

CHAPTER **4**

Rotational Spectra

4-1 OCCURRENCE OF COLLECTIVE ROTATIONAL MOTION IN QUANTAL SYSTEMS¹

A common feature of systems that have rotational spectra is the existence of a "deformation", by which is implied a feature of anisotropy that makes it possible to specify an orientation of the system as a whole. In a molecule, as in a solid body, the deformation reflects the highly anisotropic mass distribution, as viewed from the intrinsic coordinate frame defined by the equilibrium positions of the nuclei. In the nucleus, the rotational degrees of freedom are associated with the deformations in the nuclear equilibrium shape that result from the shell structure. (Evidence for these deformations will be discussed on pp. 133 ff. ($E2$ moments) and in Chapter 5 (deformed single-particle potential).) Rotational-like sequences are also observed in the hadron spectra and are referred to as Regge trajectories (see, for example, Fig. 1-13, Vol. I, p. 65), but the nature of the deformations involved has not yet been identified.

Collective motion having a structure similar to the rotations in space may occur in other dimensions, including isospace and particle-number space, if the system possesses a deformation that defines an orientation in these spaces. The rotational bands then involve sequences of states differing in the associated angular-momentum-like quantum numbers, such as isospin and nucleon number. (Such sequences occur in superfluid systems (see pp. 393 ff.) and may also occur as excitations of the nucleon (see pp. 20 ff.).)

The deformation may be invariant with respect to a subgroup of rotations of the coordinate system, as for example in the case of axially

¹Spectra associated with quantized rotational motion were first recognized in the absorption of infrared light by molecules (Bjerrum, 1912). The possible occurrence of rotational motion in nuclei became an issue in connection with the early attempts to interpret the evidence on nuclear excitation spectra (see, for example, Teller and Wheeler, 1938). The available data, as obtained, for example, from the fine structure of α decay, appeared to provide evidence against the occurrence of low-lying rotational excitations, but the discussion was hampered by the expectation that rotational motion would either be a property of all nuclei or be generally excluded, as in atoms, and by the assumption that the moment of inertia would have the classical value, as for rigid rotation. The establishment of the rotational mode in nuclei followed the recognition that such a mode was a necessary consequence of the existence of strongly deformed equilibrium shapes (Bohr, 1951); the occurrence of such deformations had been inferred at an early stage (Casimir, 1936) from the determination of nuclear quadrupole moments on the basis of atomic hyperfine structure. The analysis of $E2$ transitions gave additional evidence for collective effects associated with deformations in the nuclear shape (Goldhaber and Sunyar, 1951; Bohr and Mottelson, 1953a). The identification of rotational excitations came from the observation of level sequences proportional to $I(I+1)$ (Bohr and Mottelson, 1953b; Asaro and Perlman, 1953) and was confirmed by the evidence of the rotational intensity relations (Alaga *et al.*, 1955). The development of the Coulomb excitation process provided a powerful tool for the systematic study of the rotational spectra (Huus and Zupančič, 1953; see also the review by Alder *et al.*, 1956).

symmetric deformations. In such a situation, the deformation only partially defines the orientation of the intrinsic coordinate system, and the rotational degrees of freedom are correspondingly restricted. A first step in the analysis of the rotational spectra is therefore an analysis of the symmetry of the deformation and the resulting rotational degrees of freedom. This topic will be discussed in Sec. 4-2 for the case of axially symmetric systems, which are of special significance for nuclear spectra; systems without axial symmetry will be considered in Sec. 4-5. (The consequences of symmetry in the deformation represent a generalization of the well-known restriction of molecular rotational states imposed by identity of nuclei; see pp. 11 and 180.)

The occurrence of rotational degrees of freedom may thus be said to originate in a breaking of rotational invariance. In a similar manner, the translational degrees of freedom are based upon the existence of a localized structure. However, while the different states of translational motion of a given object are related by Lorentz invariance, there is no similar invariance applying to rotating coordinate frames. The Coriolis and centrifugal forces that act in such coordinate frames perturb the structure of a rotating object.

In a quantal system, the frequency of even the lowest rotational excitations may be so large that the Coriolis and centrifugal forces affect the structure in a major way. The condition that these perturbations be small (adiabatic condition) is intimately connected with the condition that the zero-point fluctuations in the deformation parameters be small compared with the equilibrium values of these parameters, and the adiabatic condition provides an alternative way of expressing the criterion for the occurrence of rotational spectra (Born and Oppenheimer, 1927; Casimir, 1931).

A simple illustration of this equivalence is provided by a system consisting of two particles bound together by a potential possessing a minimum for separation R (the equilibrium separation). The motion of the system can be described in terms of rotation and radial vibrations. The frequency of the rotational motion, for the lowest states, is

$$\omega_{\text{rot}} \sim \frac{\hbar}{M_0 R^2} \quad (4-1)$$

where M_0 is the reduced mass. The frequency of the vibrational motion depends on the amplitude ΔR of zero-point vibration

$$\omega_{\text{vib}} \sim \frac{\hbar}{M_0 (\Delta R)^2} \quad (4-2)$$

The condition that the fluctuations in shape be small compared with the average deformation, $\Delta R \ll R$, is therefore equivalent to the adiabatic condition $\omega_{\text{rot}} \ll \omega_{\text{vib}}$. This simple system illustrates the manner in which the rotational modes emerge as a low-frequency branch in the vibrational spectrum, in a situation where the vibrational potential energy possesses a minimum for an anisotropic shape.

The relationship between members of a rotational band manifests itself in the regularities of the energy spectra and in the intensity rules governing the transitions to different members of a band. For sufficiently small values of the rotational angular momentum, the analysis can be based on an expansion of energies and transition amplitudes in powers of the rotational frequency or angular momentum. These expressions acquire a special simplicity for systems with axially symmetric shape and in this form are found to provide a basis for the interpretation of an extensive body of data on nuclear spectra (Sec. 4-3).

The dependence of matrix elements on the rotational angular momentum reflects the response of the intrinsic motion to the Coriolis and centrifugal forces and can be analyzed in terms of the coupling between rotational bands based on different intrinsic structures, as discussed in Sec. 4-4 (see also pp. 111 ff. and pp. 130 ff.). For large values of the angular momentum, the rotational perturbations may strongly modify the intrinsic structure of the system. The structure of nuclear matter under these extreme conditions is a matter of considerable current interest (see pp. 41 ff.).

The discussion of rotational bands in the present chapter is based on the geometry of the deformed intrinsic structure. The states in a rotational band can also be characterized in terms of representations of symmetry groups; the group structure then expresses the symmetry of the rotating object. The bands described by representations of compact groups terminate after a finite number of states; thus, the U_3 symmetry group applying to particle motion in a harmonic oscillator potential has been exploited to illuminate features of nuclear rotational spectra associated with the finiteness of the number of nucleons that contribute to the anisotropy (Elliott, 1958; see also the discussion on pp. 93 ff.). Bands continuing to indefinitely large values of the angular momentum can be associated with representations of noncompact symmetry groups (see the discussion in Chapter 6, p. 411).

4-2 SYMMETRIES OF DEFORMATION. ROTATIONAL DEGREES OF FREEDOM

A separation of the motion into intrinsic and rotational components corresponds to a Hamiltonian of the form

$$H = H_{\text{intr}}(q, p) + H_{\text{rot}, \alpha}(P_{\omega}) \quad (4-3)$$

The intrinsic motion is described by the coordinates q and conjugate momenta p , which are measured relative to the body-fixed coordinate frame and are therefore scalars with respect to rotations of the external coordinate system. The orientation of the body-fixed frame, defined by the deformation of the system (see p. 1), is specified by angular variables denoted by ω . The rotational Hamiltonian does not depend on the orientation ω (if no external forces act on the system) and is a function of the conjugate angular momenta P_ω . The labeling of the rotational Hamiltonian in Eq. (4-3) indicates that the rotational motion may depend on the quantum numbers α specifying the intrinsic state.

The eigenstates of the Hamiltonian (4-3) are of the product form

$$\Psi_{\alpha,I} = \Phi_\alpha(q) \varphi_{\alpha,I}(\omega) \quad (4-4)$$

For each intrinsic state α , the spectrum involves a sequence of rotational levels, specified by a set of angular momentum quantum numbers denoted by I in Eq. (4-4).

The discussion of the consequence of symmetry in the present section is independent of the explicit relationship between the set of variables q, p, ω, P_ω , in which the Hamiltonian approximately separates, and the variables describing the position, momenta, and spins of the individual particles. This relationship is connected with the microscopic analysis of the collective rotational mode and is implicit in the treatment of this mode in terms of the intrinsic excitations, as discussed in Sec. 6-5h (see also p. 210).

4-2a Degrees of Freedom Associated with Spatial Rotations

Rotational motion in two dimensions (rotation about a fixed axis) has a very simple structure. The orientation is characterized by the azimuthal angle ϕ , and the state of motion by the eigenvalue M of the conjugate angular momentum. The associated rotational wave function is

$$\varphi_M(\phi) = (2\pi)^{-1/2} \exp \{ iM\phi \} \quad (4-5)$$

The orientation of a body in three-dimensional space involves three angular variables, such as the Euler angles, $\omega = \phi, \theta, \psi$ (see Fig. 1A-1, Vol. I, p. 76), and three quantum numbers are needed in order to specify the state of motion. The total angular momentum I and its component $M = I_z$ on a space-fixed axis provide two of these quantum numbers; the third may be obtained by considering the components of \mathbf{I} with respect to an intrinsic (or body-fixed) coordinate system with orientation ω (see Sec. 1A-6a). The

intrinsic components $I_{1,2,3}$ commute with the external components $I_{x,y,z}$, because $I_{1,2,3}$ are independent of the orientation of the external system (are scalars). The commutation rules of the intrinsic components among themselves are similar to those of $I_{x,y,z}$, but involve an opposite sign (see Eq. (1A-91)). As a commuting set of angular momentum variables, we may thus choose I^2 , I_z , and I_3 . The eigenvalues of I_3 are denoted by K (see Fig. 4-1), and have the same range of values as does M ,

$$K = I, I-1, \dots, -I \quad (4-6)$$

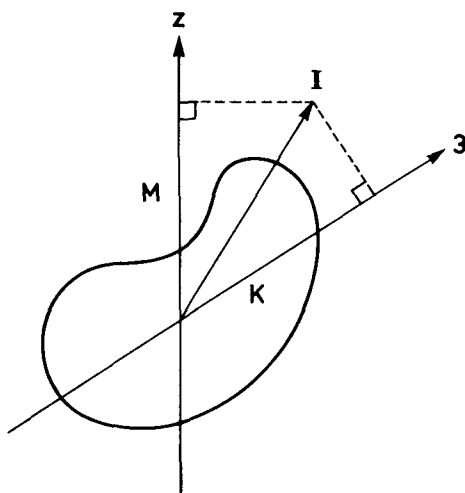


Figure 4-1 Angular momentum quantum numbers describing rotational motion in three dimensions. The z axis belongs to a coordinate system fixed in the laboratory, while the 3 axis is part of a body-fixed coordinate system (compare the \mathcal{X} and \mathcal{X}' systems defined in Fig. 1A-1, Vol. I, p. 76).

For specified values of the three quantum numbers I , K , and M , the rotational wave function is given by (see Eq. (1A-97))

$$\varphi_{IKM}(\omega) = \left(\frac{2I+1}{8\pi^2} \right)^{1/2} \mathcal{D}_{MK}^I(\omega) \quad (4-7)$$

where the functions \mathcal{D}_{MK}^I are the rotation matrices. The result (4-7) can be obtained by a transformation from the fixed coordinate system to a rotated system coinciding with the intrinsic frame (see Vol. I, p. 89). For $K=0$, the

\mathcal{D} functions reduce to spherical harmonics (see Eq. (1A-42))

$$\varphi_{I,K=0,M}(\omega) = (2\pi)^{-1/2} Y_{IM}(\theta, \phi) \quad (4-8)$$

The wave function (4-8) is independent of ψ , but normalized, as in Eq. (4-7), with respect to integration over all three Euler angles.

For $K=0$, the rotational wave function is the same as for the angular motion of a point particle with no spin. For finite K , the rotational motion corresponds to the angular motion of a particle with helicity $h=K$ (see Eq. (3A-5)).

While I^2 and I_z are constants of the motion for any rotationally invariant Hamiltonian, the commutator of I_3 with the Hamiltonian depends on intrinsic properties of the system. In general, therefore, the stationary states involve a superposition of components with different values of K ,

$$\varphi_{\tau IM}(\omega) = \left(\frac{2I+1}{8\pi^2} \right)^{1/2} \sum_K c_{\tau I}(K) \mathcal{D}_{MK}^I(\omega) \quad (4-9)$$

The third rotational quantum number is denoted by τ , and the amplitudes $c_{\tau I}(K)$ depend on the relative magnitude of the moments of inertia, as will be discussed in Sec. 4-5.

4-2b Consequences of Axial Symmetry

If the system possesses axial symmetry, two consequences ensue:

- (a) The projection I_3 on the symmetry axis is a constant of the motion.
- (b) There are no collective rotations about the symmetry axis.

The first implication is well known from classical mechanics and expresses the invariance of the Hamiltonian with respect to rotations about the symmetry axis. More generally, I_3 is a constant of the motion if the 3 axis is a symmetry axis for the tensor of inertia.

Implication (b) is a feature of the quantal description expressing the impossibility of distinguishing orientations of the intrinsic frame that differ only by a rotation about the symmetry axis. This consequence of the axial symmetry is similar to the absence of collective rotations for a spherical system. It follows that the quantum number K represents the angular momentum of the intrinsic motion and has a fixed value for the rotational band based on a given intrinsic state. (In diatomic molecules, the angular momentum of the collective rotational motion is perpendicular to the

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 ψ , 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 ψ . 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 ψ as a redundant variable, one may constrain ψ 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 ψ 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° 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 ± 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 Φ_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

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

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

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 σ .

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_{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 π_{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 Λ 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, ω) when regarded as functions of the particle coordinates x . Thus, the two sets of variables (q, ω) and (q', ω') , 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, ω) 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 π . For $K=0$ bands, the quantum numbers π 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 ω , 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 (ω, I_κ) , 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 ω is invariant while I_κ 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 Ψ_+ 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 Ψ_\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 ω_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 Ψ_+ and Ψ_- 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 Φ . 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 Φ_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 α 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^l 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 Φ_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 Λ -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 NH_3 , the tunneling frequency in the ground state is of the order of 10^{10} 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 $\mathcal{P}\mathcal{T}$),