CHAPTER 4

Rotational Spectra

4-1 OCCURRENCE OF COLLECTIVE ROTATIONAL MOTION IN QUANTAL SYSTEMS[1]

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. 133ff. ($E2$ 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-momemtum-like quantum numbers, such as isospin and nucleon number. (Such sequences occur in superfluid systems (see pp. 393ff.) and may also occur as excitations of the nucleon (see pp. 20ff.).)

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

---

[1]Spectra 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

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

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

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

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. 111ff. and pp. 130ff.). 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. 93ff.). 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

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

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

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

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

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

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 **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 $\mathbf{I}^2$, 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,

$$K = I, I-1, \ldots, -I \tag{4-6}$$

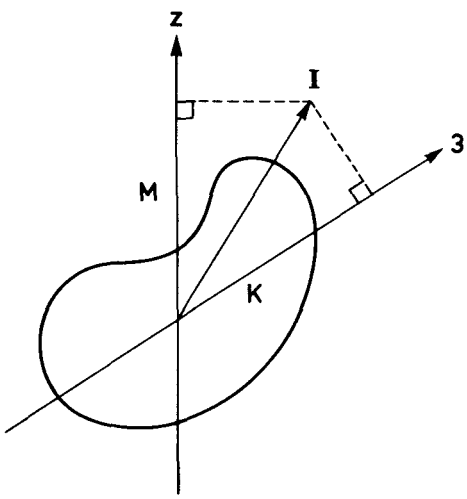

Figure 4-1 Angular momentum quantum numbers describing rotational motion in three dimensions. The z axis belongs to a coordinate system fixed in the laboratory, while the 3 axis is part of a body-fixed coordinate system (compare the $\mathscr{K}$ and $\mathscr{K}'$ systems defined in Fig. 1A-1, Vol.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

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

where the functions $\mathscr{D}^I_{MK}$ 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

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

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

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 $\mathbf{I}^2$ 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,

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

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

$$I_3 = J_3 \tag{4-10}$$

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 $\mathscr{R}$ 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 $\mathscr{R} \equiv \mathscr{R}_2(\pi)$ with respect to the 2 axis. (For systems with axial symmetry but not spherical symmetry, $\mathscr{R}$ 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 $\mathscr{R}$ invariance implies that the rotation $\mathscr{R}$ 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 $\mathscr{R}_e$, which performs the rotation $\mathscr{R}$ by acting on the collective orientation angles (external variables), is identical to the operator $\mathscr{R}_i$, which