivalent to a rotation  $\mathcal{R}$  of the entire system.

Rotors with  $\mathcal{R}$  symmetry were first encountered in the spectra of diatomic homonuclear molecules (see, for example, Herzberg, 1950; pp. 130ff.). For such a system, the quantum number  $r$ , for states with vanishing electronic angular momentum about the axis, can be expressed in the form  $r = r_{\text{el}} P(12)$ , where  $r_{\text{el}}$  represents the  $r$  quantum number of the electronic wave function, while  $P(12)$  represents the spatial exchange of the nuclei. The statistics for the identical nuclei implies the relation  $P(12) = (-1)^S$ , where  $S$  is the total nuclear spin. For the total rotational angular momentum  $L$ , exclusive of the nuclear spins, we therefore

obtain, from Eq. (4-14), the condition

$$(-1)^L = r_{el}(-1)^S \quad (4-24)$$

which expresses the restriction on the rotational motion associated with the statistics (Hund, 1927).

The conventional notation in molecular spectroscopy characterizes the electronic wave function as positive or negative with respect to reflection in a plane containing the molecular axis. The operation, denoted in the following by  $\mathcal{S}$  with eigenvalue  $s$ , is the product of  $\mathcal{R}$  and the parity operation  $\mathcal{P}$  (see p. 16). The electronic state of the molecule is labeled by the quantum numbers  $s_{el}(=+ \text{ or } -)$  and the parity  $\pi_{el}$ , which is referred to as  $g$  (gerade;  $\pi_{el}=+1$ ) or  $u$  (ungerade,  $\pi_{el}=-1$ ). Thus, for example, an electronic  ${}^1\Sigma_u^-$  state has  $\pi_{el}=s_{el}=-1$  and hence  $r_{el}=\pi_{el}s_{el}=+1$ ; the upper left-hand index is the electronic spin multiplicity, while the letters  $\Sigma, \Pi, \Delta, \dots$  give the component  $\Lambda$  of the electronic orbital angular momentum with respect to the symmetry axis ( $=0, 1, 2, \dots$ ).

The redundancy in the degrees of freedom associated with the  $\mathcal{R}$  invariance, as discussed in the present section, is associated with a lack of uniqueness of the variables  $(q, \omega)$  when regarded as functions of the particle coordinates  $x$ . Thus, the two sets of variables  $(q, \omega)$  and  $(q', \omega')$ , related by

$$\begin{aligned} q' &= \mathcal{R}_i^{-1} q \mathcal{R}_i \\ \omega' &= \mathcal{R}_e \omega \mathcal{R}_e^{-1} \end{aligned} \quad (4-25)$$

refer to the same  $x$ . The condition  $\mathcal{R}_i^{-1} \mathcal{R}_e = 1$ , therefore, expresses the requirement that wave functions and operators be single-valued functions of  $x$ . (The transformation to the variables  $(q, \omega)$  and the associated invariance conditions can be exhibited in a simple form in a model describing the dynamical degrees of freedom in terms of the amplitudes for quadrupole deformation; see Appendix 6B.)

The lack of uniqueness in the orientation angles considered as a function of the particle variables is connected with the fact that these angles are taken to be symmetric functions of the coordinates (and momenta) of the identical particles. Such a description is especially appropriate in the characterization of collective deformations in a system like the nucleus, where the particles move throughout the volume of the system and are, therefore, continually exchanging positions. In some situations, one can employ an alternative approach that involves a labeling of the constituent particles. Thus, for example, in a two-body system, the orientation is usually chosen as the direction from particle 1 to particle 2. This procedure is the one employed in characterizing the orientation of a molecule and leads to angle variables that are single-valued functions of the coordinates. The consequences of the identity of the particles are expressed in a different form in the two approaches. When the orientation angles are symmetric functions of the variables of the identical particles, the exchange of two such particles is an intrinsic operator, and the intrinsic states carry the appropriate permutation symmetry. When the definition of the orientation angles involves a labeling of the particles, the exchange acts also on the orientation angles, and the requirements of permutation symmetry may lead to restrictions in the rotational spectrum.

#### 4-2d $\mathcal{P}$ and $\mathcal{T}$ Symmetry

If the intrinsic Hamiltonian is invariant with respect to space reflection and time reversal, the operations  $\mathcal{P}$  and  $\mathcal{T}$  act on the intrinsic motion but do not affect the orientation angles.

Since  $\mathcal{P}$  commutes with  $J_3$ , the intrinsic states can be labeled by the parity quantum number

$$\begin{aligned}\mathcal{P}\Phi_K(q) &= \pi\Phi_K(q) \\ \pi &= \pm 1\end{aligned}\tag{4-26}$$

and all the states in the band have the parity  $\pi$ . For  $K=0$  bands, the quantum numbers  $\pi$  and  $r$  are distinct; each may, independently of the other, take the value  $+1$  or  $-1$ .

For a  $\mathcal{T}$ - and  $\mathcal{P}$ -invariant intrinsic Hamiltonian, we can choose phases for the intrinsic states such that  $\mathcal{P}\mathcal{T}=1$  (compare Eq. (1-39)). From Eq. (4-16) then follow

$$\begin{aligned}\mathcal{T}\Phi_K(q) &= \Phi_{\bar{K}}(q) \\ \mathcal{T}\Phi_{\bar{K}}(q) &= (-1)^{2K}\Phi_K(q) \\ \mathcal{T}\Phi_{K=0}(q) &= r\Phi_{K=0}(q)\end{aligned}\tag{4-27}$$

where the phase factor  $(-1)^{2K}$  is the value of  $\mathcal{T}^2$  (see Eq. (1-41)). Since time reversal does not affect  $\omega$ , the rotational wave function is transformed into its complex conjugate, and we obtain (see Eqs. (1A-38) and (4-19))

$$\begin{aligned}\mathcal{T}\Phi_K(q)\mathcal{D}_{MK}^I(\omega) &= \Phi_{\bar{K}}(q)(\mathcal{D}_{M\bar{K}}^I(\omega))^* \\ &= (-1)^{M-K}\Phi_{\bar{K}}(q)\mathcal{D}_{-M-K}^I(\omega) \\ \mathcal{T}\Psi_{KIM} &= (-1)^{I+M}\Psi_{\bar{K}I,-M}\end{aligned}\tag{4-28}$$

in accordance with the general phase rule (1-40).

The transformation under time reversal, combined with Hermitian conjugation, gives the relation

$$\begin{aligned}\langle K_2|F(q,p)|K_1\rangle &= -c\langle \bar{K}_1|F(q,p)|\bar{K}_2\rangle \\ (\mathcal{T}F\mathcal{T}^{-1})^\dagger &= -cF\end{aligned}\tag{4-29}$$

for the intrinsic matrix elements of an operator depending on the internal variables. The phase factor  $c$  characterizes the transformation of the operator  $F$  under particle-hole conjugation (see Eq. (3B-21)).

For the diagonal matrix element in a  $K=0$  band, the relation (4-29) yields

$$\langle K=0|F|K=0\rangle=0 \quad \text{for } c=+1 \quad (4-30)$$

For bands with  $K \neq 0$ , we obtain the selection rule

$$\langle K|F|\bar{K}\rangle=0 \quad \text{for } c(-1)^{2K}=+1 \quad (4-31)$$

for the signature-dependent term in the matrix element connecting two states in the same band (see Eq. (4-20)). (For an operator depending also on the rotational variables  $(\omega, I_\kappa)$ , the phase factor  $c$  to be used in the expressions above refers to the transformation of  $F$  in the space of the internal variables. Since  $\omega$  is invariant while  $I_\kappa$  changes sign under time reversal combined with Hermitian conjugation, the phase factor characterizing the transformation of the total operator equals  $+c$  or  $-c$  depending on whether the operator is even or odd with respect to the inversion  $I_\kappa \rightarrow -I_\kappa$ .)

In the following sections (Secs. 4-2e and 4-2f), we shall consider rotational spectra associated with deformations that are not invariant with respect to  $\mathcal{R}$ ,  $\mathcal{P}$ , and  $\mathcal{T}$ , while Sec. 4-2g deals with rotational motion resulting from a deformation that couples spin and isospin. The observed nuclear rotational spectra, at least in the great majority of cases, are found to have the full symmetry considered above, and some readers may therefore prefer to proceed directly to the discussion in Secs. 4-3 and 4-4.

#### 4-2e Deformations Violating $\mathcal{P}$ or $\mathcal{T}$ Symmetry

In a system governed by overall  $\mathcal{P}$  and  $\mathcal{T}$  invariance, the occurrence of a deformation that violates either of these symmetries is associated with a two-valued collective degree of freedom, corresponding to the equivalence of configurations with opposite sign of the deformation. The spectrum, therefore, acquires a doublet structure.

An example of a parity-violating deformation would be provided by a pseudoscalar component in the one-body potential and density, proportional to  $\mathbf{s} \cdot \mathbf{r}$ . (The possibility of a pseudoscalar deformation in the nuclear potential was considered by Bleuler, 1966; see also Burr *et al.*, 1969). The potential  $\mathbf{s} \cdot \mathbf{r}$  is rotationally invariant; in a nonspherical, but axially symmetric nucleus, the corresponding potential would involve two separate

terms, proportional to  $s_3x_3$  and  $s_1x_1 + s_2x_2$ , respectively. Parity-violating potentials of the type considered also violate  $\mathcal{T}$  symmetry, but conserve  $\mathcal{PT}$ . The assumption of overall conservation of  $\mathcal{P}$  as well as  $\mathcal{T}$  implies that deformations of either sign have the same energy, and all the states of the system therefore occur in two modifications  $\Psi_+$  and  $\Psi_- = \mathcal{P}\Psi_+$ . The two sets of states can be combined to form eigenstates of  $\mathcal{P}$ ,

$$\Psi_\pi = 2^{-1/2} \begin{cases} (\Psi_+ + \Psi_-) & \pi = +1 \\ i(\Psi_+ - \Psi_-) & \pi = -1 \end{cases} \quad (4-32)$$

(We have assumed the phases of the states  $\Psi_\pm$  to be chosen in such a manner that these states have the eigenvalue  $+1$  for the operator  $\mathcal{R}\mathcal{P}\mathcal{T}$ ; the states (4-32) then have the standard phasing,  $\mathcal{R}\mathcal{T}=1$ .) Hence, the spectrum consists of parity doublets. The doublets are connected by  $\lambda\pi=0$ —transitions of collective character, with matrix elements proportional to the pseudoscalar deformation.

The configurations with opposite sign of the deformation are separated by a potential barrier, but in a quantal system, an inversion of the deformation can take place by a “tunneling” motion. The frequency  $\omega_t$  of this inversion gives the energy separation,  $\Delta E = \hbar\omega_t$ , between the parity doublets. The treatment of the tunneling effect requires a combination of the conjugate intrinsic Hamiltonians to form a  $\mathcal{P}$ - and  $\mathcal{T}$ -conserving Hamiltonian that includes the degree of freedom associated with the tunneling motion. In this manner, the collective degree of freedom associated with the doublet structure appears as a limiting feature of the vibrational spectrum, for a potential function with two minima separated by a barrier. The eigenstates are given by Eq. (4-32), in the approximation in which the overlap of the states  $\Psi_+$  and  $\Psi_-$  can be neglected.

Similar considerations apply to deformations that violate other combinations of  $\mathcal{P}$  and  $\mathcal{T}$ . Thus, a one-body potential proportional to  $\mathbf{s} \cdot \mathbf{p}$  violates  $\mathcal{P}$ , but not  $\mathcal{T}$ , and gives rise to parity doublets, as in the case considered above. An example of a  $\mathcal{T}$ -, but not  $\mathcal{P}$ -violating deformation is provided by a potential proportional to  $\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}$ ; such a deformation leads to a spectrum consisting of doublets having the same quantum numbers  $I\pi$ .

#### 4-2f Combinations of Rotation and Reflection Symmetries

If a  $\mathcal{P}$ - or  $\mathcal{T}$ -violating deformation occurs in a nonspherical system, one obtains a doubling of all the states in the rotational band, as discussed in Sec. 4-2e. A connection between rotational motion and the degrees of



freedom associated with  $\mathcal{P}$ - and  $\mathcal{T}$ -violating deformations occurs if the system, while violating  $\mathcal{R}$  symmetry, is invariant with respect to a combination of  $\mathcal{R}$  with  $\mathcal{P}$  or  $\mathcal{T}$  symmetry.

### $\mathcal{S}$ invariance

An example is provided by an axially symmetric shape deformation containing components of odd multipole order. Such a deformation violates  $\mathcal{R}$  and  $\mathcal{P}$  symmetry, but conserves  $\mathcal{R}\mathcal{P}$ , as can be seen from the fact that this combined operation represents a reflection in a plane containing the symmetry axis. (Diatomic molecules with nuclei of different charge have deformations of this type; the possible occurrence of nuclei with stable deformations containing octupole components is discussed on p. 561.)

The invariance with respect to a reflection in a plane containing the symmetry axis is conveniently expressed in terms of the operation

$$\mathcal{S} = \mathcal{P}\mathcal{R}^{-1} \quad (4-33)$$

Such an invariance of the deformation implies that  $\mathcal{S}$  is an intrinsic variable. The parity

$$\mathcal{P} = \mathcal{S}\mathcal{R} \quad (4-34)$$

is therefore an operator that acts on the intrinsic variables through  $\mathcal{S} (= \mathcal{S}_i)$  and on the rotational variables through  $\mathcal{R} (= \mathcal{R}_e)$ .

The intrinsic states with  $K=0$  are eigenstates of  $\mathcal{S}_i$  and  $\mathcal{T}$  (assuming the intrinsic Hamiltonian to be invariant under  $\mathcal{T}$ , as in the case of shape deformations),

$$\begin{aligned} \mathcal{S}_i \Phi_{s,K=0}(q) &= s \Phi_{s,K=0}(q) \\ \mathcal{S}_i \mathcal{T} \Phi_{s,K=0}(q) &= \Phi_{s,K=0}(q) \end{aligned} \quad (4-35)$$

The last relation determines the phase of  $\Phi$ . The effect of  $\mathcal{R}_e$  on the rotational wave function is given by Eq. (4-13), and the relation (4-34) therefore yields

$$\pi = s(-1)^I \quad (4-36)$$

Hence, the band contains the states

$$\begin{aligned} \Psi_{s,K=0,IM} &= (2\pi)^{-1/2} \Phi_{s,K=0}(q) Y_{IM}(\theta, \phi) \begin{cases} 1 & \pi = +1 \\ i & \pi = -1 \end{cases} \\ I\pi &= 0+, 1-, 2+, \dots & s = +1 \\ I\pi &= 0-, 1+, 2-, \dots & s = -1 \end{aligned} \quad (4-37)$$

The factor  $i$  for  $\pi = -1$  ensures the standard transformation (4-28) under time reversal.

For  $K \neq 0$ , the intrinsic states are twofold degenerate, as a consequence of  $\mathcal{S}$  (or  $\mathcal{T}$ ) symmetry. We can choose the phases of the intrinsic states such that (compare Eqs. (4-16) and (4-27))

$$\begin{aligned}\Phi_K(q) &= \mathcal{S}_i \Phi_K \\ &= \mathcal{T} \Phi_K\end{aligned}\quad (K > 0) \quad (4-38)$$

The relation (4-34) implies that the total nuclear states of definite parity involve the following combinations of  $\Phi_K$  and  $\Phi_{\bar{K}}$ :

$$\begin{aligned}\Psi_{\pi KIM} &= \left( \frac{2I+1}{16\pi^2} \right)^{1/2} e^{i\alpha} (1 + \pi \mathcal{S}_i \mathcal{R}_e) \Phi_K \mathcal{D}_{MK}^I \\ &= \left( \frac{2I+1}{16\pi^2} \right)^{1/2} \begin{cases} \Phi_K \mathcal{D}_{MK}^I + (-1)^{I+K} \Phi_{\bar{K}} \mathcal{D}_{M-K}^I & \pi = +1 \\ i(\Phi_K \mathcal{D}_{MK}^I - (-1)^{I+K} \Phi_{\bar{K}} \mathcal{D}_{M-K}^I) & \pi = -1 \end{cases} \quad (4-39)\end{aligned}$$

The phase  $\alpha$  is chosen, in the last form of Eq. (4-39), so as to ensure the standard transformation under time reversal. (The wave functions (4-39) contain, as a special case, the helicity representation of the one-particle wave functions; the phase factor  $i$  corresponds to the phase  $i'$  in Eq. (3A-5).)

The violation of  $\mathcal{R}$  and  $\mathcal{P}$  implies that there is no constraint on the rotational or parity degrees of freedom, separately. For each intrinsic state, the band contains states with all values of  $I \geq |K|$ , and both parity values occur. However, the  $\mathcal{S}$  invariance implies a link between rotation and parity, which selects the set of states (4-37) and (4-39).

The spectrum associated with an  $\mathcal{R}\mathcal{P}$ -invariant but  $\mathcal{R}$ - and  $\mathcal{P}$ -violating deformation exhibits characteristic differences from that associated with a  $\mathcal{P}$ -violating, but  $\mathcal{R}$ -conserving, deformation. As mentioned earlier, a deformation of the latter type gives a parity doubling of all states and thus, for  $K=0$ , the rotational spectrum contains the states  $I\pi=0\pm, 2\pm, \dots$ , or  $I\pi=1\pm, 3\pm, \dots$ , depending on the value of  $r$ . Moreover, for  $K \neq 0$ , the signature-dependent terms (see Eq. (4-20)) are the same for the parity doublets, since the intrinsic states  $\Phi_K$  and  $\Phi_{\bar{K}}$  are of the type (4-32). In contrast, for the  $\mathcal{R}\mathcal{P}$ -invariant deformation, the signature-dependent terms have opposite sign for the two states (4-39) and, hence, contribute to the energy splitting of the parity doublets. (Such a splitting is

similar to the  $\Lambda$ -type doubling in molecular spectra; see, for example, Herzberg, 1950, pp. 226ff.).

A further separation between the parity doublets arises from a tunneling motion, similar to that discussed on p. 15 for a  $\mathcal{P}$ -violating deformation. For the  $\mathcal{R}\mathcal{P}$ -invariant system, the tunneling leads to an inversion of the symmetry axis through continuous variations of the shape, for fixed orientation. This effect gives rise to an energy shift  $\Delta E = \hbar\omega_t$  of the negative parity states relative to the positive parity states, which in first approximation is independent of  $I$ . The tunneling may be treated in terms of an extended,  $\mathcal{R}$ - and  $\mathcal{P}$ -invariant, intrinsic Hamiltonian, which includes the degree of freedom associated with the barrier penetration. The eigenstates of the extended intrinsic Hamiltonian consist of doublets with opposite parity, separated by the energy  $\hbar\omega_t$ . The total wave functions are given by the expressions (4-15) and (4-19), which reduce to the forms (4-37) and (4-39) if the intrinsic states are represented by symmetric and antisymmetric combinations of states referring to the two opposite directions of the  $\mathcal{R}$ - and  $\mathcal{P}$ -violating deformation (see Eq. (4-32)).






















A corresponding tunneling, or inversion, effect plays an important role in the analysis of the spectra of polyatomic molecules (see, for example, Herzberg, 1945, p. 33 and pp. 220ff.). In a simple molecule, like  $\text{NH}_3$ , the tunneling frequency in the ground state is of the order of  $10^{10} \text{ sec}^{-1}$ , which is a factor  $10^3$  smaller than the frequency of vibrations in the tunneling direction and an order of magnitude smaller than the lowest rotational frequency. The inversion frequency decreases rapidly with the mass of the atoms involved and the complexity of the configurations. For most of the organic molecules with left-right asymmetry, the lifetime for transitions between the "isomers" exceeds the time scale of biological evolution.

### *Survey of symmetries*

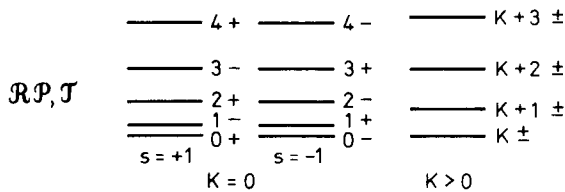
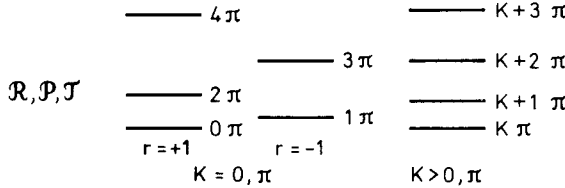
The considerations in the present and previous sections illustrate the general rules that govern the relationship between the collective degrees of freedom and the invariance of the deformation with respect to rotations and reflections. For an axially symmetric system, the invariance group of the intrinsic Hamiltonian is the product of rotations about the symmetry axis and the group  $G$  of discrete operations under which the deformation is invariant. The group may comprise up to eight elements formed out of combinations of  $\mathcal{R}$ ,  $\mathcal{P}$ , and  $\mathcal{T}$ . In the case of maximum symmetry violation, for which  $G$  contains only the identity, the intrinsic states, which can be labeled by  $K=I_3$ , are nondegenerate, and the rotational spectrum has two states for each  $I\pi$  with  $I \geq |K|$  (that is  $I\pi = (|K| \pm)^2, (|K| + 1, \pm)^2, \dots$ ). The invariance of the deformation reduces the number of states in the rotational spectrum by a factor equal to the number of elements in the group  $G$ . The two parity values occur with equal weight, except when  $G$  contains the element  $\mathcal{P}$ , in which case the entire collective spectrum has the same parity as the intrinsic state. If  $G$  includes an operation that inverts  $I_3$ , ( $\mathcal{R}$ ,  $\mathcal{T}$ ,  $\mathcal{R}\mathcal{P}$ , or  $\mathcal{P}\mathcal{T}$ ),

the intrinsic states are twofold degenerate (for  $K \neq 0$ ), and the rotational states are formed by a combination of the conjugate intrinsic states.

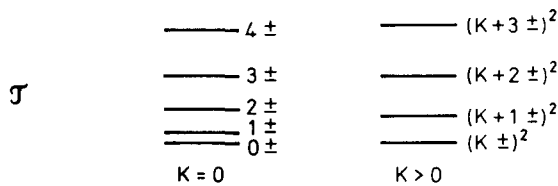
Examples of symmetry combinations are illustrated in Fig. 4-2a. In the first case, the intrinsic Hamiltonian is assumed to be invariant under  $\mathcal{R}$ ,  $\mathcal{P}$ , and  $\mathcal{T}$ ; for

Symmetry of $H_{\text{intr}}$	$K = 0$	$K$	$K \neq 0$	$\bar{K}$
$\mathcal{R}, \mathcal{P}, \mathcal{T}$	 $1, \mathcal{R}, \mathcal{P}, \mathcal{T}$	 $1, \mathcal{P}, \mathcal{R}, \mathcal{T}$	 $\mathcal{R}, \mathcal{T}$	
$\mathcal{R}, \mathcal{P}, \mathcal{T}$	  $1, \mathcal{R}, \mathcal{P}, \mathcal{T}$ $\mathcal{R}, \mathcal{P}$	  $1, \mathcal{R}, \mathcal{P}, \mathcal{T}$ $\mathcal{P}, \mathcal{R}, \mathcal{T}$	  $\mathcal{R}, \mathcal{P}, \mathcal{T}$ $\mathcal{R}, \mathcal{P}, \mathcal{T}$	
$\mathcal{T}$	    $1, \mathcal{T}$ $\mathcal{R}, \mathcal{P}$ $\mathcal{R}$ $\mathcal{P}$	    $1$ $\mathcal{R}, \mathcal{P}, \mathcal{T}$ $\mathcal{P}$ $\mathcal{R}, \mathcal{T}$	    $\mathcal{T}$ $\mathcal{R}, \mathcal{P}$ $\mathcal{P}, \mathcal{T}$ $\mathcal{R}$	

(a)



(b)



**Figure 4-2** Rotational spectra for axially symmetric systems with different combinations of  $\mathcal{R}$ ,  $\mathcal{P}$ , and  $\mathcal{T}$  invariance. The intrinsic states are illustrated in Fig. 4-2a and the associated rotational spectra in Fig. 4-2b; the quantum numbers  $I\pi$  are given to the right of the energy levels.

$K \neq 0$ , the intrinsic state is invariant under  $\mathcal{R}\mathcal{T}$  and  $\mathcal{P}$  and transforms into the degenerate state with opposite  $J_3$  under  $\mathcal{R}$  and  $\mathcal{T}$ . In the second case, the  $\mathcal{R}$  symmetry is violated, but  $H_{\text{int}}$  is assumed to be invariant under  $\mathcal{T}$  and  $\mathcal{R}\mathcal{P}$  (or  $\mathcal{I}$ ); under  $\mathcal{R}$  or  $\mathcal{P}$  separately, the states transform into eigenstates of a new equivalent Hamiltonian  $\mathcal{R}^{-1}H_{\text{int}}\mathcal{R}$ , as indicated by the dotted figures. In the third case, only  $\mathcal{T}$  but neither  $\mathcal{R}$ ,  $\mathcal{R}\mathcal{P}$ , nor  $\mathcal{P}$  is a symmetry of  $H_{\text{int}}$ . The  $\mathcal{R}\mathcal{P}$  symmetry is broken by a potential, such as  $s_3 p_3$ , symbolized by a sign ( $\pm$ ) which changes under  $\mathcal{R}\mathcal{P}$  and  $\mathcal{P}$ , but not under  $\mathcal{T}$ . The multiplicity of states in the rotational spectrum is illustrated in Fig. 4-2b for the various combinations of symmetries considered in Fig. 4-2a.

### 4-2g Rotational Motion in Isospace

The deformations considered in the previous sections refer to anisotropies in ordinary three-dimensional space. Deformations of a generalized type may occur in the dimensions associated with the specific quantal degrees of freedom such as particle number and isospin. These deformations give rise to families of states with relations similar to those involved in rotational bands.

Deformations violating particle-number conservation are characteristic of superfluid systems and lead to collective families of states with different values of the particle number. The occurrence of such spectra in superfluid nuclei ("pair rotations") will be considered in Sec. 6-3f. As an example of a deformation in isospace, we consider, in the small print below, the strong coupling model of the pion-nucleon system (Wentzel, 1940; Oppenheimer and Schwinger, 1941; Pauli and Dancoff, 1942; see also Henley and Thirring, 1962).

A rather strong interaction between the nucleon and the pseudoscalar meson field is associated with processes by which p-wave mesons are created and absorbed through the coupling to the nucleon spin  $\mathbf{s}$ . For a neutral (isoscalar) meson field, the p-wave components of given frequency  $\omega$  can be represented by a vector  $\mathbf{q}(\omega)$ , the Cartesian components of which are associated with oscillations of the meson field in the directions of the coordinate axes. (The spherical components  $q_\mu$  are associated with the creation of mesons with angular momentum component  $\mu$  and the annihilation of mesons in the time-reversed state.) For a free field, each component  $q_i(\omega)$  with  $i = 1, 2, 3$  is equivalent to a harmonic oscillator of frequency  $\omega$ . The coupling to the nucleon spin is proportional to the scalar product  $\mathbf{s} \cdot \mathbf{q}$ ,

$$H_c = \sum_{i=1}^3 s_i \int q_i(\omega) F(\omega) d\omega \quad (4-40)$$

where the strength and form factor of the coupling are expressed by the function  $F(\omega)$ . The coupling (4-40) provides a force driving the meson field oscillators from

their equilibrium position  $q_i=0$ . A coupling of sufficient strength may lead to a static deformation that is large compared with the zero-point oscillations. The deformation of the p-wave field has the character of a vector and therefore possesses axial symmetry (about the direction of this vector). In the intrinsic system, the nucleon spin is in a state of  $m'_s=1/2$  (with suitable choice of direction along the symmetry axis), and only meson field components with  $\mu'=0$  are affected. Hence, the intrinsic state has  $K\pi=1/2+$ . The deformation is  $\mathcal{RT}$  invariant (but violates  $\mathcal{R}$  and  $\mathcal{T}$  separately), and the rotational spectrum contains the states  $I\pi=1/2+, 3/2+, \dots$  (see p. 18).

For the isovector pion field, each component  $\mathbf{q}_i(\omega)$  is a vector in isospace, and the coupling takes the form

$$H_c = \sum_{i,j=1}^3 s_i t_j \int q_{ij} F(\omega) d\omega \quad (4-41)$$

where  $t$  is the isospin of the nucleon. This coupling can produce a deformation in each of the two spaces similar to that associated with the coupling to the neutral field. However, the state of lowest energy involves a correlation in the two spaces such that the deformation is invariant with respect to rotations performed simultaneously in both spaces, with the same angle and about the same intrinsic axis  $\kappa (=1, 2, 3)$ . This invariance implies that the intrinsic state is an eigenstate with eigenvalue 0 of the composite spin-isospin operator  $\mathbf{u}=\mathbf{s}+\mathbf{t}$ , defined in the intrinsic coordinate system. In such a state,  $t_\kappa = -s_\kappa$ , and hence, for each value of  $\kappa$ , the deformation  $q_{\kappa\kappa}$  is as large as the  $q_{33}$  deformation in the uncorrelated state  $m'_s=1/2, m'_t=1/2$ ; the correlation therefore gives an increase in the binding energy by a factor of three. (It is readily shown that the  $u=0$  state gives maximal binding; to this purpose, it is convenient to note that, by suitable (different) rotations in spin and isospace, it is possible to bring the coupling (4-41) to diagonal form involving only intrinsic components  $q_{\kappa\kappa'}$ , with  $\kappa'=\kappa$ . A deformation of similar symmetry is encountered in the description of superfluidity resulting from correlated pairs in  $^3P$  states ( $L=1, S=1$ ); Balian and Werthamer, 1963.) The intrinsic state with  $u=0$  does not possess axial symmetry in either of the two spaces, but is invariant with respect to arbitrary rotations performed simultaneously about any of the intrinsic axes  $\kappa$  in the two spaces. The rotational states therefore satisfy the condition  $I_\kappa + T_\kappa = 0$  for  $\kappa=1, 2, 3$ , and the spectrum consists of the series of states

$$\Psi_{IMTM_T} = \Phi_{\text{intr}} \frac{(2I+1)^{1/2}}{8\pi^2} \sum_K (-1)^{I-K} \mathcal{D}_{MK}^I(\omega) \mathcal{D}_{M_T-K}^{T=I}(\omega_T) \quad (4-42)$$

$$I = T = \frac{1}{2}, \frac{3}{2}, \dots$$

where  $\omega$  and  $\omega_T$  represent the orientations in space and isospace, respectively.

It is possible that the  $I=3/2, T=3/2$  nucleon isobar with a mass of 1236 MeV (see Fig. 1-11, Vol. I, p. 57) may correspond to the first excited state of such a generalized rotational band. This interpretation would imply relations between the properties of the nucleon and the isobar state similar to the intensity relations in nuclear rotational spectra (see Sec. 4-3), but there appears so far to be no test of

these relations. However, the rather large excitation energies, which exceed the pion rest mass, may indicate that the coupling is not sufficiently strong for a quantitative treatment in terms of a static deformation. (For a discussion of the effective coupling strength, see Henley and Thirring, 1962, pp. 192 ff.) There is at present no evidence for the existence of higher members of the sequence (4-42), with  $I = T > 5/2$ . In contrast to the  $I = T = 1/2$  and  $3/2$  members, the higher states cannot be constructed from a configuration of three quarks, each of which has spin and isospin  $1/2$  (see, for example, Vol. I, p. 41), and this circumstance might imply a discontinuity in the rotational band of a type similar to that encountered in the rotational spectra of light nuclei (see, for example, the discussion of  $^8\text{Be}$ , pp. 101 ff.).

The experimental evidence concerning the excitation spectrum of the nucleon may suggest additional rotational relationships (see the trajectories of baryon states with fixed  $T$  in Fig. 1-13, Vol. I, p. 65). Several different bands based on a given intrinsic state are possible if a corresponding number of different deformations are present.

### 4-3 ENERGY SPECTRA AND INTENSITY RELATIONS FOR AXIALLY SYMMETRIC NUCLEI

The intimate connection between states in a rotational band is reflected in the relations between the matrix elements involving different members of a given band. The separation between rotational and intrinsic motion implies that, in first approximation, the matrix elements of the various operators can be expressed in terms of products of intrinsic and rotational factors. The intrinsic factor is the same for all the members of a band, and the rotational factor gives the dependence of the total matrix element on the rotational quantum numbers. For systems with axial symmetry, the rotational wave function is completely specified by the quantum numbers  $IKM$  (see Sec. 4-2a), and the dependence of the matrix elements on the rotational quantum numbers follows from the tensorial structure of the operators (Alaga *et al.*, 1955; Bohr, Fröman, and Mottelson, 1955; Satchler, 1955; Helmers, 1960). The relations are similar to the intensity rules that govern the radiative transitions in molecular band spectra (Hönl and London, 1925).

Departures from the leading-order intensity rules arise from the Coriolis and centrifugal forces acting in the rotating body-fixed system. These effects can be analyzed in terms of a coupling between rotational and intrinsic motion giving rise to a mixing of bands, as discussed in Sec. 4-4. Alternatively, the higher-order effects can be described in terms of re-normalized, effective operators acting in the unperturbed basis; in such an approach, which provides a convenient basis for a phenomenological de-

scription, the coupling effects are represented by the dependence of the renormalized operators on the rotational angular momentum. For sufficiently small rotational frequencies, the Coriolis effects can be treated by perturbation theory, and the operators can be expanded in a power series of the rotational angular momentum. For axially symmetric systems, as discussed in the present section, the general form of such an expansion is greatly restricted by the symmetry of the rotational motion and the tensorial structure of the operators (Bohr and Mottelson, 1963). The particle-rotor model treated in Appendix 4A provides a simple explicit example illustrating many of these general relationships.

The renormalization of the operators associated with the rotational coupling effects may be expressed in terms of a canonical transformation that diagonalizes the Hamiltonian in the representation of the uncoupled motion. This transformation may also be viewed as a transformation to new intrinsic and rotational variables, in terms of which the perturbed wave functions retain the form (4-19). The explicit construction of the transformation is considered in Appendix 4A for the model consisting of a particle coupled to the motion of a rigid rotor.

### 4-3a Rotational Energies

For a slowly rotating system, the energy is given, to first approximation, by the intrinsic energy  $E_K$  associated with the state  $\Phi_K(q)$ , and is therefore the same for all the members of the band. The superimposed rotational motion gives an additional energy depending on the rotational angular momentum. Since the energy is a scalar with respect to rotations of the coordinate system, the effective Hamiltonian can only involve the components  $I_k$  of the angular momentum with respect to the intrinsic axes.

#### *Energy expansion for bands with $K=0$*

For bands with vanishing intrinsic angular momentum  $K$ , the rotational energy has an especially simple form. Such bands involve only a single intrinsic state  $\Phi_{K=0}$  (see Eq. (4-15)); the part of the energy operator acting in  $K=0$  bands is therefore diagonal with respect to  $I_3$  and can only depend on the combination  $I_1^2 + I_2^2$ .

To leading order, the rotational Hamiltonian is of the form

$$(H_{\text{rot}})_{K=0} = h_0(q, p)(I_1^2 + I_2^2) \quad (4-43)$$

where  $h_0(q, p)$  is a function of the intrinsic variables. The expectation value