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An algebraic representation of the particle-plus-rotor model ⋆

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Abstract

We investigate, using group theoretical methods, the coupling of a single particle with spin s to an axially symmetric rigid rotor by a quadrupole-quadrupole interaction. © 1998 Elsevier Science B.V.

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1. Introduction

The objective of describing nuclear collective states in terms of interacting neutrons and protons was largely achieved for even nuclei when it was shown that the collective model, for quadrupole vibrations and rotations, could be embedded in the shell model [1]. This was made possible by expressing the collective model in terms of a spectrum generating algebra (SGA), namely the symplectic algebra, which has a microscopic realization as a subalgebra of shell model observables. The present paper is part of a sequence of investigations aimed at a parallel expression of the collective states for odd nuclei.

By expressing the collective model in algebraic terms, one greatly simplifies applications of the collective model, already at the phenomenological level. This is because

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one can choose basis states which reduce suitable subalgebra chains, thereby diagonalizing a large part of the collective model Hamiltonian and facilitating the computation of matrix elements of both the Hamiltonian and other observables of the model. Then, by finding representations of the collective model algebra in the space of the shell model, one endows the collective model with microscopic wave functions; i.e. one gives the collective model a microscopic interpretation. This enables one to determine what collective model states are compatible with the microscopic many-nucleon structure of nuclei. It also enables one, at least in principle, to derive collective model parameters from corresponding shell-model observables.

In this paper, we are concerned with the particle-plus-rotor model. Various coupling schemes are possible when a rotor is coupled to a particle in a rotationally invariant manner. We first show that these coupling schemes are defined by corresponding subgroup chains. In a subsequent paper, we will consider the coupling of a microscopic rotor, described by the symplectic model, to an extra particle.

We start with the rotationally invariant Hamiltonian

$$H = H_{\rm rot} + h_{\rm s.p.} - \chi \hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{q}} \,, \tag{1}$$

where

$$H_{\rm rot} = A\hat{\boldsymbol{R}}^2 \,, \tag{2}$$

$$h_{\rm s.p.} = \frac{\hat{\boldsymbol{p}}^2}{2m} + \tfrac{1}{2} m\omega_0^2 \hat{\boldsymbol{r}}^2 + a\,\hat{\boldsymbol{l}} \cdot \hat{\boldsymbol{s}} + b\,\hat{\boldsymbol{l}} \cdot \hat{\boldsymbol{l}} \,. \tag{3}$$

$H_{\rm rot}$ is the Hamiltonian for an axially symmetric rigid rotor with angular momentum $\boldsymbol{R}$, $\hat{\boldsymbol{Q}}$ is the quadrupole tensor of the rotor and $\hat{\boldsymbol{q}}$ is the single-particle quadrupole tensor, with components

$$\hat{q}_\nu = \sqrt{\frac{16\pi}{5}}\; r^2 Y_{2\nu}(\theta, \varphi) \,. \tag{4}$$

This Hamiltonian has a SGA

$$\mathfrak{g} = [\mathbb{R}^5]\mathrm{so}(3)_R + \mathrm{sp}(3,\mathbb{R})_l + \mathrm{su}(2)_s \,, \tag{5}$$

where $[\mathbb{R}^5]\mathrm{so}(3)_R$ is a SGA for the rotor, $\mathrm{sp}(3,\mathbb{R})_l$ is a SGA for the spatial dynamics of the particle and $\mathrm{su}(2)_s$ is the spin algebra of the particle. The rotor algebra $[\mathbb{R}^5]\mathrm{so}(3)_R$ is spanned by five commuting components of the quadrupole tensor $\hat{\boldsymbol{Q}}$ and three components of the rotor angular momentum $\boldsymbol{R}$. The algebra $\mathrm{sp}(3,\mathbb{R})_l$ contains all linear combinations of the single-particle operators $p_i p_j$, $x_i x_j$ and $x_i p_j + p_j x_i$, where $\{x_i;\, i = 1, 2, 3\}$ and $\{p_i;\, i = 1, 2, 3\}$ are the components of the position and momentum vectors $\boldsymbol{r}$ and $\boldsymbol{p}$ of the single particle. In particular, $\mathrm{sp}(3,\mathbb{R})_l$ contains $\boldsymbol{p} \cdot \boldsymbol{p}$ and $\boldsymbol{r} \cdot \boldsymbol{r}$ and all components of the single particle angular momentum $\boldsymbol{l}$. $\mathrm{Sp}(3,\mathbb{R})$ has a number of important subalgebras, including those of the "shell model" chain

$$\mathrm{sp}(3,\mathbb{R}) \supset \mathrm{u}(3) \supset \mathrm{su}(3) \supset \mathrm{so}(3) \,. \tag{6}$$

All the terms of the Hamiltonian H of Eq. (1) are either elements of the Lie algebra $\mathfrak{g}$ or bilinear products of elements of $\mathfrak{g}$. Hence, eigenstates of H belong to unirreps of $\mathfrak{g}$.

A particle can be coupled to a rotor in many ways. Coupling schemes useful for computational purposes are ones whose basis states diagonalize important parts of the Hamiltonian. Such coupling schemes and the quantum numbers needed to label basis states are naturally associated with subalgebra chains of $\mathfrak{g}$, of which there are many. We mention a few of the possibilities.

1.1. Weak coupling

If the coupling constant χ is sufficiently small or if the rotor has a small intrinsic quadrupole moment, the eigenstates of H approach those of the weak coupling limit. In this limit, R, l and s are all good quantum numbers and there is no mixing of single-particle states from different spherical harmonic oscillator shells. Weak coupling ignores all observables but the angular momenta, so that weakly coupled states are simply angular momentum-coupled states. Thus, weak coupling reduces the subalgebra chains

$$\mathrm{so}(3)_l + \mathrm{su}(2)_s \supset \mathrm{su}(2)_j\,, \qquad \mathrm{so}(3)_R + \mathrm{su}(2)_j \supset \mathrm{su}(2)_I\,, \tag{7}$$

where $\mathrm{so}(3)_l$, $\mathrm{su}(2)_s$, $\mathrm{so}(3)_R$, $\mathrm{su}(2)_j$ and $\mathrm{su}(2)_I$ are the angular momentum algebras spanned, respectively, by the components of $\boldsymbol{l}$, $\boldsymbol{s}$, $\boldsymbol{R}$, $\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s}$, and $\boldsymbol{I} = \boldsymbol{R} + \boldsymbol{j}$. Note that so(3) is isomorphic to su(2).

Among the multiplets of weakly coupled states, which are degenerate in the $\chi = 0$ limit, the most interesting are the so-called *rotationally aligned* states for which $I = R + j$. Because of Coriolis decoupling, these states are particularly important at high angular momentum I and when the single particle angular momentum j is large.

1.2. Intermediate coupling

Intermediate coupling occurs when the interaction $-\chi\hat{\boldsymbol{Q}}\cdot\hat{\boldsymbol{q}}$ is small compared to energy differences between single particle states but large compared to energy differences of the rotor (at sufficiently low angular momentum). We then have a variety of possible coupling schemes in which the particle is strongly coupled to an adiabatic rotor; the following are three special cases.

1.2.1. Strong j coupling

In strong j coupling [2], the angular momentum j of the particle is a good quantum number. This coupling scheme reduces the subalgebra chain

$$[\mathbb{R}^5]\mathrm{so}(3)_R + \mathrm{su}(2)_j \supset [\mathbb{R}^5]\mathrm{su}(2)_I \supset \mathrm{su}(2)_I\,. \tag{8}$$

This coupling makes use of the fact that the direct sum Lie algebra $[\mathbb{R}^5]\mathrm{so}(3)_R + \mathrm{su}(2)_j$, spanned by the quadrupole moments and angular momentum operators $\{\hat{Q}_\nu, \hat{R}_k, \hat{j}_k\}$, has a subalgebra, $[\mathbb{R}^5]\mathrm{su}(2)_I$, spanned by the subset of operators $\{\hat{Q}_\nu, \hat{I}_k = \hat{R}_k + \hat{j}_k\}$. It also makes use of the fact that the rotor algebra $[\mathbb{R}^5]\mathrm{so}(3)$, like so(3), has representations comprising states of half odd integer spins.

1.2.2. Strong l coupling

In strong l coupling [2], the primary coupling is between the rotor and the orbital angular momentum l of the extra particle. Strong l coupling reduces the subalgebra chains

$$\left[\mathbb{R}^5\right] \mathrm{so}(3)_R + \mathrm{so}(3)_l \supset \left[\mathbb{R}^5\right] \mathrm{so}(3)_L \,, \tag{9}$$

$$\left[\mathbb{R}^5\right] \mathrm{so}(3)_L + \mathrm{su}(2)_s \supset \left[\mathbb{R}^5\right] \mathrm{su}(2)_I \supset \mathrm{su}(2)_I \,, \tag{10}$$

where $[\mathbb{R}^5]\mathrm{so}(3)_L$ is the algebra spanned by the operators $\{\hat{Q}_\nu, \hat{L}_k = \hat{R}_k + \hat{l}_k\}$. It is a double coupling in which the spin degree of freedom $\boldsymbol{s}$ are strongly coupled to the rotor with SGA $[\mathbb{R}^5]\mathrm{so}(3)_L$. Like strong j coupling, strong l coupling makes use of the fact that the rotor algebra $[\mathbb{R}^5]\mathrm{so}(3)$ has spinor representations.

1.2.3. Strong su(3) coupling

Strong su(3) coupling is essentially the coupling scheme in which Nilsson model states, computed with suppression of major harmonic oscillator shell mixing, are strongly coupled to a rotor. This limit was treated algebraically in a previous paper [3]. It uses the fact that a rotor can be regarded as an asymptotic su(3) irrep; i.e.,

$$[\mathbb{R}^5]\mathrm{so}(3)_R \equiv \lim \mathrm{su}(3)_R \,. \tag{11}$$

To see this, consider the su(3) operators $\{\hat{Q}_\nu^{\mathrm{su}(3)}, \hat{L}_\alpha\}$, where $\hat{Q}_\nu^{\mathrm{su}(3)}$ is an su(3) quadrupole moment and $\hat{L}_\alpha$ is an angular momentum, and rescale the su(3) quadrupole moments such that

$$\hat{Q}_\nu^{\mathrm{su}(3)} \to \hat{\mathcal{Q}}_\nu = \hat{Q}_\nu^{\mathrm{su}(3)}/\sqrt{\Lambda} \,, \tag{12}$$

where $\Lambda = 4(\lambda^2 + \sigma^2 + \lambda\sigma + 3\lambda + 3\sigma)$ is the eigenvalue of the second order su(3) Casimir operator when acting on any state of a representation (λ, σ). In the limit in which λ (and hence Λ) goes to $\to \infty$, the commutation relations for the rescaled operators become [4]

$$\begin{aligned}
\left[\hat{\mathcal{Q}}_\nu, \hat{\mathcal{Q}}_\mu\right] &= \frac{1}{\Lambda} \left[\hat{Q}_\nu^{\mathrm{su}(3)}, \hat{Q}_\mu^{\mathrm{su}(3)}\right] \\
&= \frac{1}{\Lambda}\, 3\sqrt{10}\big(2\,\nu; 2\,\mu|1\,\nu+\mu\big)\, \hat{L}_{\nu+\mu} \to 0 \quad \text{as } \Lambda \to \infty \,, \\
\left[\hat{\mathcal{Q}}_\nu, \hat{L}_\alpha\right] &= \frac{-1}{\sqrt{\Lambda}}\, \sqrt{6}\, \big(2\,\alpha; 1\,\nu|2\,\alpha+\nu\big)\, \hat{Q}_{\alpha+\nu}^{\mathrm{su}(3)} \\
&= -\sqrt{6}\, \big(2\,\alpha; 1\,\nu|2\,\alpha+\nu\big)\, \hat{\mathcal{Q}}_{\alpha+\nu} \,, \\
\left[\hat{L}_\nu, \hat{L}_\mu\right] &= -\sqrt{2}\, \big(1\,\nu; 1\,\mu|1\,\nu+\mu\big)\, \hat{L}_{\nu+\mu} \,,
\end{aligned} \tag{13}$$

i.e. they contract to the commutation relations of the rigid rotor algebra $[\mathbb{R}^5]\mathrm{so}(3)$.

With this contraction, we obtain a coupling scheme which reduces the subalgebra chain

$$[\mathbb{R}^5]\,\mathrm{so}(3)_R + \mathrm{su}(3)_l + \mathrm{su}(2)_s \equiv \lim_{\Lambda\to\infty} \mathrm{su}(3)_R + \mathrm{su}(3)_l + \mathrm{su}(2)_s$$
$$\supset \lim_{\Lambda\to\infty} \mathrm{su}(3)_L + \mathrm{su}(2)_s \supset [\mathbb{R}^5]\,\mathrm{su}(2)_I \supset \mathrm{su}(2)_I\,. \quad (14)$$

1.3. Strong coupling

This limit occurs when the coupling interaction $\chi\hat{\boldsymbol{Q}}\cdot\hat{\boldsymbol{q}}$ is dominant. The coupling scheme that emerges reduces the subalgebra chain

$$[\mathbb{R}^5]\,\mathrm{so}(3)_R + \mathrm{sp}(3,\mathrm{R})_l + \mathrm{su}(2)_s \supset [\mathbb{R}^5]\,\mathrm{su}(2)_I \supset \mathrm{su}(2)_I\,. \quad (15)$$

It corresponds to a rotationally invariant version of the Nilsson model. The primary objective of the present paper is to give an algorithm for implementing strong coupling in a rotationally invariant manner.

2. The strong coupling scheme

2.1. Basis states for a rotor

To describe the dynamics of a rotor, we must construct a unirrep of its spectrum generating algebra, $[\mathbb{R}^5]\mathrm{su}(2)$. This is accomplished by the method of induced representations [5].

In the context of the rotor model, the inducing construction can be seen as a systematic algorithm for implementing the traditional Bohr-Mottelson construction. In both approaches, one makes use of two frames of references: a laboratory (or space-fixed) frame and an intrinsic (or body-fixed) frame which rotates with the rotor.

The first step of the construction is to choose an irrep ρ of the $\mathbb{R}^5$ subalgebra. This subalgebra is spanned by the five quadrupole moment operators $\{\hat{Q}_\nu\,, \nu = \pm 2, \pm 1, 0\}$. Since $\mathbb{R}^5$ is Abelian, the irrep ρ is one-dimensional and corresponds to an assignment of numerical values $\{\overline{Q}_\nu\,, \nu = \pm 2, \pm 1, 0\}$ to each of the quadrupole operators $\{\hat{Q}_\nu\}$, i.e.

$$\rho(\hat{Q}_\nu) = \overline{Q}_\nu\,. \quad (16)$$

The quadrupole moments $\{\overline{Q}_\nu\}$ are interpreted as moments relative to an intrinsic (i.e. body-fixed) frame. We assume that an intrinsic frame for the rotor is chosen such that

$$\overline{Q}_\nu = \overline{Q}_0\delta_{\nu,0} + \overline{Q}_2(\delta_{\nu,2} + \delta_{\nu,-2})\,. \quad (17)$$

The next step in the construction of an $[\mathbb{R}^5]\mathrm{su}(2)_J$ unirrep is to identify the intrinsic symmetry group $\mathcal{S}$ of the rotor. This group is the subgroup of rotations that leave the intrinsic quadrupole moments invariant, i.e.

$$\mathcal{S} = \{\omega \in \mathrm{SU}(2) | \hat{R}(\omega)\,\overline{Q}_\nu\,\hat{R}(\omega^{-1}) = \overline{Q}_\nu\}\,, \quad (18)$$

where

$$\hat{R}(\omega)\,\bar{Q}_\nu\,\hat{R}(\omega^{-1}) = \sum_\mu \bar{Q}_\mu\,\mathcal{D}^2_{\mu\nu}(\omega)\,. \tag{19}$$

One sees that, if both $\bar{Q}_0$ and $\bar{Q}_2$ are non-zero, the rotor is triaxial and $\mathcal{S}$ is the group D_2 of rotations through multiples of π about any of its axes, i.e. D_2 comprises $\bar{\Gamma}(\pm\pi_y) = R(0,\pm\pi,0)$, $\bar{\Gamma}(\pm\pi_z) = R(\pm\pi,0,0)\}$, and all products of these two elements, with $R(\alpha,\beta,\gamma)$ denoting an element of SU(2) parametrized by the three Euler angles (α,β,γ). However, if $\bar{Q}_0 \neq 0$ but $\bar{Q}_2 = 0$, the rotor has a symmetry axis and $\mathcal{S}$ is the group D_∞ comprising rotations about the symmetry axis and rotations through angle π about perpendicular axes, i.e. D_∞ contains $\bar{\Gamma}(\gamma_z) = R(0,0,\pm\gamma)$, $\bar{\Gamma}(\pm\pi_y) = R(0,\pm\pi,0)$ and all their products. Rotors with D_∞ intrinsic symmetry are often referred to as symmetric tops.

A two-dimensional irrep $\bar{\Gamma}_K$ of D_∞ with basis states $\{\varphi_K,\varphi_{\bar{K}}\}$ is defined, for $2K$ a positive integer, by the equations

$$\bar{\Gamma}_K(\gamma_z)\varphi_K = e^{-i\gamma K}\varphi_K\,,\quad \bar{\Gamma}_K(\gamma_z)\varphi_{\bar{K}} = e^{i\gamma K}\varphi_{\bar{K}}\,, \tag{20}$$

$$\bar{\Gamma}_K(\pi_y)\varphi_K = \varphi_{\bar{K}}\,,\qquad \bar{\Gamma}_K(\pi_y)\varphi_{\bar{K}} = (-1)^{2K}\varphi_K\,,\quad K>0\,. \tag{21}$$

D_∞ also has one-dimensional irreps with $K = 0$ and basis state $\{\varphi_0^\varepsilon\}$ that satisfy

$$\bar{\Gamma}_0(\gamma_z)\,\varphi_0^\varepsilon = \varphi_0^\varepsilon\,,\qquad \bar{\Gamma}_0(\pi_y)\,\varphi_0^\varepsilon = \varphi_{\bar{0}}^\varepsilon \equiv \varepsilon\varphi_0^\varepsilon\,, \tag{22}$$

with $\varepsilon = \pm 1$.

Thus, a symmetric top rotor has an intrinsic state φ_0 (if $K = 0$), or a pair of intrinsic states $\{\varphi_K,\varphi_{\bar{K}}\}$ if $(K > 0)$, which are eigenstates of the quadrupole operators with identical eigenvalue $\bar{Q}_0$;

$$\hat{Q}_\nu\,\varphi_K = \delta_{\nu,0}\bar{Q}_0\varphi_K\,,\quad \hat{Q}_\nu\,\varphi_{\bar{K}} = \delta_{\nu,0}\bar{Q}_0\varphi_{\bar{K}}\,. \tag{23}$$

Note that, since the intrinsic quadrupole moments $\rho(\hat{Q}_\nu) = \bar{Q}_\nu$ are invariant under the subgroup $\mathcal{S}$ of SU(2), the two irreps ρ of $\mathbb{R}^5$ and $\bar{\Gamma}_K$ of $\mathcal{S}$ are compatible one with the other and give an irrep of the semi-direct product group $[\mathbb{R}^5]\mathcal{S}$. It remains to induce an irrep of $[\mathbb{R}^5]\mathrm{SU}(2)$ from this $[\mathbb{R}^5]\mathcal{S}$ irrep.

Consider a general product of intrinsic and rotational wave functions of the form

$$\Psi^I_{\eta KM}(\Omega) = \varphi_K \sum_N a^{\eta I}_{KN}\,\mathcal{D}^I_{NM}(\Omega) + \varphi_{\bar{K}} \sum_N a^{\eta I}_{\bar{K}N}\,\mathcal{D}^I_{NM}(\Omega)\,, \tag{24}$$

where $\Omega \in \mathrm{SU}(2)$ is the rotation which defines the orientation of the body-fixed axes relative to the laboratory axes, and where η denotes all additional quantum numbers needed to label the state. It is known from Mackey's theory that, if the $a^{\eta I}_{KN}$ coefficients are chosen such that the $\Psi^I_{\eta KM}$ wave functions satisfy the consistency equation

$$\bar{\Gamma}_K(\omega)\Psi^I_{\eta KM}(\Omega) = \Psi^I_{\eta KM}(\omega\Omega)\,,\qquad \omega\in\mathcal{S}\,, \tag{25}$$

where

$$\bar{\Gamma}_K(\omega)[\varphi_K \mathcal{D}^I_{NM}(\Omega)] = [\bar{\Gamma}_K(\omega)\varphi_K]\ \mathcal{D}^I_{NM}(\Omega)\,, \tag{26}$$

then the wave functions $\{\Psi^I_{\eta KM}\}$ are a basis for an irreducible $[\mathbb{R}^5]\mathrm{su}(2)_I$ representation.

For a symmetric top rotor we have the familiar wave functions:

$$\Psi^I_{KM}(\Omega) = \sqrt{\frac{2I+1}{16\pi^2(1+\delta_{K0})}}\{\varphi_K \mathcal{D}^I_{KM}(\Omega) + (-1)^{I+K}\varphi_{\tilde{K}}\mathcal{D}^I_{-KM}(\Omega)\}\,,\ K \geqslant 0\,, \tag{27}$$

where the relative phase of the two terms is determined from the self-consistency condition. They are labeled by the quantum number K, which can be taken to be non-negative since the wave function Ψ^I_{-KM}, with $K \geqslant 0$, differs from Ψ^I_{KM} by only a phase factor. Note that if $K = 0$, the irrep of the intrinsic symmetry group becomes one-dimensional with $\varphi_{\tilde{0}} = \varepsilon\varphi_0$ and $\varepsilon = \pm 1$. We then regain the familiar result that a $K = 0$ band comprises a $I = 0, 2, 4, \ldots$ sequence of states, if $\varepsilon = 1$, and a $I = 1, 3, 5, \ldots$ sequence, if $\varepsilon = -1$.

2.2. Strongly coupled particle-plus-rotor states

We now consider wave functions for a rotor-plus-particle system in the limit in which the inertial parameter A in the Hamiltonian of Eq. (3) is small relative to the strength (in suitable units) of the particle-rotor interaction $-\chi\hat{\boldsymbol{Q}}\cdot\hat{\boldsymbol{q}}$. In this limit, eigenfunctions of H can be found which reduce the subalgebra chain (15).

When A is small, it is appropriate to replace the angular momentum of the rotor $\hat{\boldsymbol{R}}$ by the difference $\hat{\boldsymbol{I}} - \hat{\mathbf{j}} = \hat{\boldsymbol{R}}$ and express H in the form

$$H = A\,\hat{\boldsymbol{I}}\cdot\hat{\boldsymbol{I}} + h + V\,, \tag{28}$$

where

$$\begin{aligned} h &= h_{\text{s.p.}} - \chi\hat{\boldsymbol{Q}}\cdot\hat{\boldsymbol{q}} \\ &= \frac{\hat{\boldsymbol{p}}^2}{2m} + \tfrac{1}{2}m\omega_0^2\,\hat{\boldsymbol{r}}^2 + a\,\hat{\boldsymbol{l}}\cdot\hat{\mathbf{s}} + b\,\hat{\boldsymbol{l}}\cdot\hat{\boldsymbol{l}} - \chi\,\hat{\boldsymbol{Q}}\cdot\hat{\boldsymbol{q}}\,, \end{aligned} \tag{29}$$

and

$$V = A\,\hat{\mathbf{j}}\cdot(\hat{\mathbf{j}} - 2\hat{\boldsymbol{I}})\,. \tag{30}$$

We obtain strong coupling of the particle to the rotor when A is small and the Coriolis interaction, $-2A\,\hat{\mathbf{j}}\cdot\hat{\boldsymbol{I}}$, can either be neglected or treated as a first order perturbation. For this reason, the Coriolis interaction is known as a *decoupling interaction*.

All terms in the Hamiltonian H are rotationally invariant. Moreover, h is independent of the total angular momentum. Thus, its energy levels can be determined in any frame of reference. In particular, they can be determined in the intrinsic frame of the rotor in which the components of the quadrupole tensor $\hat{Q}$ are replaced by their intrinsic values: $\hat{Q}_\nu \to \rho(\hat{Q}_\nu) = \overline{Q}_\nu = \delta_{\nu 0}\overline{Q}_0$. In this frame

$$h \to \overline{h} = h_{\text{s.p.}} - \chi \overline{\boldsymbol{Q}} \cdot \hat{\boldsymbol{q}} = h_{\text{s.p.}} - \chi \overline{Q}_0 \ (2z^2 - x^2 - y^2) \,, \tag{31}$$

and $\overline{h}$ can be identified with the Nilsson model Hamiltonian

$$\overline{h} = \frac{\hat{\boldsymbol{p}}^2}{2m} + \tfrac{1}{2}m(\omega_\perp^2 x^2 + \omega_\perp^2 y^2 + \omega_z^2 z^2) + a\,\hat{\boldsymbol{l}} \cdot \hat{\boldsymbol{s}} + b\,\hat{\boldsymbol{l}} \cdot \hat{\boldsymbol{l}} \,, \tag{32}$$

where

$$\omega_\perp^2 = \omega_0^2\,(1 + 2\alpha) \,, \qquad \omega_z^2 = \omega_0^2\,(1 - 4\alpha) \,, \tag{33}$$

and α is the dimensionless parameter

$$\alpha = \frac{\chi \overline{Q}_0}{m\omega_0^2} \,. \tag{34}$$

When h is replaced by $\overline{h}$, it ceases to be rotationally invariant. However, it remains invariant under $\mathrm{D}_\infty^j \subset \mathrm{SU}(2)_j$ and has the dynamical subgroup chain

$$\mathrm{Sp}(3,\mathbb{R})_l + \mathrm{SU}(2)_s \supset \mathrm{D}_\infty^j \supset \mathrm{U}(1)_j \,. \tag{35}$$

Eigenstates $\{\psi_{\eta k}, \psi_{\eta \tilde{k}}\}$ of $\overline{h}$ can then be defined which reduce the subgroup chain of Eq. (35) and satisfy the equations

$$\overline{h}\psi_{\eta k} = \varepsilon_{\eta k}\psi_{\eta k} \,, \quad \overline{h}\psi_{\eta \tilde{k}} = \varepsilon_{\eta k}\psi_{\eta \tilde{k}} \,, \tag{36}$$

$$\overline{\Gamma}_k(\gamma_z)\psi_{\eta k} = e^{-\mathrm{i}\gamma k}\psi_{\eta k} \,, \quad \overline{\Gamma}_k(\gamma_z)\psi_{\eta \tilde{k}} = e^{\mathrm{i}\gamma k}\psi_{\eta \tilde{k}} \,, \tag{37}$$

$$\overline{\Gamma}_k(\pi_y)\psi_{\eta \tilde{k}} = \psi_{\eta k} \,, \quad \overline{\Gamma}_k(\pi_y)\psi_{\eta k} = (-1)^{2k}\psi_{\eta \tilde{k}} \,. \tag{38}$$

Basis states for the combined rotor-plus-particle system, which span irreps of $[\mathbb{R}^5]\,\mathrm{SU}(2)_I$ and reduce the subgroup chain

$$[\mathbb{R}^5]\mathrm{SO}(3)_R \times \mathrm{Sp}(3,\mathbb{R})_l \times \mathrm{SU}(2)_s \supset [\mathbb{R}^5]\mathrm{SU}(2)_I \supset \mathrm{SU}(2)_I \,, \tag{39}$$

can now be constructed by inducing from irreps of $[\mathbb{R}^5]\mathrm{D}_\infty^I$ in the chain

$$[\mathbb{R}^5]\mathrm{D}_\infty^R \times \mathrm{D}_\infty^l \times \mathrm{D}_\infty^s \supset [\mathbb{R}^5]\mathrm{D}_\infty^R \times \mathrm{D}_\infty^j \supset [\mathbb{R}^5]\mathrm{D}_\infty^I \,, \tag{40}$$

where $\mathrm{D}_\infty^R \subset \mathrm{SO}(3)_R$ is the intrinsic symmetry group of the rotor and $\mathrm{D}_\infty^j \subset \mathrm{SU}(2)_j$ is the intrinsic symmetry group of the particle.

With the help of the D_∞ branching rules and coupling coefficients to be found in Appendix B, we find that, if φ_0 is an intrinsic state for a $(K = 0)$ band of the rotor core, we obtain strongly coupled wave functions $\{\Psi_{\eta k M}^I\}$ for the particle plus rotor in the standard rotor model form with

$$\Psi_{\eta k M}^I(\Omega) = \sqrt{\frac{2I+1}{16\pi^2}}\ \{\varphi_{\eta k}\mathcal{D}_{kM}^I(\Omega) + (-1)^{I+k}\varphi_{\eta \tilde{k}}\mathcal{D}_{-kM}^I(\Omega)\} \,, \quad k \geqslant \tfrac{1}{2} \,, \tag{41}$$

where $k = |k|$ is a good quantum number, and where, according to Eq. (B.13), $\varphi_{\eta k} = \varphi_0 \cdot \psi_{\eta k}$ and $\varphi_{\eta \tilde{k}} = \varphi_{\tilde{0}} \cdot \psi_{\eta \tilde{k}}$ span a 2-dimensional representation of D_∞, with

$$\bar{\Gamma}_k(\gamma_z)\varphi_{\eta k} = e^{-i\gamma k}\varphi_{\eta k}, \quad \bar{\Gamma}_k(\gamma_z)\varphi_{\eta \tilde{k}} = e^{i\gamma k}\varphi_{\eta \tilde{k}},$$
$$\bar{\Gamma}_k(\pi_y)\varphi_{\eta \tilde{k}} = \varphi_{\eta k}, \quad \bar{\Gamma}_k(\pi_y)\varphi_{\eta k} = (-1)^{2k}\varphi_{\eta \tilde{k}}. \tag{42}$$

3. Coupling coefficients for intermediate couplings

The schemes for coupling a particle to a rotor can be expressed in terms of group theoretically defined coupling coefficients. There are several couplings for which the coefficients have analytic expressions derivable by group theoretical means. These include: weak coupling and the several intermediate-coupling limits defined in Section 1. As we show in the following sections, we can also derive analytic coupling coefficients for the asymptotic limit of strong coupling.

For weak coupling, the rotor-plus-particle states are simply SU(2)-coupled;

$$[\Phi_R \times \psi_{\eta lj}]_{IM} = \sum_{M_r m} (R\, M_r; j\, m|I\, M)\; \Phi_{RM_r}\, \psi_{\eta\, ljm}. \tag{43}$$

Thus, the coupling coefficients $\{(R\, M_r; j\, m|I\, M)\}$ are SU(2) Clebsch Gordan coefficients. For other coupling schemes, the coefficients are products of SU(2) coefficients and reduced coupling coefficients. The reduced coupling coefficients $\{C^{Rlj}_{\eta I}\}$ for an arbitrary state $|\eta IM\rangle$ are then given by the expansion

$$\Psi_{\eta IM} = \sum_{Rlj} C^{Rlj}_{\eta I}\; [\Phi_R \times \psi_{\eta\, lj}]_{IM}. \tag{44}$$

3.1. Strong-j coupling

For strong-j coupling, we start with Eq. (41) but replace $\varphi_{\eta k}$ by the D_∞ product wave function

$$\varphi_{\eta ljk} = \psi_{\eta ljk} \cdot \varphi_0^+, \tag{45}$$

where $\psi_{\eta ljk}$ is a single-particle state of angular momentum jk and φ_0^+ is the intrinsic state for the core. (N.B., the group D_∞ has two $K = 0$ irreps, $\bar{\Gamma}_0^{\pm}$, cf., Appendix B, where the superscript $\pm$ indicates that the basis states for the two representations are, respectively, even and odd under rotation through angle π about the $\bar{y}$ axis.) The corresponding coupled wave functions are then given [6,2] by

$$\Psi_{\eta ljkIM} = \sum_R \sqrt{\frac{2\,(2R+1)}{(2I+1)}}\; (R\,0; j\,k|I\,k)\; [\Phi_R \times \psi_{\eta lj}]_{IM}, \quad k \geqslant \tfrac{1}{2}. \tag{46}$$

Once again, we can restrict to k positive because the wave functions with $k < 0$ differ from the former by only a phase factor. For rigid rotor core states of a $K^\pi = 0^+$ band, the sum extends over even values of R only. Thus, we determine that

$$C^{Rlj}_{\eta kI} = \sqrt{\frac{2\,(2R+1)}{(2I+1)}}\,\left(R\,0; j\,k|I\,k\right). \tag{47}$$

3.2. Strong-l coupling

For strong-l coupling, the possible intrinsic states are constructed as follows. We first couple the rotor to the orbital part of the single particle wave function. In accordance with Eq. (B.12), the D_∞ coupling decomposes as $\bar{\Gamma}_k \otimes \bar{\Gamma}^+_0 = \bar{\Gamma}_k$ $(k \geqslant 0)$ with intrinsic states $\{\psi_{\eta lk} \cdot \varphi^+_0, \quad \psi_{\eta l\tilde{k}} \cdot \varphi^+_0\}$, where the single particle state $\psi_{\eta lk}$ has integral orbital angular momentum quantum numbers lk.

These intrinsic states are then coupled to states $\{\zeta_{sk_s}\}$ of spin angular momentum s. Whenever s is a half odd integer (as we assume in this paper), i.e. $s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$ etc., the possible values of k_s are also half odd integer, so that it is impossible to have $k_s = k_l$. The appropriate D_∞ couplings are therefore

$$\bar{\Gamma}_{k_s} \otimes \bar{\Gamma}_k = \begin{cases} \bar{\Gamma}_{k_s} & \text{if} \quad k = 0\,, \\ \bar{\Gamma}_{k_s+k} \oplus \bar{\Gamma}_{|k_s-k|} & \text{if} \quad k>0\,. \end{cases} \tag{48}$$

Using Eqs. (B.5), (B.6) or (B.7), we find that the appropriate intrinsic states are given by

$$\varphi_{\eta(lk)sK} = \begin{cases} \zeta_{sk_s} \cdot \left[\psi_{\eta lk} \cdot \varphi^+_0\right] & \text{if} \quad K = k + k_s\,, \\ \zeta_{sk_s} \cdot \left[\psi_{\eta l\tilde{k}} \cdot \varphi^+_0\right] & \text{if} \quad K = k_s - k > 0 \\ \zeta_{s\tilde{k}_s} \cdot \left[\psi_{\eta lk} \cdot \varphi^+_0\right] & \text{if} \quad K = k - k_s > 0\,, \end{cases} \tag{49}$$

with $\varphi_{\eta(lk)s\tilde{K}}$ obtained using $\bar{\Gamma}_K(\pi_y)\,\varphi_{\eta(lk)sK} = \varphi_{\eta(lk)s\tilde{K}}$, along with $\psi_{\eta l\tilde{0}} = (-1)^l\,\psi_{\eta l0}$ if $k = 0$.

The three cases can be handled simultaneously if we allow the intermediate labels k and k_s to take negative, as well as positive, values. In the last case of Eq. (49), for example, one would have $k_s < 0$ and $k \geqslant 0$. This allows us to write all lab frame expressions of strong-l wave functions in the common form

$$\Psi_{\eta(lk)sKIM} = \sum_{RL} \sqrt{\frac{2\,(2R+1)}{(2I+1)}}\left(R\,0; l\,k|L\,k\right)\left(L\,k; s\,k_s|I\,K\right) \times [\,[\Phi_R \times \psi_{\eta l}] \times \zeta_s]_{IM}\,, \qquad K = k + k_s > 0\,. \tag{50}$$

It follows that the coupling coefficients for strong-l coupling are given by

$$C^{Rlj}_{\eta kKI} = \sum_{Lj} \sqrt{\frac{2\,(2R+1)(2L+1)(2j+1)}{(2I+1)}} \times \left(R\,0; l\,k|L\,k\right)\,\left(L\,k; s\,k_s|I\,K\right)W(RlIs; Lj)\,, \tag{51}$$

where $W(RlIs; Lj)$ is a Racah recoupling coefficient.

3.3. Strong-su(3) coupling

Strong-su(3) coupling is based on the observation that the coupling of a rotor and an su(3) particle is given by the $\Lambda \to \infty$ limit of the su(3) coupling $(\Lambda, 0) \otimes (\lambda, 0)$ for a single particle in the shell λ. From the work of Elliott [7], it is known that only the highest weight state of an su(3) representation is required to generate the states of a rotor band. Thus, we first consider the highest weight states for the su(3) irreps in the tensor product

$$(\Lambda, 0) \otimes (\lambda, 0) = \sum_{\sigma'} (\Lambda + \lambda - 2\sigma', \sigma') . \tag{52}$$

Let ϕ_{n_z, n_x, n_y} denote a single-particle (spherical harmonic oscillator) state with (n_x, n_y, n_z) quanta associated with the (x, y, z) directions, respectively. From previous work [8] we know that the simple product $\phi_{\lambda-\sigma,\sigma,0} \cdot \varphi_0^+$, where φ_0^+ is a rotor intrinsic state, is a highest weight state for the su(3) representation $(\Lambda+\lambda-2\sigma, \sigma)$ in the $\Lambda \to \infty$ limit. The state $\phi_{\lambda-\sigma,\sigma,0}$ is an eigenstate of the su(3) quadrupole moment $q_0^{\mathrm{su}(3)}$ with eigenvalue $(2\lambda - 3\sigma)$. It has also been shown [7] that, in the $\Lambda \to \infty$ limit, the representation $(\Lambda + \lambda - 2\sigma, \sigma)$ becomes indistinguishable from a sum of axially symmetric rigid rotor reps, i.e.

$$\lim_{\Lambda \to \infty} (\Lambda + \lambda - 2\sigma, \sigma) = \sum_{k_L} \bar{\Gamma}_{k_L} , \qquad k_L = \sigma , \sigma - 2 , \sigma - 4 , 0 \text{ or } 1 , \tag{53}$$

with $\varepsilon = (-1)^\lambda$ when $k_L = 0$ occurs.

It follows from this that the asymptotic su(3) highest weight state $\phi_{\lambda-\sigma,\sigma,0} \cdot \varphi_0^+$ must be a sum of $k_L \geqslant 0$, D_∞ states. Since φ_0^+ carries a 1-dimensional irrep of D_∞, we can use the branching rules of Appendix B to express [3] $\phi_{\lambda-\sigma,\sigma,0}$ as a sum of such states. This decomposition can be inferred if we first expand $\phi_{\lambda-\sigma,\sigma,0}$ in a complete set of angular momentum states

$$\phi_{\lambda-\sigma,\sigma,0} = \sum_{k=-\lambda}^{\lambda} \sum_{l=0}^{\lambda} \psi_{\lambda lk}(\omega_0) \langle \psi_{\lambda lk}(\omega_0) | \phi_{\lambda-\sigma,\sigma,0} \rangle , \tag{54}$$

and define $\{\Theta_{\lambda\sigma k}, \Theta_{\lambda\sigma\tilde{k}}\}$, $k \geqslant 0$ by

$$\Theta_{\lambda\sigma k} = \sum_l \psi_{\lambda lk}(\omega_0) \langle \psi_{\lambda lk}(\omega_0) | \Theta_{\lambda-\sigma,\sigma,0} \rangle ,$$
$$\Theta_{\lambda\sigma\tilde{k}} = (-1)^{\lambda-k} \sum_l \psi_{\lambda l,-k}(\omega_0) \langle \psi_{\lambda l,-k}(\omega_0) | \phi_{\lambda-\sigma,\sigma,0} \rangle , \qquad k \geqslant 0 . \tag{55}$$

(The argument ω_0 of $\psi_{\lambda lk}(\omega_0)$ specifies the original frequency of the shell model potential (cf., Eq. (29).) It can then be verified, using the elements of D_∞, that $\{\Theta_{\lambda\sigma k}, \Theta_{\lambda\sigma\tilde{k}}\}$ span a two-dimensional representation $\bar{\Gamma}_k$ of D_∞ when $k > 0$, whereas $\Theta_{\lambda\sigma 0}$ is a basis vector for a 1-dimensional irrep $\bar{\Gamma}_0$ with $\varepsilon = (-1)^\lambda$.

The branching rule of Eq. (53) is satisfied because the overlaps

$$\langle\psi_{\lambda l,-k}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle = (-1)^{\sigma-k}\langle\psi_{\lambda lk}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle\,, \qquad k\geqslant 0\,, \tag{56}$$

which were evaluated in Ref. [8], are different from zero only when k is one of the possible values of k_L, i.e. $k=\sigma,\sigma-2$ etc. Therefore,

$$\langle\psi_{\lambda l,-k}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle = \langle\psi_{\lambda lk}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle\,, \qquad k\geqslant 0\,. \tag{57}$$

Thus, the asymptotic su(3) highest weight state $\phi_{\lambda-\sigma,\sigma,0}\cdot\varphi_0^+$ is a sum of $k\geqslant 0$, D_∞-coupled intrinsic states

$$\{\Theta_{\lambda\sigma k}\cdot\varphi_0^+,\ \Theta_{\lambda\sigma\tilde{k}}\cdot\varphi_0^+\}\,, \qquad k=\sigma,\sigma-2,\sigma-4,0 \text{ or } 1\,. \tag{58}$$

The overlaps $\langle\psi_{\lambda lk}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle$, $k\geqslant 0$, are given [8] by

$$\langle\psi_{\lambda lk}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle = \sqrt{\frac{2^\sigma}{\binom{\sigma}{\frac{1}{2}(\sigma-k)}}}\sqrt{\frac{(\lambda-\sigma)!}{\lambda!\sigma!}}\,F(\lambda,\sigma lk)\,, \qquad k\geqslant 0\,, \tag{59}$$

where

$$F(\lambda,\sigma lk) = \sigma!\,2^k\sqrt{\frac{\{\frac{1}{2}(\lambda-l)\}!\{(l+k)!\,(l-k)!\,\{\frac{1}{2}(\lambda+l)\}!\,\lambda!\,2^l}{(\lambda+l+1)!}}$$
$$\times\sum_{q=k}^{\frac{1}{2}(\sigma+k)}\frac{(-1)^q}{2^{2q}q!(q-k)!(l+k-2q)!\{\frac{1}{2}(\sigma+k)-q\}!\{q-\frac{1}{2}(\sigma+k)+\frac{1}{2}(\lambda-l)\}!}\,. \tag{60}$$

With the inclusion of spin, the relevant $K\geqslant 0$, D_∞ states for the coupling of a particle in shell λ to a rigid rotor are given by

$$\varphi_{\lambda\sigma ksK} = \begin{cases} \sum_l \zeta_{sk_s}\cdot\left[\psi_{\lambda lk}(\omega_0)\cdot\varphi_0^+\right]\cdot\langle\psi_{\lambda lk}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle & \text{if} \quad K=k+k_s \\ \sum_l \zeta_{sk_s}\cdot\left[\psi_{\lambda l\tilde{k}}(\omega_0)\cdot\varphi_0^+\right]\cdot\langle\psi_{\lambda lk}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle & \text{if} \quad K=k_s-k>0 \\ \sum_l \zeta_{s\tilde{k}_s}\cdot\left[\psi_{\lambda lk}(\omega_0)\cdot\varphi_0^+\right]\cdot\langle\psi_{\lambda lk}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle & \text{if} \quad K=k-k_s>0\,, \end{cases} \tag{61}$$

where the order of the coupling reflects the fact that the asymptotic SU(3) coupling is to be done first, with the resultant coupled to spin.

The intrinsic state $\varphi_{\lambda\sigma ksK}$ is seen to be a sum of strong-l states. Thus, we obtain the lab frame wave functions

$$\Psi_{\lambda\sigma ksKIM} = \sum_l \Psi_{\lambda(lk)sKIM}\ \langle\psi_{\lambda lk}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle\,, \qquad K>0\,, \tag{62}$$

where we follow the rules detailed in Section 3.2 to determine the signs of k and k_s required to evaluate $\langle\psi_{\lambda lk}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle$ and the Clebsch–Gordan coefficients that enter in the construction of strong-l states. It follows that the coupling coefficients for strong-SU(3) coupling are given by

$$C^{Rlj}_{\lambda\sigma ksKI} = \sum_L \sqrt{\frac{2\,(2R+1)(2L+1)(2j+1)}{2I+1}}\;(R0;lk|Lk)(Lk;sk_s|IK) \times W(RlIs;Lj)\langle\psi_{\lambda lk}(\omega_0)|\phi_{\lambda-\sigma,\sigma,0}\rangle\,. \tag{63}$$

4. The asymptotic Nilsson basis

The eigenfunctions of the full Nilsson Hamiltonian, Eq. (32), are generally only partially defined by a dynamical subgroup chain. An exception occurs when the parameters a and b of the Hamiltonian are put equal to zero or when the term

$$a\,\hat{\boldsymbol{l}}\cdot\hat{\mathbf{s}} + b\,\hat{\boldsymbol{l}}\cdot\hat{\boldsymbol{l}} \tag{64}$$

in the Hamiltonian is treated as a first order perturbation. The Nilsson model wave functions then reduce the subgroup chains

$$\mathrm{Sp}(3,\mathbb{R})_l \supset \mathrm{U}(1)\times\mathrm{U}(2)_l \supset \mathrm{D}^l_\infty\,,\quad \mathrm{SU}(2)_s \supset \mathrm{D}^s_\infty\,,\quad \mathrm{D}^l_\infty\times\mathrm{D}^s_\infty \supset \mathrm{D}^j_\infty\,, \tag{65}$$

and there are no missing quantum numbers. The basis that results is the well-known *asymptotic Nilsson* basis.

4.1. The Hamiltonian

When using the asymptotic basis, it is convenient to express the rotor-plus-particle Hamiltonian of Eq. (1) in the form

$$H = H_{\mathrm{rot.}} + h_0 + V\,, \tag{66}$$

with

$$\begin{aligned} H_{\mathrm{rot.}} &= A\,\hat{\boldsymbol{I}}\cdot\hat{\boldsymbol{I}}\,,\\ h_0 &= \frac{\hat{\boldsymbol{p}}^2}{2m} + \tfrac{1}{2}m\omega_0^2\hat{\boldsymbol{r}}^2 - \chi\,\hat{\boldsymbol{Q}}\cdot\hat{\boldsymbol{q}}\,, \end{aligned} \tag{67}$$

and

$$V = a\,\hat{\boldsymbol{l}}\cdot\hat{\mathbf{s}} + b\,\hat{\boldsymbol{l}}\cdot\hat{\boldsymbol{l}} + A\,(\hat{\mathbf{j}}\cdot\hat{\mathbf{j}} - 2\hat{\boldsymbol{I}}\cdot\hat{\mathbf{j}})\,. \tag{68}$$

The components H_{rot} and h_0 are then diagonal in the asymptotic basis.

4.2. The asymptotic basis as a deformed spherical basis

The Hamiltonian $H_{\rm rot.} + h_0$ commutes with the total orbital angular momentum $\boldsymbol{L} = \boldsymbol{R} + \boldsymbol{l}$ operator for the system; this makes it possible to construct eigenstates of good total orbital angular momentum.

One starts by diagonalizing h_0 in the intrinsic frame of the rotor. In this frame, the quadrupole moments of the rotor are replaced by their intrinsic values; i.e. $\hat{Q}_\nu \to \rho(\hat{Q}_\nu) = \overline{Q}_\nu$. We suppose that the intrinsic quadrupole moments are those of an axially symmetric $K_R^\pi = 0^+$ rotor. Thus, $\overline{Q}_\nu = \delta_{\nu 0}\overline{Q}_0$ and

$$h_0 \to \overline{h}_{\rm cyl.} = \frac{\hat{\boldsymbol{p}}^2}{2m} + \tfrac{1}{2}m\omega_0^2\hat{\boldsymbol{r}}^2 - \chi\overline{Q}_0\ (2z^2 - x^2 - y^2)\ , \tag{69}$$

In terms of the familiar creation and destruction operators

$$a_j^\dagger = \sqrt{\frac{m\omega_0}{2\hbar}}\left(x_j - \frac{{\rm i}p_j}{m\omega_0}\right)\ , \qquad a_j = \sqrt{\frac{m\omega_0}{2\hbar}}\left(x_j + \frac{{\rm i}p_j}{m\omega_0}\right)\ , \tag{70}$$

this gives

$$\begin{aligned}\overline{h}_{\rm cyl.} = &\hbar\omega_0\left[(1-2\alpha)(a_z^\dagger a_z + \tfrac{1}{2}) - \alpha\,(a_z^\dagger a_z^\dagger + a_z a_z)\right]\\ &+\hbar\omega_0\left[(1+\alpha)(a_x^\dagger a_x + \tfrac{1}{2}) + \tfrac{1}{2}\alpha\,(a_x^\dagger a_x^\dagger + a_x a_x)\right]\\ &+\hbar\omega_0\left[(1+\alpha)(a_y^\dagger a_y + \tfrac{1}{2}) + \tfrac{1}{2}\alpha\,(a_y^\dagger a_y^\dagger + a_y a_y)\right].\end{aligned} \tag{71}$$

The Hamiltonian $\overline{h}_{\rm cyl.}$ is an element of the single particle ${\rm sp}(3,\mathbb{R})_l$ algebra (cf. Appendix A). Moreover, $\overline{h}_{\rm cyl.}$ is diagonalized by an ${\rm Sp}(3,\mathbb{R})_l$ group transformation of the spherical basis. Since $\overline{h}_{\rm cyl.}$ is a sum of three simple harmonic oscillator Hamiltonians, the transformation $\mathcal{O}$ which diagonalizes $\overline{h}_{\rm cyl.}$ is carried out by eliminating the shell mixing terms for each of the three components separately. The desired transformation is of the form

$$\mathcal{O} = \mathcal{S}_z(\epsilon)\,\mathcal{S}_y(\delta)\,\mathcal{S}_x(\delta)\ , \tag{72}$$

where

$$\mathcal{S}_j(\beta) = e^{-\frac{1}{2}\beta(a_j^\dagger a_j^\dagger - a_j a_j)}\ . \tag{73}$$

$\mathcal{O}$ is an asymmetric scale transformation in which the parameters ϵ and δ are fixed by the requirement that the mixing of different single particle shells is suppressed in the transformed Hamiltonian $\mathcal{O}\overline{h}_{\rm cyl.}\mathcal{O}^{-1}$. One also notes that $\mathcal{O}$ is ${\rm D}_\infty$ invariant; thus, it preserves the ${\rm D}_\infty$ invariance of $\overline{h}_{\rm cyl.}$

We determine that

$$\begin{aligned}\mathcal{S}_j(\beta)\,a_j^\dagger\,\mathcal{S}_j(-\beta) &= a_j^\dagger\,\cosh\beta + a_j\,\sinh\beta\,,\\ \mathcal{S}_j(\beta)\,a_j\,\mathcal{S}_j(-\beta) &= a_j\cosh\beta + a_j^\dagger\sinh\beta\,.\end{aligned} \tag{74}$$

Thus, under the action of $\mathcal{O}$, which maps an operator $\hat{X} \mapsto \mathcal{O}\,\hat{X}\,\mathcal{O}^{-1}$,

$$
\begin{aligned}
a_z^\dagger a_z^\dagger &\mapsto a_z^\dagger a_z^\dagger \cosh^2\epsilon + a_z a_z \sinh^2\epsilon + 2(a_z^\dagger a_z + \tfrac{1}{2})\cosh\epsilon\sinh\epsilon\,,\\
a_z a_z &\mapsto a_z a_z \cosh^2\epsilon + a_z^\dagger a_z^\dagger \sinh^2\epsilon + 2(a_z^\dagger a_z + \tfrac{1}{2})\cosh\epsilon\sinh\epsilon\,,\\
(a_z^\dagger a_z + \tfrac{1}{2}) &\mapsto (a_z^\dagger a_z + \tfrac{1}{2})(\cosh^2\epsilon + \sinh^2\epsilon) + (a_z^\dagger a_z^\dagger + a_z a_z)\cosh\epsilon\sinh\epsilon\,. \qquad (75)
\end{aligned}
$$

Similar formulae hold for the x and y operators with the replacement $\epsilon \to \delta$.

To evaluate the parameters ϵ and δ, we use Eq. (71) to obtain $\mathcal{O}\,\overline{h}_{\text{cyl.}}\mathcal{O}^{-1}$ explicitly. Requiring that the shell mixing terms vanish then leads to the equations for ϵ and δ:

$$\tfrac{1}{2}(1-2\alpha)\sinh 2\epsilon - \alpha\cosh 2\epsilon = 0\,, \qquad \tfrac{1}{2}(1+\alpha)\sinh 2\delta + \tfrac{1}{2}\alpha\cosh 2\delta = 0\,. \qquad (76)$$

These are easily solved to give

$$e^\epsilon = \frac{1}{[1-4\alpha]^{1/4}} = \sqrt{\frac{\omega_0}{\omega_z}} \qquad \text{and} \qquad e^\delta = \frac{1}{[1+2\alpha]^{1/4}} = \sqrt{\frac{\omega_0}{\omega_\perp}}\,. \qquad (77)$$

The transformed Hamiltonian is diagonal in the basis of eigenstates of a harmonic oscillator with frequency ω_0,

$$\mathcal{O}\overline{h}_{\text{cyl.}}\mathcal{O}^{-1} = \hbar\omega_0\left[\sqrt{1-4\alpha}(a_z^\dagger a_z + \tfrac{1}{2}) + \sqrt{1+2\alpha}(a_x^\dagger a_x + a_y^\dagger a_y + 1)\right]. \qquad (78)$$

Thus, as a result of the transformation, $\mathcal{O}\,\overline{h}_{\text{cyl.}}\mathcal{O}^{-1}$ has become $\mathrm{u}(1)+\mathrm{u}(2)$ invariant, where $\mathrm{u}(1)$ is the Lie algebra spanned by $a_z^\dagger a_z$ and $\mathrm{u}(2)$ is spanned by $\{a_i^\dagger a_j,\ i,j = x,y\}$.

$\mathcal{O}\overline{h}_{\text{cyl.}}\mathcal{O}^{-1}$ can be related to the strong-su(3) problem if we rewrite

$$
\begin{aligned}
\mathcal{O}\,\overline{h}_{\text{cyl.}}\mathcal{O}^{-1} = \hbar\omega_0\,\tfrac{1}{3}\,&(\sqrt{1-4\alpha}+2\sqrt{1+2\alpha})\,(a_z^\dagger a_z + a_x^\dagger a_x + a_y^\dagger a_y + \tfrac{3}{2})\\
&+\tfrac{1}{3}\,(\sqrt{1-4\alpha}-\sqrt{1+2\alpha})\,\hat{q}_0^{\mathrm{su}(3)}\,, \qquad (79)
\end{aligned}
$$

where

$$\hat{q}_0^{\mathrm{su}(3)} = \hbar\omega_0\,(2a_z^\dagger a_z - a_x^\dagger a_x - a_y^\dagger a_y) \qquad (80)$$

is the $\nu = 0$ component of the su(3) quadrupole tensor. Thus, in the intrinsic frame, the transformed Hamiltonian is the strong-su(3) Hamiltonian of Ref. [3] plus a diagonal, spherically symmetric term.

4.3. Asymptotic strong-coupling coefficients

4.3.1. Intrinsic states

We have shown in Section 3.3 that to generate strong-SU(3) particle-plus-core states, it is sufficient to combine the intrinsic state of the rotor with a single particle U(3) state $\phi_{p-\sigma,\sigma,0}$ which is an eigenstate of $\hat{q}_0^{\mathrm{su}(3)}$. Since, as pointed out earlier, $\mathcal{O}\,\overline{h}_{\text{cyl.}}\mathcal{O}^{-1}$ is basically a strong-su(3) Hamiltonian, the particle-plus-core states for $\overline{h}_{\text{cyl.}}$ are to be inferred from its eigenstates $\mathcal{O}^{-1}\phi_{p-\sigma,\sigma,0}$. Thus, as in Eq. (55), we define the asymptotic intrinsic states $\{\xi_{p\sigma k}, \xi_{p\sigma\tilde{k}}\}$ for the particle by

$$\xi_{p\sigma k} = \sum_{\lambda l} \psi_{\lambda lk}(\omega_0)\, \langle \psi_{\lambda lk}(\omega_0)|\, \mathcal{O}^{-1}\, |\phi_{p-\sigma,\sigma,0}\rangle\,,$$
$$\xi_{p\sigma\tilde{k}} = (-1)^{p-k} \sum_{\lambda l} \psi_{\lambda l,-k}(\omega_0)\, \langle \psi_{\lambda l,-k}(\omega_0)|\, \mathcal{O}^{-1}\, |\phi_{p-\sigma,\sigma,0}\rangle\,,$$
$$k = \sigma, \sigma-2, \ldots, 1 \text{ or } 0\,, \tag{81}$$

where $\psi_{\lambda lk}(\omega_0)$ is an eigenstate of a spherical harmonic oscillator of frequency ω_0.

When combined with spin wave function and the wave function of the rotor, the strongly coupled intrinsic states are given by the immediate generalization of Eq. (61). For instance, with $K = k + k_s$, we find

$$\varphi_{p\sigma ksK} = \zeta_{sk_s} \cdot [\xi_{p\sigma k} \cdot \varphi_0^+] = \sum_{\lambda l} \zeta_{sk_s} \cdot \left[\psi_{\lambda lk}(\omega_0) \cdot \varphi_0^+\right] \langle \psi_{\lambda lk}(\omega_0)|\, \mathcal{O}^{-1}\, |\phi_{p-\sigma,\sigma,0}\rangle\,. \tag{82}$$

Hence, a lab frame wave function with this intrinsic state is given by

$$\Psi_{p\sigma ksKIM} = \sum_{\lambda l} \Psi_{\lambda(lk)sKIM}\, \langle \psi_{\lambda lk}(\omega_0)|\, \mathcal{O}^{-1}\, |\phi_{p-\sigma,\sigma,0}\rangle\,, \tag{83}$$

and the corresponding coupling coefficients are

$$C^{Rlj}_{\lambda\sigma ksKI} = \sum_L \sqrt{\frac{2\,(2R+1)(2L+1)(2j+1)}{2I+1}}\, (R0; lk|Lk)(Lk; sk_s|IK)$$
$$\times W(RlIs; Lj) \langle \psi_{\lambda lk}(\omega_0)|\, \mathcal{O}^{-1}\, |\phi_{p-\sigma,\sigma,0}\rangle\,. \tag{84}$$

4.3.2. Overlap integrals

First, we claim that

$$(-1)^{l+k} \langle \psi_{\lambda l,-k}(\omega_0)|\, \mathcal{O}^{-1}\, |\phi_{p-\sigma,\sigma,0}\rangle = (-1)^{p-\sigma} \langle \psi_{\lambda lk}(\omega_0)|\, \mathcal{O}^{-1}\, |\phi_{p-\sigma,\sigma,0}\rangle\,, \tag{85}$$
$$k \geqslant 0\,.$$

For this, we note that

$$(-1)^{l-k} \langle \psi_{\lambda lk}(\omega_0)|\, \mathcal{O}^{-1}\, |\phi_{p-\sigma,\sigma,0}\rangle = \langle \psi_{\lambda l,-k}(\omega_0)|\, R_y(\pi)\, \mathcal{O}^{-1}\, |\phi_{p-\sigma,\sigma,0}\rangle$$
$$= \langle \psi_{\lambda l,-k}(\omega_0)|\, \mathcal{O}^{-1}\, R_y(\pi) |\phi_{p-\sigma,\sigma,0}\rangle\,, \tag{86}$$

since $\mathcal{O}^{-1}$, being D_∞-invariant, commutes with $R_y(\pi) \in D_\infty$. If we now write

$$R_y(\pi) |\phi_{p-\sigma,\sigma,0}\rangle = R_y(\pi)\, \frac{(a_z^\dagger)^{p-\sigma}}{\sqrt{(p-\sigma)!}}\, \frac{(a_y^\dagger)^\sigma}{\sqrt{\sigma!}}\, |\phi_{000}\rangle$$
$$= \left[R_y(\pi)\, \frac{(a_z^\dagger)^{p-\sigma}}{\sqrt{(p-\sigma)!}}\, R_y^{-1}(\pi) \right] \frac{(a_y^\dagger)^\sigma}{\sqrt{\sigma!}}\, R_y(\pi) |\phi_{000}\rangle\,, \tag{87}$$

then, since

$$R_y(\pi)\, a_y^\dagger\, R_y^{-1}(\pi) = a_y^\dagger\,, \tag{88}$$

and $a_z^\dagger$ transforms as the $m = 0$ component of an $l = 1$ tensor operator, we find

$$R_y(\pi)(a_z^\dagger)^{p-\sigma}R_y^{-1}(\pi) = (-1)^{p-\sigma}(a_z^\dagger)^{p-\sigma}, \tag{89}$$

which completes the proof of the claim.

As a result of the claim, we need only evaluate $\langle\psi_{\lambda lk}(\omega_0)|\,\mathcal{O}^{-1}\,|\phi_{p-\sigma,\sigma,0}\rangle$ for $k \geqslant 0$. To this end, it is convenient to rewrite $\mathcal{O}$ as a z-scaling transformation, $\mathcal{S}_z(\epsilon-\delta)$, times a rotationally invariant volume change $\mathcal{V}(\delta)$, i.e.

$$\mathcal{O} = \mathcal{S}_z(\epsilon-\delta)\,\mathcal{V}(\delta), \tag{90}$$

where

$$\mathcal{V}(\delta) = e^{-\frac{1}{2}\delta\sum_i(a_i^\dagger a_i^\dagger - a_i a_i)} \qquad \text{and} \qquad \mathcal{S}_z(\epsilon-\delta) = e^{-\frac{1}{2}(\epsilon-\delta)\,(a_z^\dagger a_z^\dagger - a_z a_z)}. \tag{91}$$

Note that the transformations $\mathcal{V}(\delta)$ and $\mathcal{S}_z(\epsilon-\delta)$ commute with one another. Thus we obtain

$$\begin{aligned}\langle\psi_{\lambda lk}(\omega_0)|\mathcal{O}^{-1}|\phi_{p-\sigma,\sigma,0}\rangle &= \langle\psi_{\lambda lk}(\omega_0)|\mathcal{V}^{-1}(\delta)\,\mathcal{S}_z^{-1}(\epsilon-\delta)|\phi_{p-\sigma,\sigma,0}\rangle,\\ &= \sum_q \langle\psi_{\lambda lk}(\omega_0)|\mathcal{V}^{-1}(\delta)\,|\phi_{q-\sigma,\sigma,0}\rangle\\ &\quad\times\langle\phi_{q-\sigma,\sigma,0}|\mathcal{S}_z^{-1}(\epsilon-\delta)|\phi_{p-\sigma,\sigma,0}\rangle,\\ &= \sum_q\langle\psi_{\lambda lk}(\omega_0)|\mathcal{V}^{-1}(\delta)\,|\psi_{qlk}(\omega_0)\rangle\,\langle\psi_{qlk}(\omega_0)|\phi_{q-\sigma,\sigma,0}\rangle\\ &\quad\times\langle\phi_{q-\sigma,\sigma,0}|\mathcal{S}_z^{-1}(\epsilon-\delta)|\phi_{p-\sigma,\sigma,0}\rangle,\end{aligned} \tag{92}$$

where we have used Eq. (59) and the fact that $\mathcal{V}$ commutes with the components of $\boldsymbol{l}$.

The matrix elements $\langle\phi_{q-\sigma,\sigma,0}|\mathcal{S}_z(\epsilon-\delta)|\phi_{p-\sigma,\sigma,0}\rangle$ can be evaluated by observing that the three binomials

$$J_+ = \tfrac{1}{2}\,a_z^\dagger a_z^\dagger, \qquad J_0 = \tfrac{1}{4}\,(a_z^\dagger a_z + a_z a_z^\dagger) \qquad \text{and} \qquad J_- = \tfrac{1}{2}\,a_z a_z \tag{93}$$

are the generators of an su(1,1) subalgebra.

Following Ui [9], we have

$$\langle\mathcal{J}\,\mathcal{M}'|e^{-\frac{1}{4}\beta\,(a^\dagger a^\dagger - aa)}|\mathcal{J}\,\mathcal{M}\rangle = (-1)^{\tilde{\mathcal{M}}'-\tilde{\mathcal{M}}}d^{\mathcal{J}}_{\mathcal{M}'\mathcal{M}}(\beta), \tag{94}$$

where $d^{\mathcal{J}}_{\mathcal{M}'\mathcal{M}}(\beta)$ is an su(1,1) d-function. Depending on whether $p-\sigma$ is even or odd, we are dealing with the unirrep $\mathcal{J} = \frac{1}{4}$ or $\frac{3}{4}$ of su(1,1) and we find that

$$\begin{aligned}\mathcal{A}_{q,p,\sigma}(\epsilon-\delta) &\equiv \langle\phi_{q-\sigma,\sigma,0}|\mathcal{S}_z^{-1}(\epsilon-\delta)|\phi_{p-\sigma,\sigma,0}\rangle,\\ &= \langle\phi_{q-\sigma,\sigma,0}|e^{\frac{1}{2}(\epsilon-\delta)\,(a_z^\dagger a_z^\dagger - a_z a_z)}|\phi_{p-\sigma,\sigma,0}\rangle,\\ &= \begin{cases}(-1)^{\mathcal{M}_z'-\mathcal{M}_z}d^{1/4}_{\mathcal{M}_z'\,\mathcal{M}_z}(2(\delta-\epsilon)) & \text{if } p-\sigma \text{ is even,}\\ (-1)^{\mathcal{M}_z'-\mathcal{M}_z}d^{3/4}_{\mathcal{M}_z'\,\mathcal{M}_z}(2(\delta-\epsilon)) & \text{if } p-\sigma \text{ is odd,}\end{cases}\end{aligned} \tag{95}$$

where

$$\mathcal{M}_z' = \tfrac{1}{2}(q - \sigma + \tfrac{1}{2}), \quad \mathcal{M}_z = \tfrac{1}{2}(p - \sigma + \tfrac{1}{2}), \quad e^{\delta-\epsilon} = \left[\frac{1-4\alpha}{1+2\alpha}\right]^{1/4} = \sqrt{\frac{\omega_z}{\omega_\perp}}. \quad (96)$$

Ui [9] has also given the analytic expression for the su(1,1) d-function:

$$\begin{aligned} d^{\mathcal{J}}_{\mathcal{M}'\mathcal{M}}(\beta) &= \sqrt{\frac{\Gamma(\mathcal{M}'+\mathcal{J})\Gamma(\mathcal{M}'-\mathcal{J}+1)}{\Gamma(\mathcal{M}+\mathcal{J})\Gamma(\mathcal{M}-\mathcal{J}+1)}}\frac{1}{\Gamma(\mathcal{M}'-\mathcal{M}+1)} \\ &\quad\times(\cosh\tfrac{1}{2}\beta)^{-2\mathcal{J}+\mathcal{M}-\mathcal{M}'}(\sinh\tfrac{1}{2}\beta)^{\mathcal{M}'-\mathcal{M}} \\ &\quad\times{}_2F_1(-\mathcal{M}+\mathcal{J},\mathcal{M}'+\mathcal{J};\mathcal{M}'-\mathcal{M}+1;\tanh^2\tfrac{1}{2}\beta), \quad (\mathcal{M}'\geqslant\mathcal{M}), \\ &= (-1)^{\mathcal{M}'-\mathcal{M}}d^{\mathcal{J}}_{\mathcal{M}\mathcal{M}'}(\beta), \qquad (\mathcal{M}>\mathcal{M}'), \end{aligned} \quad (97)$$

where ${}_2F_1(a,b;c;z)$ is a hypergeometric function.

The matrix elements $\langle\psi_{\lambda lk}(\omega_0)|\,\mathcal{V}(\delta)^{-1}|\psi_{qlk}(\omega_0)\rangle$ are also related to su(1,1) d-functions. This time, however, the relevant su(1,1) subalgebra is spanned by the rotationally invariant operators

$$\tilde{J}_+ = \tfrac{1}{2}\sum_{i=x,y,z} a_i^\dagger a_i^\dagger, \qquad \tilde{J}_0 = \tfrac{1}{4}\sum_{i=x,y,z}\left(a_i^\dagger a_i + a_i a_i^\dagger\right), \qquad \tilde{J}_- = \tfrac{1}{2}\sum_{i=x,y,z} a_i a_i. \quad (98)$$

To discover which representation is appropriate, consider the state $\psi_{llk}(\omega_0)$ of angular momentum l with $\lambda = l$ quanta. Since $\tilde{J}_-$ commutes with $\boldsymbol{l}$ and $\tilde{J}_-$ removes two quanta from any state, $\tilde{J}_-\psi_{llk}(\omega_0)$ is proportional to a state with $l-2$ quanta and angular momentum l. But there is no such state. Thus, $\tilde{J}_-\psi_{llk}(\omega_0) = 0$, implying that $\psi_{llk}(\omega_0)$ is a lowest weight state for a representation of su(1,1) labeled by the eigenvalue $\tilde{\mathcal{J}} = \frac{1}{2}(l+\frac{3}{2})$ of $\tilde{J}_0$. Furthermore, since $\tilde{J}_+$ and $\tilde{J}_0$ both commute with $\boldsymbol{l}$, states sharing common lk labels belong to the same su(1,1) unirrep. The su(1,1) weight $\tilde{\mathcal{M}}$ of the state $\psi_{\lambda lk}(\omega_0)$ is just the eigenvalue of $\tilde{J}_0$, i.e. $\tilde{\mathcal{M}} = \frac{1}{2}(\lambda+\frac{3}{2})$, so that we have the correspondence $\psi_{\lambda lk}(\omega_0) \leftrightarrow |\tilde{\mathcal{J}}\,\tilde{\mathcal{M}}\,k\rangle$ with k distinguishing multiple occurrences of the su(1,1) unirrep $\tilde{\mathcal{J}}$ in our Hilbert space of harmonic oscillator states.

Thus, we have

$$\langle\psi_{\lambda lk}(\omega_0)|\mathcal{V}^{-1}(\delta)|\psi_{qlk}(\omega_0)\rangle = (-1)^{\tilde{\mathcal{M}}'-\tilde{\mathcal{M}}}d^{\tilde{\mathcal{J}}}_{\tilde{\mathcal{M}}'\tilde{\mathcal{M}}}(-2\delta), \quad (99)$$

where

$$\tilde{\mathcal{J}} = \tfrac{1}{2}(l+\tfrac{3}{2}), \quad \tilde{\mathcal{M}}' = \tfrac{1}{2}(\lambda+\tfrac{3}{2}), \quad \tilde{\mathcal{M}} = \tfrac{1}{2}(q+\tfrac{3}{2}), \quad e^{-\delta} = [1+2\alpha]^{1/4}, \quad (100)$$

and the d-function is given in Eq. (97). Note that the overlap

$$\langle\psi_{\lambda lk}(\omega_0)|\mathcal{V}^{-1}(\delta)|\psi_{qlk}(\omega_0)\rangle$$

does not depend on the “multiplicity” label k.

The final expression for $\langle\psi_{\lambda lk}(\omega_0)|\,\mathcal{O}^{-1}\,|\phi_{p-\sigma,\sigma,0}\rangle$ is therefore

$$\langle\psi_{\lambda lk}(\omega_0)|\,\mathcal{O}^{-1}\,|\phi_{p-\sigma,\sigma,0}\rangle = \sum_q (-1)^{\tilde{\mathcal{M}}'-\tilde{\mathcal{M}}} d^{\tilde{\mathcal{J}}}_{\tilde{\mathcal{M}}'\tilde{\mathcal{M}}}(-2\delta)\,\langle\psi_{qlk}(\omega_0)|\phi_{q-\sigma,\sigma,0}\rangle \times\mathcal{A}_{q,p,\sigma}(\epsilon-\delta)\,, \quad (101)$$

where $\langle\psi_{\lambda lk}(\omega_0)|\phi_{q-\sigma,\sigma,0}\rangle$ is given by Eq. (59).

Note: The phases of the d-function $(-1)^{\tilde{\mathcal{M}}'-\tilde{\mathcal{M}}} d^{\tilde{\mathcal{J}}}_{\tilde{\mathcal{M}}'\tilde{\mathcal{M}}}(-2\delta)$ for the rotationally invariant operators of Eq. (98) and of the overlap $\langle\psi_{qlk}(\omega_0)|\phi_{q-\sigma,\sigma,0}\rangle$ are consistent with the su(3) states defined by Sharp et al. [11]. If one uses the harmonic oscillator states of [12] or [13], then the change $\langle\psi_{qlk}(\omega_0)|\phi_{q-\sigma,\sigma,0}\rangle \to (-1)^{(q-l)/2}\langle\psi_{qlk}(\omega_0)|\phi_{q-\sigma,\sigma,0}\rangle$ should be made.

Coming back to the claim made in Eq. (85), we see that the phases are such that

$$\langle\psi_{\lambda l,-k}(\omega_0)|\,\mathcal{O}^{-1}\,|\phi_{p-\sigma,\sigma,0}\rangle = \langle\psi_{\lambda lk}(\omega_0)|\,\mathcal{O}^{-1}|\phi_{p-\sigma,\sigma,0}\rangle\,, \qquad k\geqslant 0\,, \quad (102)$$

since, if p is even (resp. odd), only even (resp. odd) values of λ will occur, which in turns implies that only even (resp. odd) values of l will occur, while non-zero overlaps $\langle\psi_{\lambda lk}(\omega_0)|\phi_{q-\sigma,\sigma,0}\rangle$ only occur when $k-\sigma$ is even. This completes the calculation of all overlaps required for the construction of the strong symplectic wave functions.

4.4. Matrix elements in the asymptotic Nilsson basis

The computation of matrix elements of $a\hat{\boldsymbol{l}}\cdot\hat{\mathbf{s}}+b\hat{\boldsymbol{l}}\cdot\hat{\boldsymbol{l}}$ and $A\hat{\boldsymbol{R}}^2$ is straightforward now that we have explicit expressions for the asymptotic Nilsson basis in terms of states of good angular momentum with coefficients given by Eq. (101). The matrix elements simplify further when the operator under consideration commutes with the volume transformation $\mathcal{V}(\delta)$, as is the case for $a\hat{\boldsymbol{l}}\cdot\hat{\mathbf{s}}+b\hat{\boldsymbol{l}}\cdot\hat{\boldsymbol{l}}$ and $A\hat{\boldsymbol{R}}^2$. For then $\mathcal{O}=\mathcal{S}_z(\epsilon-\delta)\,\mathcal{V}(\delta)$ can be replaced by just $\mathcal{S}_z(\epsilon-\delta)$ and, from Eq. (83), we obtain, for example,

$$\begin{aligned}&\langle\Psi_{p'\sigma'k'sK'I'M'}|a\hat{\boldsymbol{l}}\cdot\hat{\mathbf{s}}+b\hat{\boldsymbol{l}}\cdot\hat{\boldsymbol{l}}\,|\Psi_{p\sigma ksKIM}\rangle\\ &\quad=\sum_{\lambda l}\langle\Psi_{\lambda(lk')sK'I'M'}|a\hat{\boldsymbol{l}}\cdot\hat{\mathbf{s}}+b\hat{\boldsymbol{l}}\cdot\hat{\boldsymbol{l}}\,|\Psi_{\lambda(lk)sKIM}\rangle\\ &\quad\times\left[\langle\psi_{\lambda lk'}(\omega_0)|\mathcal{S}_z(\epsilon-\delta)|\phi_{p'-\sigma',\sigma',0}\rangle^*\,\langle\psi_{\lambda lk}(\omega_0)|\mathcal{S}_z(\epsilon-\delta)|\phi_{p-\sigma,\sigma,0}\rangle\right]\\ &\quad\times\delta_{II'}\delta_{KK'}\delta_{MM'}\,,\end{aligned} \quad (103)$$

with

$$\langle\Psi_{\lambda(lk')sKIM}|\,\hat{\boldsymbol{l}}\cdot\hat{\mathbf{s}}\,|\Psi_{\lambda(lk)sKIM}\rangle = \sum_j \left(s\,k_s';l\,k'|j\,K\right)\left(s\,k_s;l\,k|j\,K\right)\tfrac{1}{2}[\,j(j+1)-l(l+1)-s(s+1)\,]\,. \quad (104)$$

The su(2) Clebsch–Gordan coefficients in the above matrix element arise from the relation

$$\zeta_{sk_s} \cdot \left[\psi_{\lambda lk}(\omega_0) \cdot \varphi_0^+\right] = \sum_j \left(s\, k_s; l\, k|j\, K\right) \varphi_{\lambda ljk} \cdot \varphi_0^+ \tag{105}$$

used convert strong-l states into a sum of strong-j states.

Matrix elements of $\hat{\boldsymbol{R}}^2 = \hat{\boldsymbol{I}} \cdot \hat{\boldsymbol{I}} - \hat{\jmath} \cdot \hat{\jmath} - 2\,\hat{\boldsymbol{I}} \cdot \hat{\jmath}$ are evaluated in a similar way with

$$\langle \Psi_{\lambda(lk')sK'IM} | \hat{\boldsymbol{I}} \cdot \hat{\jmath} | \Psi_{\lambda(lk)sKIM} \rangle = \sum_j \left(s\, k_s'; l\, k'|j\, K\right) \left(s\, k_s; l\, k|j\, K\right) \times \langle \Psi_{\lambda ljK'IM} | \hat{\boldsymbol{I}} \cdot \hat{\jmath}\, | \Psi_{\lambda ljKIM} \rangle\,, \tag{106}$$

where $\langle \Psi_{\lambda ljK'IM} | \hat{\boldsymbol{I}} \cdot \hat{\jmath}\, | \Psi_{\lambda ljKIM} \rangle$ is a familiar Coriolis matrix element.

5. Conclusion

The strategy of this paper, that of expressing the rotationally invariant Hamiltonian

$$H = H_{\rm rot} + h_{\rm s.p.} - \chi\, \hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{q}}$$

of Eq. (1) in terms of generators of the dynamical algebra $\mathfrak{g}$ of Eq. (5), has allowed us to go beyond the standard methods of the Nilsson model. In particular, by identifying $\mathrm{sp}(3,\mathbb{R})_l$ as the dynamical algebra of the deformed as well as the spherical harmonic oscillator, it has become possible to diagonalize exactly the Hamiltonian $A\ \hat{\boldsymbol{I}} \cdot \hat{\boldsymbol{I}} + h_0$, where

$$h_0 = \frac{\hat{\boldsymbol{p}}^2}{2m} + \tfrac{1}{2} m\omega_0 \hat{\boldsymbol{r}}^2 - \chi\, \hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{q}}\,,$$

by a group transformation $\mathcal{O}$. As a result, we have been able to express asymptotic Nilsson model states as sums of angular momentum-coupled rotor-plus-particle states

$$\Psi_{p\sigma ksKIM} = \sum_{\lambda Rlj} C^{Rlj}_{\lambda\sigma ksKI} [\Phi_R \times \psi_{\lambda\, lj}]_{IM}\,,$$

with group theoretically defined coupling coefficients $\{C^{Rlj}_{\lambda\sigma ksKI}\}$, given explicitly by Eqs. (84) and (101).

In arriving at this result, we were able to solve the problem of labeling angular momentum states IM by using the index K, which labels irreps of the intrinsic symmetry subgroup $[\mathbb{R}^5]\mathrm{D}^I_\infty \subset \mathfrak{G}$ of the coupled rotor-plus-particle system. Multiple occurrences of the irreps K are distinguished by considering the D_∞ couplings of the subgroups in the chains

$$\begin{aligned} [\mathbb{R}^5]\mathrm{SO}(3)_R &\supset [\mathbb{R}^5]\mathrm{D}^R_\infty\,, \\ \mathrm{SU}(2)_s &\supset \mathrm{D}^s_\infty\,, \\ \mathrm{Sp}(3,\mathbb{R})_l \supset \mathrm{U}(1)\times\mathrm{U}(2) &\supset \mathrm{U}(1)\times \mathrm{D}^l_\infty\,, \end{aligned} \tag{107}$$

which completely specify the construction of the various K irreps through the labels $(p\sigma ks)$.

The problem of handling infinitely many states with given angular momentum labels lk, in the expansion of deformed single-particle wave functions, was solved by the use of the non-compact group SU(1,1) and its associated d-functions.

Although the formalism presented here was derived for the case of a single extra nucleon coupled to an axially symmetric core, many extensions can be considered without too much difficulty. The mathematical framework pertinent to these more general cases has been discussed elsewhere [8].

Appendix A. Review of the symplectic algebra

We assume throughout this paper that we are dealing with harmonic series representations of the non-compact symplectic algebra sp(3,$\mathbb{R}$), which is spanned by the 21 operators

$$A_{ij} = \sum_{a=1}^{\mathrm{A}} a^\dagger_{ia} a^\dagger_{ja} , \qquad C_{ij} = \tfrac{1}{2} \sum_{a=1}^{\mathrm{A}} (a^\dagger_{ia} a_{ja} + a_{ja} a^\dagger_{ia}) , \qquad B_{ij} = \sum_{a=1}^{\mathrm{A}} a_{ia} a_{ja} , \tag{A.1}$$

where a labels the particle number, A is the total number of particles, $i, j = x, y, z$ label the directions of space and the operators $a^\dagger_{ja}$ and a_{ja} are defined in the usual way by

$$a^\dagger_{ja} = \sqrt{\frac{m\omega_0}{2\hbar}} \left(x_{ja} - \frac{\mathrm{i} p_{ja}}{m\omega_0} \right) , \qquad a_{ja} = \sqrt{\frac{m\omega_0}{2\hbar}} \left(x_{ja} + \frac{\mathrm{i} p_{ja}}{m\omega_0} \right) , \tag{A.2}$$

The harmonic series are unitary representations carried by subspaces of many-particle harmonic oscillator states. They are characterized by lowest but not highest weight states.

The Cartan subalgebra of sp(3,$\mathbb{R}$) coincides with that of the u(3) subalgebra spanned by the nine C_{ij} operators. Thus, sp(3,R) irreps are labeled by three integers, which can be chosen to be $N(\Lambda,\mu)$. N is the eigenvalue of $C_{11}+C_{22}+C_{33}$, which is equal to the number of quanta plus the zero point energy for A nucleons, 3A/2. (Λ,μ) are the usual su(3) labels. The symplectic operators A_{ij} and B_{ij} are u(3) tensors of the type $2(2,0)$ and $-2(0,2)$ respectively, and all the states of an sp(3,$\mathbb{R}$) representation $N(\Lambda,\mu)$ can be generated by laddering up with the A_{ij} operators from the states of the lowest u(3) subspace, labeled by $N(\Lambda,\mu)$.

There are two one-particle harmonic series irrep; they are distinguished by parity. For a single particle representation, the sums in (A.1) contain only a single term (i.e. A=1). Single particle operators will be denoted by lower case letters, so that we have

$$a_{ij} = a^\dagger_i a^\dagger_j , \qquad c_{ij} = \tfrac{1}{2}(a^\dagger_i a_j + a_j a^\dagger_i) , \qquad b_{ij} = a_i a_j . \tag{A.3}$$

Single particle lowest weight states, i.e. states annihilated by b_{ij}, belong to the su(3) irrep $(0,0)$ or $(1,0)$. Hence, single particle irreps of sp(3,$\mathbb{R}$) are labeled by $\frac{3}{2}(0,0)$ (positive parity) or $\frac{5}{2}(1,0)$ (negative parity). These representations contain, respectively, the u(3) shells $(2n+\frac{3}{2})(2n,0)$ and $(2n+\frac{5}{2})(2n+1,0)$ with $n = 0,1,2,\dots$

Appendix B. Branching rules and basis states for D_∞ coupling

A generic irrep $\bar{\Gamma}_K$ $(K > 0)$ of D_∞ is two-dimensional with basis states $\{\varphi_K, \varphi_{\tilde{K}}\}$ that satisfy Eqs. (20) and (21). D_∞ also has one-dimensional irreps with $K = 0$ and basis state $\{\varphi_0^\varepsilon\}$ that satisfy

$$\bar{\Gamma}(\gamma_z)\,\varphi_0^\varepsilon = \varphi_0^\varepsilon\,, \qquad \bar{\Gamma}(\pi_y)\,\varphi_0^\varepsilon = \varphi_{\tilde{0}}^\varepsilon \equiv \varepsilon\varphi_0^\varepsilon\,, \tag{B.1}$$

where ε is either $+1$ or -1.

To find the Clebsch–Gordan series

$$\bar{\Gamma}_{K_1} \otimes \bar{\Gamma}_{K_2} = \sum_K c_K \bar{\Gamma}_K\,, \qquad K \geqslant 0\,, \tag{B.2}$$

where c_K is the multiplicity of the irrep $\bar{\Gamma}_K$ in the decomposition of the above product, we first determine the possible values of the K quantum number in the space spanned by the products of basis states of $\bar{\Gamma}_{K_1}$ and $\bar{\Gamma}_{K_2}$.

If $K_1 > 0$ and $K_2 > 0$, so that $\bar{\Gamma}_{K_1}$ and $\bar{\Gamma}_{K_2}$ are both two-dimensional, the representation space for $\bar{\Gamma}_{K_1} \otimes \bar{\Gamma}_{K_2}$ is spanned by the 4 states $\{\varphi_{K_1}\cdot\varphi_{K_2}, \varphi_{K_1}\cdot\varphi_{\tilde{K}_2}, \varphi_{\tilde{K}_1}\cdot\varphi_{K_2}, \varphi_{\tilde{K}_2}\cdot\varphi_{\tilde{K}_1}\}$. Acting with $\bar{\Gamma}(\gamma_z)$ on these states, we find, using Eq. (20), that

$$\begin{aligned}
\bar{\Gamma}(\gamma_z)\left[\varphi_{K_1}\cdot\varphi_{K_2}\right] = \left[\Gamma(\gamma_z)\,\varphi_{K_1}\right]\cdot\left[\Gamma(\gamma_z)\,\varphi_{K_2}\right] &= e^{-i(K_1+K_2)\gamma}\ \varphi_{K_1}\cdot\varphi_{K_2}\,,\\
\bar{\Gamma}(\gamma_z)\left[\varphi_{K_1}\cdot\varphi_{\tilde{K}_2}\right] &= e^{-i(K_1-K_2)\gamma}\ \varphi_{K_1}\cdot\varphi_{\tilde{K}_2}\,,\\
\bar{\Gamma}(\gamma_z)\left[\varphi_{\tilde{K}_1}\cdot\varphi_{K_2}\right] &= e^{i(K_1-K_2)\gamma}\ \varphi_{\tilde{K}_1}\cdot\varphi_{K_2}\,,\\
\bar{\Gamma}(\gamma_z)\left[\varphi_{\tilde{K}_1}\cdot\varphi_{\tilde{K}_2}\right] &= e^{i(K_1+K_2)\gamma}\ \varphi_{\tilde{K}_1}\cdot\varphi_{\tilde{K}_2}\,.
\end{aligned} \tag{B.3}$$

Thus, if $K_1 \neq K_2$, the representation $\bar{\Gamma}_{K_1+K_2}$ will occur once in (B.2), along with one copy of the representation $\bar{\Gamma}_{|K_1-K_2|}$, i.e.

$$\bar{\Gamma}_{K_1} \otimes \bar{\Gamma}_{K_2} = \bar{\Gamma}_{K_1+K_2} \oplus \bar{\Gamma}_{|K_1-K_2|}\,, \qquad K_1 \neq K_2\,, \quad K_1, K_2 > 0\,. \tag{B.4}$$

Basis states for $\bar{\Gamma}_{K_1+K_2}$ are given simply by

$$\{\varphi_K = \varphi_{K_1}\cdot\varphi_{K_2}\,, \quad \varphi_{\tilde{K}} = \varphi_{\tilde{K}_1}\cdot\varphi_{\tilde{K}_2}\}\,, \qquad K = K_1 + K_2, \quad K_1, K_2 > 0\,. \tag{B.5}$$

For the irrep $\bar{\Gamma}_{|K_1-K_2|}$, we choose the basis states

$$\{\varphi_K = \varphi_{K_1}\cdot\varphi_{\tilde{K}_2}, \varphi_{\tilde{K}} = \varphi_{\tilde{K}_1}\cdot\varphi_{K_2}\} \quad \text{for} \quad K = K_1 - K_2 > 0, \quad K_1 > K_2 > 0\,, \tag{B.6}$$

and

$$\{\varphi_K = \varphi_{\tilde{K}_1}\cdot\varphi_{K_2}, \varphi_{\tilde{K}} = \varphi_{K_1}\cdot\varphi_{\tilde{K}_2}\} \quad \text{for} \quad K = K_2 - K_1 > 0, \quad K_2 > K_1 > 0\,. \tag{B.7}$$

If $K_1 = K_2$, the representation $\bar{\Gamma}_K$ with $K = 2K_1$ occurs once, and there are two $\bar{\Gamma}_0$ irreps. The latter can be distinguished by the $\bar{\Gamma}(\pi_y) \in D_\infty$ operator. Thus, if we set

$$\varphi_0^\varepsilon = \frac{1}{\sqrt{2}}\left[\varphi_{K_1}\cdot\varphi_{\tilde{K}_1} + \varepsilon\cdot\varphi_{\tilde{K}_1}\cdot\varphi_{K_1}\right]\,, \qquad K_1 = K_2 > 0\,, \tag{B.8}$$

it can be verified that $\overline{\Gamma}(\pi_y)\,\varphi_0^{\varepsilon} = \varepsilon\varphi_0^{\varepsilon} = \varphi_{\tilde{0}}^{\epsilon}$ in accordance with Eq. (B.1). Thus, we find

$$\overline{\Gamma}_{K_1} \otimes \overline{\Gamma}_{K_1} = \overline{\Gamma}_{2K_1} \oplus \overline{\Gamma}_0^{+} \oplus \overline{\Gamma}_0^{-}, \qquad K_1 = K_2 > 0\,, \tag{B.9}$$

with basis states given by Eq. (B.5) with $K_1 = K_2$ for $\overline{\Gamma}_{2K_1}$ and by Eq. (B.8) for $\overline{\Gamma}_0^{\varepsilon}$.

Suppose now that $K_1 > 0$ but $K_2 = 0$. The resulting two-dimensional space $\overline{\Gamma}_{K_1} \otimes \overline{\Gamma}_0^{\varepsilon}$ is spanned by $\{\varphi_{K_1}\cdot\varphi_0^{\varepsilon}, \varphi_{\tilde{K}_1}\cdot\varphi_0^{\varepsilon}\}$. It follows from the action of $\overline{\Gamma}(\gamma_z)$ on these states that the only possible value of K is $K = K_1$, i.e.

$$\overline{\Gamma}_{K_1} \otimes \overline{\Gamma}_0^{\varepsilon} = \overline{\Gamma}_{K_1}\,, \qquad K_1 > 0\,, \quad K_2 = 0\,, \tag{B.10}$$

with basis states

$$\{\varphi_{K_1}\cdot\varphi_0^{\varepsilon}\,, \quad \varphi_{\tilde{K}_1}\cdot\varphi_{\tilde{0}}^{\varepsilon}\}\,, \qquad K_1 > 0\,, \quad K_2 = 0\,, \tag{B.11}$$

where the phase of the second basis state has been adjusted so that Eq. (21) is verified. If $K_1 = 0$ but $K_2 > 0$, then

$$\overline{\Gamma}_0^{\varepsilon} \otimes \overline{\Gamma}_{K_2} = \overline{\Gamma}_{K_2}\,, \tag{B.12}$$

with basis states

$$\{\varphi_0^{\varepsilon}\cdot\varphi_{K_2}\,, \quad \varphi_{\tilde{0}}^{\varepsilon}\cdot\varphi_{\tilde{K}_2}\}\,, \qquad K_2 > 0\,, \quad K_1 = 0\,. \tag{B.13}$$

Finally, if $K_1 = K_2 = 0$, we have

$$\overline{\Gamma}_0^{\varepsilon_1} \otimes \overline{\Gamma}_0^{\varepsilon_2} = \overline{\Gamma}_0^{\varepsilon}\,, \qquad \varepsilon = \varepsilon_1\cdot\varepsilon_2\,, \qquad K_1 = K_2 = 0\,, \tag{B.14}$$

with basis state

$$\varphi_0^{\varepsilon} = \varphi_0^{\varepsilon_1}\cdot\varphi_0^{\varepsilon_2}\,. \tag{B.15}$$

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