

## Reformulation of the two-rotor model

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The two-rotor model of deformed nuclei which predicts an isovector collective  $M1$  state owing to orbital motion is reformulated by a different quantization procedure. This new formulation leads to an eigenvalue equation for the intrinsic motion which is identical to that found in the interacting boson approximation. The close correspondence to the vibrating potential model is also stressed. The values of the excitation energy and  $B(M1)$  strength are now in reasonable agreement with the estimates of those models.

[ NUCLEAR STRUCTURE Two-rotor picture, deformed nuclei, collective  
isovector orbital magnetic excitations. ]

### I. INTRODUCTION

A few years ago a two-rotor model of deformed nuclei had been considered.<sup>1</sup> In such a model, protons and neutrons are assumed to form separate rigid bodies of ellipsoidal shape. The restoring force generated by their relative displacement can give rise, classically, either to relative rotational oscillations or to a configuration where the nucleus rotates as a whole, while the proton neutron symmetry axes stay at a fixed angle, as shown in Fig. 1.

The model, which has been studied for simplicity only for  $N=Z$ , predicts collective states only in the region of heavy deformed nuclei. In such a region for  $A=180$  and deformation parameter  $|\delta| \sim 0.25$ , there are two  $K=1$  states with  $I=1,2$  at about 12 MeV with  $B(M1) \uparrow \sim 15(e/2m)^2$ , and  $B(E2) \uparrow \sim 0.6$  W.u., respectively.

A collective state interpreted in terms of the two-rotor model has been predicted in the framework of the vibrating potential model (VPM) (Ref. 2) and the interacting boson approximation (IBA) (Ref. 3). In both cases the energy of the  $M1$  state is much lower than the one estimated in Ref. 1.

One of the motivations of the present paper is to investigate the origin of such a discrepancy. In this connection, we reconsider the quantization procedure of the two-rotor model.

In Ref. 1, to be referred to as I, the classical Hamiltonian has been quantized after the transformation to intrinsic frame variables. Now it is known that quantization in a different system of coordinates gives rise, in general, to different results.<sup>4</sup> Since the model is to be considered an approximation to a nuclear Hamiltonian expressed in terms of the fixed-frame nucleon coordinates, it is more appropriate to quantize in the fixed-frame variables and then to transform to intrinsic frame variables.

As shown in a preliminary report,<sup>5</sup> this latter procedure leads to results which are qualitatively similar but quantitatively different from the previous ones, and closer to the predictions of the VPM and the IBA.

We also extend the model to the case  $N \neq Z$  in order to account for the neutron excess and discuss our numerical estimate of the restoring force constant. While the first effect turns out to be negligible, we find that there are large uncertainties in the estimate of the restoring force constant inherent to the semiclassical nature of the model.

In Sec. II we illustrate the new quantization procedure whose derivation is given in Appendix A. In Sec. III, we solve the eigenvalue problem; in Sec. IV we evaluate transition probabilities and the  $M1$  form factor; in Sec. V, we discuss the numerical estimate of the restoring force constant and compare the new version of the two-rotor model with the VPM and the IBA. We use  $\hbar=c=1$  u.

### II. THE MODEL

If relative translational motion is neglected, the classical Hamiltonian of the two-rotor model is

$$H = \frac{1}{2\mathcal{I}_p} \vec{I}^{(p)2} + \frac{1}{2\mathcal{I}_n} \vec{I}^{(n)2} + V, \tag{2.1}$$

where  $\vec{I}^{(p)}$ ,  $\vec{I}^{(n)}$ ,  $\mathcal{I}_p$ , and  $\mathcal{I}_n$  are the angular momenta and moments of inertia of protons and neutrons, while  $V$  is the potential energy.

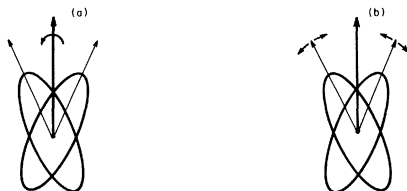


FIG. 1. Classical motions in the two-rotor model: (a) rotation around the  $\xi$  axis; (b) rotational oscillation around the  $\xi$  axis.

It is now convenient to introduce the total angular momentum  $I$

$$\begin{aligned}\vec{I} &= \vec{I}^{(p)} + \vec{I}^{(n)}, \\ \vec{S} &= \vec{I}^{(p)} - \vec{I}^{(n)},\end{aligned}\quad (2.2)$$

and rewrite  $H$  as

$$H = \frac{1}{2\mathcal{I}}(\vec{I}^2 + \vec{S}^2) + \frac{\mathcal{I}_n - \mathcal{I}_p}{4\mathcal{I}_n\mathcal{I}_p}\vec{I} \cdot \vec{S} + V, \quad (2.3)$$

where

$$\mathcal{I} = \frac{4\mathcal{I}_p\mathcal{I}_n}{\mathcal{I}_p + \mathcal{I}_n}. \quad (2.4)$$

We assume the potential to depend on the angle  $\theta$  between the symmetry axes  $\hat{\xi}^{(p)}, \hat{\xi}^{(n)}$  of the proton and neutron ellipsoids

$$\cos(2\theta) = \hat{\xi}^{(p)} \cdot \hat{\xi}^{(n)}. \quad (2.5)$$

It is therefore natural to introduce this variable along with a set of other variables necessary to identify  $\hat{\xi}^{(p)}, \hat{\xi}^{(n)}$ . These variables may be the Euler angles  $\alpha, \beta, \gamma$  of the intrinsic frame defined by

$$\begin{aligned}\hat{\xi} &= \frac{\hat{\xi}^{(p)} \times \hat{\xi}^{(n)}}{\sin(2\theta)}, \\ \hat{\eta} &= \frac{\hat{\xi}^{(p)} - \hat{\xi}^{(n)}}{2\sin\theta}, \\ \hat{\xi} &= \frac{\hat{\xi}^{(p)} + \hat{\xi}^{(n)}}{2\cos\theta}.\end{aligned}\quad (2.6)$$

The correspondence  $\{\hat{\xi}^{(p)}, \hat{\xi}^{(n)}\} = \{\alpha, \beta, \gamma, \theta\}$  is one to one and regular for  $0 < \theta < \pi/2$ .

The variables  $(\xi^{(p)}, \xi^{(n)}) = (\alpha, \beta, \gamma, \theta)$  are not sufficient to describe the configurations of the classical system. However, they describe uniquely the quantized system owing to the constraints

$$I_{\xi^{(p)}}^{(p)} = I_{\xi^{(n)}}^{(n)} = 0, \quad (2.7)$$

appropriate to rigid bodies with axial symmetry. These constraints are automatically satisfied if we take wave functions depending on  $\hat{\xi}^{(p)}, \hat{\xi}^{(n)}$  only.

In I we have first expressed the Hamiltonian through the classical components of  $\vec{I}$  and  $\vec{S}$  along the intrinsic axes, and then quantized it by replacing such components by their operator realizations. The latter are well known for  $\vec{I}$ , while for  $\vec{S}$  they resulted to be

$$S_{\xi} = i\frac{\partial}{\partial\theta}, \quad S_{\eta} = -\cot\theta I_{\xi}, \quad S_{\zeta} = -\tan\theta I_{\eta}. \quad (2.8)$$

Following the alternative procedure mentioned in the Introduction, we first quantize by replacing  $\vec{I}$  and  $\vec{S}$  by their Cartesian operator realizations and then perform the change of variables  $(\hat{\xi}^{(p)}, \hat{\xi}^{(n)}) \rightarrow (\alpha, \beta, \gamma, \theta)$ . This change of variables is a unitary transformation provided the scalar product in the new variables is defined by

$$\langle \psi | \psi' \rangle = \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma \int_0^{\pi/2} d(2\theta) \sin(2\theta) \psi^*(\alpha\beta\gamma\theta) \psi'(\alpha\beta\gamma\theta). \quad (2.9)$$

The properties of this transformation are given in Appendix A. We show there that the transformed  $\vec{S}$  operator coincides with (2.8), while the transformed Hamiltonian is

$$H = \frac{1}{2\mathcal{I}}I^2 + H_I, \quad (2.10)$$

$$H_I = \frac{1}{2\mathcal{I}} \left[ \cot^2\theta I_{\xi}^2 + \tan^2\theta I_{\eta}^2 - \frac{\partial^2}{\partial\theta^2} - 2\cot(2\theta) \frac{\partial}{\partial\theta} \right] + \frac{\mathcal{I}_n - \mathcal{I}_p}{4\mathcal{I}_p\mathcal{I}_n} \left[ -\tan\theta I_{\xi} I_{\eta} - \cot\theta I_{\eta} I_{\xi} + i I_{\xi} \frac{\partial}{\partial\theta} \right]. \quad (2.11)$$

$H_I$  for  $N=Z$  differs from the intrinsic Hamiltonian of  $I$  by the term

$$-\frac{1}{\mathcal{I}} \cot(2\theta) \frac{\partial}{\partial\theta}.$$

### III. THE EIGENVALUE PROBLEM

The general expression for the eigenfunctions is

$$\psi_{IM\sigma} = \left( \frac{2I+1}{8\pi^2} \right)^{1/2} \sum_K \mathcal{D}_{MK}^I(\alpha\beta\gamma) \Phi_{IK\sigma}(\theta), \quad (3.1)$$

where  $\sigma$  stands for all necessary quantum numbers.

These eigenfunctions must satisfy the constraints

$$R_{\xi}^{(p)}(\pi) \Psi_{IM\sigma} = R_{\xi}^{(n)}(\pi) \Psi_{IM\sigma} = \Psi_{IM\sigma}, \quad (3.2)$$

owing to the fact that configurations of the system differing by a rotation of  $\pi$  around the  $\xi$  axis are indistinguishable. The other symmetries imposed in I are absent for  $N \neq Z$ .

In Appendix B we derive two sets of relations. The first one is

$$\Phi_{IK\sigma}(\theta) = (-1)^J \Phi_{I-K\sigma}(\theta). \quad (3.3)$$

Using this relation we can rewrite the eigenfunctions as

$$\Psi_{IM\sigma} = \left( \frac{2I+1}{16\pi^2} \right)^{1/2} \sum_{K \geq 0} \frac{1}{\sqrt{1+\delta_{K0}}} [\mathcal{D}_{MK}^I + (-)^I \mathcal{D}_{M-K}^I] \Phi_{IK\sigma}(\theta). \quad (3.4)$$

The second set of constraints relates the values of the  $\Phi$ 's in the regions  $0 \leq \theta \leq \pi/4$  and  $\pi/4 \leq \theta \leq \pi/2$ ,

$$\begin{aligned} \Phi_{00\sigma} \left[ \frac{\pi}{2} - \theta \right] &= \Phi_{00\sigma}(\theta), \\ \Phi_{1K\sigma} \left[ \frac{\pi}{2} - \theta \right] &= -\Phi_{1K\sigma}(\theta), \\ \Phi_{22\sigma} \left[ \frac{\pi}{2} - \theta \right] &= \frac{1}{2} \Phi_{22\sigma}(\theta) - \frac{1}{2} \sqrt{3/2} \Phi_{20\sigma}(\theta), \\ \Phi_{21\sigma} \left[ \frac{\pi}{2} - \theta \right] &= \Phi_{21\sigma}(\theta), \\ \Phi_{20\sigma} \left[ \frac{\pi}{2} - \theta \right] &= -\sqrt{3/2} \Phi_{22\sigma}(\theta) - \frac{1}{2} \Phi_{20\sigma}(\theta). \end{aligned} \quad (3.5)$$

It is therefore sufficient to solve the eigenvalue problem for  $0 \leq \theta \leq \pi/4$ . The solution of the eigenvalue problem is simplified by the following transformation, which eliminates the term linear in the  $\theta$  derivative from the Hamiltonian (2.10),

$$(U\phi_{IK\sigma})(\theta) = \sqrt{\sin(2\theta)} \Phi_{IK\sigma}(\theta) \stackrel{\text{def}}{=} \varphi_{IK\sigma}(\theta), \quad (3.6)$$

$$\begin{aligned} H' = UHU^{-1} &= \frac{1}{2\mathcal{J}} \left\{ \cot^2 \theta I_\xi^2 + \tan^2 \theta I_\eta^2 - \frac{\partial^2}{\partial \theta^2} - [2 + \cot^2(\theta)] \right\} \\ &+ \frac{\mathcal{J}_n - \mathcal{J}_p}{4\mathcal{J}_n \mathcal{J}_p} \left[ \frac{1}{2} (\cot \theta + \tan \theta) (I_\xi I_\eta + I_\eta I_\xi) - i I_\xi \frac{\partial}{\partial \theta} \right] + V(\theta). \end{aligned} \quad (3.7)$$

We assume an harmonic approximation for the potential

$$V(\theta) = \begin{cases} \frac{1}{2} C \theta^2, & 0 \leq \theta \leq \frac{\pi}{4}, \\ \frac{1}{2} C \left[ \frac{\pi}{2} - \theta \right]^2, & \frac{\pi}{4} \leq \theta \leq \frac{\pi}{2}, \end{cases} \quad (3.8)$$

as imposed by the geometry of the system and we consistently expand  $H'$  in powers of  $\theta$  up to second order

$$H' = \frac{1}{2\mathcal{J}} \left[ \frac{1}{\theta^2} (I_\xi^2 - \frac{1}{4}) - \frac{\partial^2}{\partial \theta^2} - 2 \right] + \frac{1}{2} C \theta^2 + \frac{1}{2\mathcal{J}} \theta^2 I_\eta^2 + \frac{\mathcal{J}_n - \mathcal{J}_p}{4\mathcal{J}_n \mathcal{J}_p} \left[ \frac{1}{2} \left[ \frac{1}{\theta} + \theta \right] (I_\xi I_\eta + I_\eta I_\xi) - i I_\xi \frac{\partial}{\partial \theta} \right], \quad 0 \leq \theta \leq \frac{\pi}{4}. \quad (3.9)$$

Let us introduce the definitions

$$\theta_0 = (\mathcal{J}C)^{-1/4}, \quad x = \frac{\theta}{\theta_0}. \quad (3.10)$$

Omitting the constant term  $-1/\mathcal{J}$ ,  $H'$  can be rewritten

$$H' = \frac{1}{2}\omega \left[ -\frac{\partial^2}{\partial x^2} + \frac{1}{x^2} (I_\xi^2 - \frac{1}{4}) + x^2 \right] + \frac{1}{2}\omega \theta_0^4 x^2 I_\eta^2 + \omega \theta_0 \frac{\mathcal{J}_n - \mathcal{J}_p}{\mathcal{J}_n + \mathcal{J}_p} \left[ \frac{1}{2} \left[ x + \theta_0^2 \frac{1}{x} \right] (I_\xi I_\eta + I_\eta I_\xi) - i I_\xi \frac{\partial}{\partial x} \right]. \quad (3.11)$$

According to the estimates made in I for a heavy nucleus (see also Sec. IV)  $\theta_0 \sim 0.03$ , so that  $[(\mathcal{J}_n - \mathcal{J}_p)/(\mathcal{J}_n + \mathcal{J}_p)]\theta_0$  is of the order of 1%, and we can neglect the last term in the Hamiltonian

$$H' = \frac{1}{2}\omega \left[ -\frac{\partial^2}{\partial x^2} + \frac{1}{x^2} (I_\xi^2 - \frac{1}{4}) + x^2 \right], \quad 0 \leq x \leq \frac{\pi}{4\theta_0}, \quad (3.12)$$

which coincides with that obtained by Dieperink<sup>3</sup> in the framework of the IBA. This Hamiltonian does not contain any coupling between states with different  $K$ . In the region  $\pi/4 \leq \theta \leq \pi/2$  states with different  $K$  are instead coupled, because in that region, writing  $[(\pi/2) - \theta]/\theta_0 = y$ , we have

$$H' = \frac{1}{2}\omega \left[ -\frac{\partial^2}{\partial y^2} + \frac{1}{y^2} \left( I_\eta^2 - \frac{1}{4} \right) + y^2 \right]. \quad (3.13)$$

Constraints (3.5) can be shown to be in agreement with the above approximate expression of the Hamiltonian. In this approximation the nucleus still has axial symmetry.

Note, however, that the terms we have neglected in  $H'$ , while small with respect to the intrinsic excitation energies, are comparable to the rotational energy, so that deviation from pure rotational spectrum might be expected.

The eigenfunctions of  $H'$  are

$$\begin{aligned} \varphi_{IKn}(\theta) = \varphi_{Kn}(\theta) &= \left[ \frac{n!}{(n+K+1)\theta_0} \right]^{1/2} \left[ \frac{\theta}{\theta_0} \right]^{K+(1/2)} \\ &\times e^{-(1/2)(\theta/\theta_0)^2} L_n^K(\theta^2/\theta_0^2), \end{aligned} \quad (3.14)$$

with eigenvalues

$$\epsilon_{Kn} = \omega(2n + K + 1). \quad (3.15)$$

The total eigenfunctions are

$$\Psi_{IMKn} = \left[ \frac{2I+1}{16\pi^2(1+\delta_{K0})} \right]^{1/2} [\mathcal{D}_{MK}^I + (-1)^I \mathcal{D}_{M-K}^I] \frac{\varphi_{K\sigma}}{\sqrt{2\theta}}. \quad (3.16)$$

We remark that states with  $n=1, K=0$ , correspond to the classical vibrations shown in Fig. 1(a), while states with  $n=0, K=1$ , correspond to the classical rotations shown in Fig. 1(b).

#### IV. TRANSITION PROBABILITIES AND M1 FORM FACTOR

The electromagnetic radiation excites only states with quantum numbers  $I=K=1, n=0$  and  $I=2, K=1$ , and  $n=0$ , through  $M1$  and  $E2$  multipoles, respectively. The  $n=1, K=0$  states have, in fact, a negligible strength of the order of  $\theta_0^4$ .

##### A. M1 transition

The  $M1$  operator has the following form:

$$\begin{aligned} \mathcal{M}(M1, \mu) &= \sqrt{3/4\pi} \frac{e}{2} \int d\vec{r} [g_p \rho_p(\vec{r}) + g_n \rho_n(\vec{r})] [\vec{r} \times \vec{v}_p(\vec{r})]_\mu \\ &= \sqrt{3/4\pi} \frac{e}{2m} [g_p I_\mu^{(p)} + g_n I_\mu^{(n)}] = \mathcal{M}_0(M1, \mu) + \mathcal{M}_\theta(M1, \mu), \end{aligned} \quad (4.1)$$

where  $\vec{v}_p(\vec{r})$  is the proton velocity field,

$$\mathcal{M}_0(M1, \mu) = \frac{1}{2} \sqrt{3/4\pi} I_\mu (g_p + g_n) \frac{e}{2m}, \quad (4.2)$$

is the isoscalar part which is  $\theta$  independent, and

$$\mathcal{M}_\theta(M1, \mu) = \frac{1}{2} \sqrt{3/4\pi} S_\mu (g_p - g_n) \frac{e}{2m}, \quad (4.3)$$

is the isovector part which is  $\theta$  dependent.

Equation (4.1) shows that the  $M1$  transition is entirely owing to orbital motion. Furthermore, Eq. (4.3) shows that the  $M1$  transition operator does not depend on  $N-Z$  explicitly.

The only nonvanishing reduced amplitude is

$$\begin{aligned} \langle I=K=1, n=0 || \mathcal{M}_\theta(M1, K=1) || I=K=n=0 \rangle &= -i\sqrt{3/16\pi} \int_0^{\pi/2} d\theta \sin(2\theta) \Phi_{110}(\theta) \frac{d}{d\theta} \Phi_{000}(\theta) (g_p - g_n) \frac{e}{2m} \\ &\simeq i\sqrt{3/16\pi} \theta_0^{-1} (g_p - g_n) \frac{e}{2m}, \end{aligned} \quad (4.4)$$

where we used Eqs. (3.14) and (3.5) to evaluate the integral.

The transition probability is therefore

$$B(M1) \uparrow \simeq \frac{3}{16\pi} \theta_0^{-2} (g_p - g_n)^2 \left[ \frac{e}{2m} \right]^2 = \frac{3}{16\pi} \mathcal{I} \omega (g_p - g_n)^2 \left[ \frac{e}{2m} \right]^2, \quad (4.5)$$

which coincides with the expression obtained in the framework of the VPM by Lipparini and Stringari.<sup>6</sup>

### B. $E2$ transition

The  $E2$  operator is

$$\begin{aligned} \mathcal{M}(E2, \mu) &= e \int d\vec{r} \rho_p(R_\theta^{-1} \vec{r}) \vec{r} Y_{2\mu}(\hat{r}) \\ &= e \int d\vec{r} \rho_p(\vec{r}) r^2 Y_{2\mu}(R_\theta \vec{r}) = e \sum_{\nu} Q_{2\nu}^{(p)} \langle 2\nu | \exp(-i\theta I_\xi) | 2\mu \rangle, \end{aligned} \quad (4.6)$$

where

$$Q_{2\nu}^{(p)} = \int d\vec{r} \rho_p(\vec{r}) r^2 Y_{2\mu}(\hat{r}). \quad (4.7)$$

For an ellipsoidal shape  $Q_{2\nu} = Q_{20} \delta_{\nu 0}$ . To first order in  $\theta$  and  $[(\pi/2) - \theta]$ , Eq. (4.6) becomes

$$\mathcal{M}(E2, \mu) = \mathcal{M}_0(E2, \mu) + \mathcal{M}_\theta(E2, \mu), \quad (4.8)$$

where

$$\mathcal{M}_0(E2, \mu) \simeq e Q_{20}^{(p)} \left[ \delta_{\mu 0} S \left[ \theta - \frac{\pi}{4} \right] + \left\langle 20 \left| \exp \left[ -i \frac{\pi}{4} I_\xi \right] \right| 2\mu \right\rangle S \left[ \frac{\pi}{4} - \theta \right] \right], \quad (4.9)$$

$$\mathcal{M}_\theta(E2, \mu) \simeq -ie Q_{20}^{(p)} \sqrt{3/2} \delta_{\mu 1} \left[ \theta S \left[ \theta - \frac{\pi}{4} \right] + \left[ \frac{\pi}{2} - \theta \right] S \left[ \frac{\pi}{4} - \theta \right] \right], \quad (4.10)$$

and

$$S(x) = \begin{cases} 1, & x < 0, \\ 0, & x > 0. \end{cases}$$

Using Eqs. (3.14) and (3.5) we get

$$\langle I = 2K = 1, n = 0 | \mathcal{M}(E2, K = 1) | I = K = n = 0 \rangle \simeq -ie Q_{20}^{(p)} 2\sqrt{3} \int_0^{\pi/4} d\theta \varphi_{210}(\theta) \theta \varphi_{000}(\theta) \simeq -i\sqrt{3} Q_{20}^{(p)} \theta_0 e. \quad (4.11)$$

The  $E2$  transition probability results

$$B(E2) \uparrow \simeq 3 Q_{20}^{(p)2} \theta_0^2 e^2 = 3 Q_{20}^{(p)2} \frac{1}{\mathcal{I}_\omega} e^2. \quad (4.12)$$

### C. The $M1$ form factor

The expression of the orbital part of the  $M1$  operator for electron scattering<sup>7</sup> is, in Born approximation,

$$\hat{T}_{1\mu}^{(m)}(q) = -\frac{i}{\sqrt{2}} \int d\vec{r} [\vec{r} \times \vec{\nabla} j_1(qr) Y_{1\mu}(\hat{r})] [\rho_p(\vec{r}) \vec{v}_p(\vec{r})]. \quad (4.13)$$

Introducing the angular velocity  $\vec{\Gamma}^{(p)}/\mathcal{I}_p = \vec{\Omega}$ , we can relate  $\vec{v}_p$  to  $\vec{\Gamma}^{(p)}$  through the relation

$$\vec{v}_p = -\vec{r} \times \vec{\Omega} = -\frac{1}{\mathcal{I}_p} \vec{r} \times \vec{\Gamma}^{(p)}. \quad (4.14)$$

After performing the angular integrations in Eq. (4.13), approximating  $\rho_p(\vec{r})$  by a spherical density  $\rho_p(r)$ , we get

$$\hat{T}_{1\mu}^{(m)}(q) = \delta_{|\mu| 1} i \sqrt{4\pi/3} \frac{\mathcal{I}_\xi^{(p)}}{\mathcal{I}_p} \int_0^\infty dr r^3 \rho_p(r) j_1(qr), \quad (4.15)$$

as a consequence of the fact that  $\vec{\Omega} \parallel \vec{\xi}$ . We have checked that the first order correction in the deformation is of the order of 1%.

The only nonvanishing matrix element of the above operator is

$$\begin{aligned} \langle I = K = 1, n = 0 | \hat{T}_{1\mu}^{(m)}(q) | I = K = n = 0 \rangle &= -\sqrt{\pi/3} \frac{1}{\mathcal{I}_\theta} \int_0^\infty dr r^3 \rho(r) j_1(qr) \\ &= -\sqrt{\pi/3} \sqrt{\omega/\mathcal{I}} \int_0^\infty dr r^3 \rho(r) j_1(qr), \end{aligned} \quad (4.16)$$

where we have introduced the nuclear density  $\rho(r)$  with normalization

$$\int d\vec{r} \rho(r) = A. \quad (4.17)$$

## V. NUMERICAL ESTIMATES AND RESULTS

In I we have determined the value of the restoring force constant  $C$  by extending the procedure adopted by Goldhaber and Teller.<sup>8</sup> This procedure starts from the observation that when  $\theta$  is larger than a critical value  $\theta_C$ ,  $\frac{1}{2}\rho\Delta v(\theta_C)$  neutron-proton pairs do not interact any longer, causing an increase of the nuclear potential energy

$$V(\theta_C) = \frac{1}{2}\rho\Delta v(\theta_C)v_0, \quad (5.1)$$

where  $v_0$  is the neutron-proton interaction potential, and  $\Delta v(\theta_C)$  is the volume filled by protons or neutrons only as a consequence of the relative proton-neutron rotation, whose expression is<sup>6</sup>

$$\Delta v(\theta) = \frac{32}{3}R^3 |\delta| \theta. \quad (5.2)$$

In I,  $C$  was determined by imposing  $\frac{1}{2}C\theta_C^2 = \frac{1}{2}\rho\Delta v(\theta_C)v_0$ . Since  $\Delta v(\theta)$  is not quadratic, however, in contrast to the harmonic form assumed for the potential, by equating forces rather than energies at  $\theta = \theta_C$ , we would obtain a value of  $C$  smaller by a factor of 2. The latter is a generally adopted criterion so that we must divide by 2 the value obtained in I for  $C$ , getting

$$C = 26A^{4/3}\delta^2 \text{ MeV}. \quad (5.3)$$

Following such a procedure, the value of  $C$  does not depend on  $N - Z$ , provided  $\rho_p(\vec{r}) = Z/N\rho_n(\vec{r})$ . The value of  $C$  could depend on  $N - Z$  if protons and neutrons had a different form for the density. If, for instance, protons had a smaller radius,  $C$  would decrease. In view of the experimental uncertainty in proton-neutron radii we do not evaluate this effect.

Assuming rigid-body values for  $\mathcal{I}_p$  and  $\mathcal{I}_n$ , we obtain

$$\omega = \left[ \left( \frac{A^2}{4NZ} \right) \frac{C}{\mathcal{I}_p + \mathcal{I}_n} \right]^{1/2} \simeq \left( \frac{C}{\mathcal{I}_p + \mathcal{I}_n} \right)^{1/2} \simeq 42 |\delta| A^{-1/6} \text{ MeV}. \quad (5.4)$$

Owing to the combined effect of the new quantization and of different evaluation of  $C$ , the excitation energy is reduced by more than a factor of 2 with respect to I.

The electromagnetic transitions are accordingly modified

$$B(M1)\uparrow \simeq 0.035 |\delta| A^{3/2} (g_p - g_n)^2 \left( \frac{e}{2m} \right)^2, \quad (5.5)$$

$$B(E2)\uparrow \simeq 0.32 \left( \frac{Z^3}{N} \right)^{1/2} |\delta| A^{5/6} e^2 \text{ fm}^4. \quad (5.6)$$

We note that only the  $B(E2)\uparrow$  depends explicitly on  $N - Z$ . The  $M1$  form factor of  $^{156}\text{Gd}$  is shown in Fig. 2 for a hard sphere of radius  $R = 1.2A^{1/3}$  and a Fermi density distribution of parameters  $R = 1.2A^{1/3}$  and  $a = 0.54$  fm. The practical insensitiveness to the diffuseness of the nu-

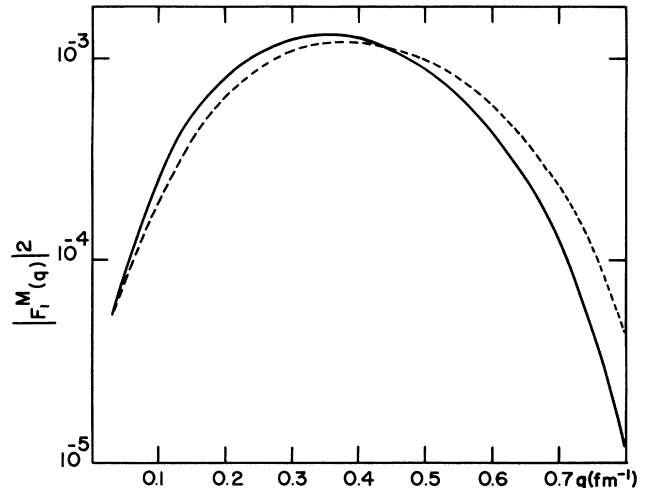


FIG. 2. The  $M1$  form factor of  $^{156}\text{Gd}$  for a Fermi density distribution (full line) and a hard sphere density distribution (dotted line).

clear surface should be noted.

A comparison with the VPM and the IBA shows that our estimates of the excitation energy as well as of  $B(M1)\uparrow$  are larger. We should stress that we have developed a semiclassical model where by assumption the coupling of the present collective mode with other modes is ignored. Now, Suzuki and Rowe,<sup>2</sup> and more explicitly, Lipparini and Stringari<sup>6</sup> have found that the coupling of this  $M1$  state with quadrupole surface vibrations reduces its frequency by a factor of 2. Our formula (4.5) shows that  $B(M1)$  is proportional to the excitation energy, so that it should be proportionally reduced, as confirmed in Ref. 6.

## APPENDIX A

In this appendix we perform the change of variables  $(\hat{\zeta}^{(p)}, \hat{\zeta}^{(n)}) \rightarrow (\alpha, \beta, \gamma, \theta)$  and derive the expression of the transformed operators. We will omit the vector and versor symbols from here on for simplicity.

Let us denote by  $(e_i)$ ,  $i = 1, 2, 3$ , a fixed right-handed orthonormal (RHON) frame in a three-dimensional space, and by  $\text{SO}(3)$  the group of proper rotations. A rotation of an angle  $\varphi$  around the unit vector  $n$  will be indicated by  $R_n(\varphi)$  [if  $n = e_k$  we simply write  $R_k(\varphi)$ ], and its action on a vector  $y$  is given by

$$R_n(\varphi)y = (n \cdot y)n + \cos\varphi[n \times (n \cdot y)n] + \sin\varphi n \times y. \quad (A1)$$

For any rotation  $R$  the unit vectors  $V_i$  defined by

$$V_i = R e_i \quad (i = 1, 2, 3) \quad (A2)$$

form a RHON frame, and, conversely, any given RHON frame  $(V_i)$  uniquely defines a rotation  $R$  through Eqs. (A1) and (A2). Hence, (A2) gives a one to one correspondence between the group  $\text{SO}(3)$  and the set of RHON frames  $(V_i)$ .

As it is well known, one can specify any frame  $(V_i)$ , and hence, the rotation defined by it, by means of the

Euler angles  $(\alpha, \beta, \gamma)$ , which can be chosen so that

$$\begin{aligned} R(\alpha, \beta, \gamma)e_i &= V_i(\alpha, \beta, \gamma) = R_3(\alpha)R_2(\beta)R_3(\gamma)e_i, \\ 0 \leq \alpha \leq 2\pi, \quad 0 \leq \beta \leq \pi, \quad 0 \leq \gamma \leq 2\pi. \end{aligned} \quad (\text{A3})$$

According to (A3),  $(\alpha, \beta)$  are simply the polar angles of  $V_3$  with respect to  $(e_i)$ .

The correspondence between  $(\alpha, \beta, \gamma)$  and  $V_i(\alpha, \beta, \gamma)$  is one to one if the angles are restricted to vary in  $0 < \alpha < 2\pi$ ,  $0 < \beta < \pi$ , and  $0 < \gamma < 2\pi$ . Hence, apart from exceptional cases, (A3) gives a parametrization in terms of  $(\alpha, \beta, \gamma)$  of the rotations  $R \in \text{SO}(3)$ . We recall that on the group  $\text{SO}(3)$  an invariant measure  $d\mu(R)$  exists

$$\begin{aligned} \int_{\text{SO}(3)} f(RS) d\mu(R) &= \int_{\text{SO}(3)} f(SR) d\mu(R) \\ &= \int_{\text{SO}(3)} f(R) d\mu(R) \quad \forall S \in \text{SO}(3). \end{aligned} \quad (\text{A4})$$

In terms of  $\alpha, \beta, \gamma$ , the measure is  $d\mu(\alpha, \beta, \gamma) = \sin\beta d\alpha d\beta d\gamma$  and the transformations  $R \rightarrow SR, R \rightarrow RS$  of  $\text{SO}(3)$  into itself become

$$\begin{aligned} (\alpha, \beta, \gamma) &\rightarrow (\alpha', \beta', \gamma') \text{ if } R(\alpha', \beta', \gamma') = SR(\alpha, \beta, \gamma), \\ (\alpha, \beta, \gamma) &\rightarrow (\alpha'', \beta'', \gamma'') \text{ if } R(\alpha'', \beta'', \gamma'') = R(\alpha, \beta, \gamma)S, \end{aligned}$$

so that the invariance of the measure in (A4) means

$$\begin{aligned} \int_0^{2\pi} d\alpha \int_0^\pi d\beta \sin\beta \int_0^{2\pi} d\gamma f(\alpha', \beta', \gamma') &= \int_0^{2\pi} d\alpha \int_0^\pi d\beta \sin\beta \int_0^{2\pi} d\gamma f(\alpha'', \beta'', \gamma'') \\ &= \int_0^{2\pi} d\alpha \int_0^\pi d\beta \sin\beta \int_0^{2\pi} d\gamma f(\alpha, \beta, \gamma). \end{aligned}$$

We finally note that from (A3) any unit vector  $\zeta$  of polar angles  $\theta_\zeta \Phi_\zeta$  can be obtained as

$$\zeta = R(\zeta)e_3 = R_3(\phi_\zeta)R_2(\theta_\zeta)e_3. \quad (\text{A5})$$

The measure  $d\mu(\zeta) = \sin\theta_\zeta d\theta_\zeta d\Phi_\zeta$  is rotationally invariant in the sense that

$$\int f(S\zeta) d\mu(\zeta) = \int f(\zeta) d\mu(\zeta) \quad \forall S \in \text{SO}(3). \quad (\text{A6})$$

We want to use as variables, instead of the two unit vectors  $\zeta^{(p)}, \zeta^{(n)}$ , the angle  $2\theta$  between them and the Euler angles  $(\alpha, \beta, \gamma)$  of the intrinsic frame  $(\xi, \eta, \zeta)$ . To this end, we consider the correspondence  $\tau: (\zeta^{(p)}, \zeta^{(n)}) \rightarrow [\theta(\zeta^{(p)}, \zeta^{(n)}), \mathcal{R}(\zeta^{(p)}, \zeta^{(n)})]$  defined by

$$\begin{aligned} \cos[2\theta(\zeta^{(p)}, \zeta^{(n)})] &= \zeta^{(p)} \cdot \zeta^{(n)}, \\ \mathcal{R}(\zeta^{(p)}, \zeta^{(n)})e_3 &= V_3(\zeta^{(p)}, \zeta^{(n)}) = \zeta = \frac{1}{2\cos\theta}(\zeta^{(p)} + \zeta^{(n)}), \\ \mathcal{R}(\zeta^{(p)}, \zeta^{(n)})e_2 &= V_2(\zeta^{(p)}, \zeta^{(n)}) = \eta = \frac{1}{2\sin\theta}(\zeta^{(p)} - \zeta^{(n)}), \\ \mathcal{R}(\zeta^{(p)}, \zeta^{(n)})e_1 &= V_1(\zeta^{(p)}, \zeta^{(n)}) = \xi = \frac{1}{\sin(2\theta)}\zeta^{(p)} \times \zeta^{(n)}. \end{aligned} \quad (\text{A7})$$

Through Eq. (A3) the above equations define the Euler angles  $(\alpha, \beta, \gamma)$ , which we will denote simply by  $R$ .

It is easy to see that apart from  $\theta = 0, \pi/2$ ,  $\tau$  is a one to one correspondence. Its inverse  $\tau^{-1}(\theta, \mathcal{R}) \rightarrow (\zeta^{(p)}, \zeta^{(n)})$  is

$$\begin{aligned} \zeta^{(p)}(\theta, \mathcal{R}) &= \cos\theta V_3(\mathcal{R}) + \sin\theta V_2(\mathcal{R}), \\ \zeta^{(n)}(\theta, \mathcal{R}) &= \cos\theta V_3(\mathcal{R}) - \sin\theta V_2(\mathcal{R}). \end{aligned} \quad (\text{A8})$$

Our aim is now to relate wave functions and operators from the  $(\zeta^{(p)}, \zeta^{(n)})$  representation, in which our Hamiltonian has been defined, to those in the  $(\theta, \alpha, \beta, \gamma)$  or, equivalently,  $(\theta, \mathcal{R})$  representation. Using (A8), if  $F(\zeta^{(p)}, \zeta^{(n)})$  is a wave function in the  $(\zeta^{(p)}, \zeta^{(n)})$  representation, the corresponding wave function in the  $(\theta, \mathcal{R})$  representation is

$$(VF)(\theta, \mathcal{R}) \stackrel{\text{def}}{=} F[\zeta^{(p)}(\theta, \mathcal{R}), \zeta^{(n)}(\theta, \mathcal{R})]. \quad (\text{A9})$$

The inverse transformation, if  $G(\theta, \mathcal{R})$  is a wave function in the  $(\theta, \mathcal{R})$  representation, is

$$(V^{-1}G)(\zeta^{(p)}, \zeta^{(n)}) = G[\theta(\zeta^{(p)}, \zeta^{(n)}), \mathcal{R}(\zeta^{(p)}, \zeta^{(n)})]. \quad (\text{A10})$$

$V$  will be a unitary transformation if we define the scalar product in the  $(\theta, \mathcal{R})$  representation as

$$(G_1, G_2) = \int G_1^*(\theta, \mathcal{R}) G_2(\theta, \mathcal{R}) \rho(\theta, \mathcal{R}) d\theta d\mu(\mathcal{R}),$$

where  $d\mu(\mathcal{R})$  is the invariant measure on  $\text{SO}(3)$ , and  $\rho(\theta, \mathcal{R})$  is a (non-negative) function to be chosen so that

$$\begin{aligned} \int |F(\zeta^{(p)}, \zeta^{(n)})|^2 d\mu(\zeta^{(p)}) d\mu(\zeta^{(n)}) &= \int |(VF)(\theta, \mathcal{R})|^2 \rho(\theta, \mathcal{R}) d\theta d\mu(\mathcal{R}) \\ &= \int |F[\zeta^{(p)}(\theta, \mathcal{R}), \zeta^{(n)}(\theta, \mathcal{R})]|^2 \rho(\theta, \mathcal{R}) d\theta d\mu(\mathcal{R}). \end{aligned}$$

In the present situation, it is possible to determine  $\rho$  without going through the evaluation of the Jacobian of the

transformation  $\tau$ . Observe, in fact, that we must also have

$$\begin{aligned} \int |G(\theta, R)|^2 \rho(\theta, R) d\theta d\mu(R) &= \int |(V^{-1}G)(\zeta^{(p)}, \zeta^{(n)})|^2 d\mu(\zeta^{(p)}) d\mu(\zeta^{(n)}) \\ &= \int d\mu(\zeta^{(p)}) \int |(V^{-1}G)(\zeta^{(p)}, \zeta^{(n)})|^2 d\mu(\zeta^{(n)}) \\ &= \int d\mu(\zeta^{(p)}) \int |(V^{-1}G)(\zeta^{(p)}, S\zeta^{(n)})|^2 d\mu(\zeta^{(n)}), \end{aligned} \quad (\text{A11})$$

where  $S$  is any rotation in  $\text{SO}(3)$ .

In the last step we used the rotation invariance of  $d\mu(\zeta^{(n)})$ . Note that  $S$  is allowed to depend on  $\zeta^{(p)}$ , as it actually will. Let  $(\theta_p, \phi_p)$  and  $(\theta_n, \phi_n)$  be the polar angles of  $\zeta^{(p)}$  and  $\zeta^{(n)}$ , and

$$\zeta^{(p)} = R_3(\phi_p)R_2(\theta_p)e_3 = S(\zeta_p)e_3.$$

It follows from (A7) that, calling  $\theta_S = \theta[\zeta^{(p)}, S(\zeta^{(p)})\zeta^{(n)}]$

$$\begin{aligned} \cos(2\theta_S) &= \zeta^{(p)}[S(\zeta^{(p)})\zeta^{(n)}] \\ &= [S(\zeta^{(p)})e_3][S(\zeta^{(p)})\zeta^{(n)}] \\ &= e_3 \cdot \zeta^{(n)} = \cos\theta_n. \end{aligned}$$

In other words, with the choice we made of  $S(\zeta^{(p)})$ , the angle  $2\theta$  between  $\zeta^{(p)}$  and  $S(\zeta^{(p)})\zeta^{(n)}$  is precisely the azimuthal angle  $\theta_n$  of  $\zeta^{(n)}$ . Using this, our formula (A11) becomes

$$\begin{aligned} \int |G(\theta, R)|^2 \rho(\theta, R) d\theta d\mu(R) &= \int d\mu(\zeta^{(p)}) \int_0^\pi d\theta_n \sin\theta_n \int_0^{2\pi} d\phi_n |G\{\theta[\zeta^{(p)}, S(\zeta^{(p)})\zeta^{(n)}], R[\zeta^{(p)}, S(\zeta^{(p)})\zeta^{(n)}]\}|^2 \\ &= \int d\mu(\zeta^{(p)}) \int_0^\pi d\theta_n \sin\theta_n \int_0^{2\pi} d\phi_n \left| G\left\{\frac{\theta_n}{2}, R[\zeta^{(p)}, S(\zeta^{(p)})\zeta^{(n)}]\right\} \right|^2 \\ &= \int_0^{\pi/2} d(2\theta) \sin(2\theta) \int d\mu(\zeta^{(p)}) \int_0^{2\pi} d\phi_n |G\{\theta, R[\zeta^{(p)}, S(\zeta^{(p)})\zeta^{(n)}]\}|^2. \end{aligned}$$

We will show in a moment that

$$R[\zeta^{(p)}, S(\zeta^{(p)})\zeta^{(n)}] = R_3(\phi_p)R_2(\theta_p)R_3(\phi_n)R(\theta),$$

where  $R(\theta)$  is a rotation depending on the intrinsic angle  $\theta$ . Taking this result for granted, we have

$$\int |G(\theta, R)|^2 \rho(\theta, R) d\theta d\mu(R) = \int_0^{\pi/2} d(2\theta) \sin(2\theta) \int_0^{2\pi} d\phi_n \int_0^\pi d\theta_p \sin\theta_p \int_0^{2\pi} d\phi_p |G[\theta, R(\phi_p, \theta_p, \phi_n)R(\theta)]|^2,$$

where

$$R(\phi_p, \theta_p, \phi_n) = R_3(\phi_p)R_2(\theta_p)R_3(\phi_n).$$

As  $\phi_p$ ,  $\theta_p$ , and  $\phi_n$  vary over their allowed ranges,  $R$  describes the full group  $\text{SO}(3)$ . Furthermore,  $\sin\theta_p d\theta_p d\phi_p d\phi_n$  is just the invariant measure on  $\text{SO}(3)$  for the parametrization we are using. Hence

$$\begin{aligned} \int |G(\theta, R)|^2 \rho(\theta, R) d\theta d\mu(R) &= \int_0^{\pi/2} d(2\theta) \sin(2\theta) \int d\mu(R) |G[\theta, RR(\theta)]|^2 \\ &= \int_0^{\pi/2} d(2\theta) \sin(2\theta) \int d\mu(R) |G(\theta, R)|^2. \end{aligned}$$

We have used in the last step the invariance of  $d\mu(R)$  to get rid of  $R(\theta)$ . This shows that  $\rho(\theta, R) = 2 \sin(2\theta)$ .

The assertion we used in this proof must now be verified. From (A7),

$$R[\zeta^{(p)}, S(\zeta^{(p)})\zeta^{(n)}]e_3 = \frac{1}{2 \cos\theta} [\zeta^{(p)} + S(\zeta^{(p)})\zeta^{(n)}],$$

$$R[\zeta^{(p)}, S(\zeta^{(p)})\zeta^{(n)}]e_2 = \frac{1}{2 \sin\theta} [\zeta^{(p)} - S(\zeta^{(p)})\zeta^{(n)}],$$

with  $\zeta^{(p)} = S(\zeta^{(p)})e_3$  and  $\theta = \theta_n/2$ . Hence

$$R[\zeta^{(p)}, S(\zeta^{(p)})\zeta^{(n)}]e_3 = S(\zeta^{(p)})R_3(\phi_n) \left\{ \frac{1}{2 \cos\theta} [e_3 + R_2(2\theta)e_3] \right\} = S(\zeta^{(p)})R_3(\phi_n)V'_3,$$

$$R[\zeta^{(p)}, S(\zeta^{(p)})\zeta^{(n)}]e_2 = S(\zeta^{(p)})R_3(\phi_n) \left\{ \frac{1}{2 \sin\theta} [e_3 - R_2(2\theta)e_3] \right\} = S(\zeta^{(p)})R_3(\phi_n)V'_2.$$

The vectors  $V'_3, V'_2$ , and  $V'_1 = V'_2 \times V'_3$  are orthonormal and hence can be written as  $V'_K = R(\theta)e_K$ . Finally,



$$\begin{aligned} R[\zeta^{(p)}, S(\zeta^{(p)})\zeta^{(n)}] &= S(\zeta^{(p)})R_3(\phi_n)R(\theta) \\ &= R_3(\phi_p)R_2(\theta_p)R_3(\phi_n)R(\theta). \end{aligned}$$

We now want to transform the operators  $I^{(p)}, I^{(n)}$ , to the  $(\theta, R)$  representation. This can be done most easily if we remember that  $I^{(p)}, I^{(n)}$  are the generators of rotations on the vectors  $\zeta^{(p)}, \zeta^{(n)}$ . To be precise, if  $R_n(\varphi)$  is a rotation of an angle  $\varphi$  around the unit vector  $n$ , we have, on suitably regular functions of  $\zeta^{(p)}, \zeta^{(n)}$ ,

$$[(-in \cdot I^{(p)})F](\zeta^{(p)}, \zeta^{(n)}) = \frac{\partial}{\partial \varphi} F[R_n^{-1}(\varphi)\zeta^{(p)}, \zeta^{(n)}] \Big|_{\varphi=0} = \dot{F}[R_n^{-1}(\varphi)\zeta^{(p)}, \zeta^{(n)}],$$

$$[(-in \cdot I^{(n)})F](\zeta^{(p)}, \zeta^{(n)}) = \dot{F}[\zeta^{(p)}, R_n^{-1}(\varphi)\zeta^{(n)}],$$

where the dot will be used to indicate  $(\partial/\partial\varphi) \Big|_{\varphi=0}$  from here on. If  $I_\epsilon = I^{(p)} + \epsilon I^{(n)}$  and  $\epsilon = \pm 1$ , it follows that

$$[(-in \cdot I_\epsilon)F](\zeta^{(p)}, \zeta^{(n)}) = \dot{F}[R_n^{-1}(\varphi)\zeta^{(p)}, R_n^{-1}(\epsilon\varphi)\zeta^{(n)}].$$

With the notation used in the paper,  $I_1 = I$ , the total angular momentum operator, and  $I_{-1} = S$ .

It turns out that the calculations are simpler if we specialize the axis  $n$  introduced above to be one of the unit vectors  $V_K(\zeta^{(p)}, \zeta^{(n)})$  of the intrinsic frame. We consider then the operators  $-iV_K \cdot I_\epsilon$  whose action on  $F(\zeta^{(p)}, \zeta^{(n)})$  is

$$[(-iV_K \cdot I_\epsilon)F](\zeta^{(p)}, \zeta^{(n)}) = [V_K(\zeta^{(p)}, \zeta^{(n)})]_r [(-ie_r \cdot I_\epsilon)F](\zeta^{(p)}, \zeta^{(n)}) = \dot{F}[R_{V_K(\zeta^{(p)}, \zeta^{(n)})}^{-1}(\varphi)\zeta^{(p)}, R_{V_K(\zeta^{(p)}, \zeta^{(n)})}^{-1}(\epsilon\varphi)\zeta^{(n)}], \quad (\text{A12})$$

the  $V_K(\zeta^{(p)}, \zeta^{(n)})$ 's being defined in (A7). If  $V$  is the unitary transformation introduced in (A9) and (A10), we must evaluate

$$\begin{aligned} [V(-iV_K \cdot I_\epsilon)V^{-1}G](\theta, R) &= [(-iV_K \cdot I_\epsilon)V^{-1}G][\zeta^{(p)}(\theta, R), \zeta^{(n)}(\theta, R)] \\ &= (\partial/\partial\varphi)_{\varphi=0} (V^{-1}G)[R_{V_K(R)}^{-1}(\varphi)\zeta^{(p)}(\theta, R), R_{V_K(R)}^{-1}(\epsilon\varphi)\zeta^{(n)}(\theta, R)] \\ &= \dot{G}[\theta^{(K)}(\epsilon, \varphi), \alpha^{(K)}(\epsilon, \varphi), \beta^{(K)}(\epsilon, \varphi), \gamma^{(K)}(\epsilon, \varphi)]. \end{aligned} \quad (\text{A13})$$

where

$$\cos[2\theta^{(K)}(\epsilon, \varphi)] = [R_{V_K(R)}^{-1}(\varphi)\zeta^{(p)}(\theta, R)] \cdot [R_{V_K(R)}^{-1}(\epsilon\varphi)\zeta^{(n)}(\theta, R)], \quad (\text{A14})$$

and where  $\alpha^{(K)}(\epsilon, \varphi)$ ,  $\beta^{(K)}(\epsilon, \varphi)$ , and  $\gamma^{(K)}(\epsilon, \varphi)$  are the Euler angles of the frame

$$V_i^{(K)}(\epsilon, \varphi) = V_i [R_{V_K(R)}^{-1}(\varphi)\zeta^{(p)}(\theta, R), R_{V_K(R)}^{-1}(\epsilon\varphi)\zeta^{(n)}(\theta, R)]. \quad (\text{A15})$$

In deriving the previous relations use has been made of (A9) and (A10), and, of course, of the definitions (A7) and (A8).

If we indicate temporarily as  $\overline{-iV_K \cdot I_\epsilon}$  the operators  $V(-iV_K \cdot I_\epsilon)V^{-1}$  we have from (A13), on suitably regular functions  $G(\theta, \alpha, \beta, \gamma)$ ,

$$\begin{aligned} [(\overline{-iV_K \cdot I_\epsilon})G](\theta, \alpha, \beta, \gamma) &= \frac{\partial}{\partial \theta} G(\theta, \alpha, \beta, \gamma) \dot{\theta}^{(K)}(\epsilon, \varphi) + \frac{\partial G}{\partial \alpha}(\theta, \alpha, \beta, \gamma) \dot{\alpha}^{(K)}(\epsilon, \varphi) + \frac{\partial}{\partial \beta} G(\theta, \alpha, \beta, \gamma) \dot{\beta}^{(K)}(\epsilon, \varphi) \\ &\quad + \frac{\partial}{\partial \gamma} G(\theta, \alpha, \beta, \gamma) \dot{\gamma}^{(K)}(\epsilon, \varphi). \end{aligned} \quad (\text{A16})$$

This formula explicitly gives the operators  $\overline{-iV_K \cdot I_\epsilon}$  as differential operators with respect to  $\theta$  and the Euler angles, once the  $\dot{\alpha}^{(K)}(\epsilon, \varphi), \dots$ , etc., are known.

It is easy to relate the derivatives of Eq. (A16) to  $\dot{V}_i^{(K)}$ . Recalling, in fact, the definition (A3) and using (A1) one gets

$$\begin{aligned} e_3 \cdot V_3 &= \cos \beta, \\ e_1 \cdot V_3 &= \cos \alpha \cos \beta, \\ e_3 \cdot V_1 &= -\sin \beta \cos \gamma. \end{aligned}$$

Applying these relations to the vectors of the transformed frame  $V_i^{(K)}(\epsilon, \varphi)$  (A15) we obtain the following:

$$\begin{aligned} \dot{\beta}^{(K)}(\epsilon) &= -\frac{1}{\sin \beta} e_3 \cdot \dot{V}_3^{(K)}(\epsilon), \\ \dot{\alpha}^{(K)}(\epsilon) &= -\frac{1}{\sin \alpha \sin \beta} [e_1 \cdot \dot{V}_3^{(K)}(\epsilon) + \cot \beta \cos \alpha e_3 \cdot \dot{V}_3^{(K)}(\epsilon)], \\ \dot{\gamma}^{(K)}(\epsilon) &= \frac{1}{\sin \beta \sin \gamma} [e_3 \cdot \dot{V}_1^{(K)}(\epsilon) - \cot \beta \cos \gamma e_3 \cdot \dot{V}_3^{(K)}(\epsilon)]. \end{aligned} \quad (\text{A17})$$

(Note that, clearly,  $\alpha^{(K)}(\epsilon, 0) = \alpha, \dots$ , etc.) The evaluation of  $\dot{\theta}^{(K)}(\epsilon)$  and  $\dot{V}_i^{(K)}(\epsilon)$  is straightforward. From (A1),  $\dot{R}_n^{-1}(\varphi)y = -n \times y$ . Using this and (A7) and (A8), we obtain from (A14) and (A15),

$$\begin{aligned}\dot{\theta}^{(K)}(\epsilon) &= \frac{1}{2}(1-\epsilon)\delta_{K1}, \\ \dot{V}_3^{(K)}(\epsilon) &= -\frac{1}{2}(1+\epsilon)V_K \times V_3 - \frac{1}{2}(1-\epsilon)\tan\theta(-\delta_{K1}V_3 + V_K \times V_2), \\ \dot{V}_2^{(K)}(\epsilon) &= -\frac{1}{2}(1+\epsilon)V_K \times V_2 - \frac{1}{2}(1-\epsilon)\cot\theta(\delta_{K1}V_2 + V_K \times V_3), \\ \dot{V}_1^{(K)}(\epsilon) &= -\frac{1}{2}(1+\epsilon)V_K \times V_1 - \frac{1}{2}(1-\epsilon)\{(\cot\theta - \tan\theta)\delta_{K1}V_1 + \tan\theta[V_K - (V_K \cdot V_2)V_2] - \cot\theta[V_K - (V_K \cdot V_3)V_3]\}.\end{aligned}\quad (\text{A18})$$

[We have written  $V_K$  instead of the complete notation  $V_K(\alpha, \beta, \gamma)$ .] From these formulas we can draw, by inspection, the following conclusions:

$$\dot{\theta}^{(K)}(\epsilon=1)=0, \quad \dot{V}_i^{(K)}(\epsilon=1)=-V_K \times V_i, \\ \dot{\theta}^{(K)}(\epsilon=-1)=\delta_{K1}, \quad \dot{V}_i^{(1)}(\epsilon=-1)=0, \quad (\text{A19})$$

$$\dot{V}_i^{(2)}(\epsilon=-1)=-\cot\theta\dot{V}_i^{(3)}(\epsilon=1), \quad (\text{A20})$$

$$\dot{V}_i^{(3)}(\epsilon=-1)=-\tan\theta\dot{V}_i^{(2)}(\epsilon=1).$$

Since, for fixed values of  $\alpha, \beta$ , and  $\gamma$ , the relations (A17) are linear in the  $\dot{V}_i^{(K)}(\epsilon)$ 's, we have immediately from (A16), using (A20),

$$\overline{V_3 \cdot I_{-1}} = -\tan\theta \overline{V_2 \cdot I_1},$$

$$V_2 \cdot I_{-1} = -\cot\theta \overline{V_3 \cdot I_1},$$

$$\overline{V_1 \cdot I_{-1}} = i \frac{\partial}{\partial \theta}.$$

In the notation used in the main text,  $I_1 = I, I_{-1} = S, V_3 = \zeta, V_2 = \eta$ , and  $V_1 = \xi$ ; this means

$$\zeta \cdot S = -\tan\theta \eta \cdot I, \quad \eta \cdot S = -\cot\theta \zeta \cdot I, \quad \xi \cdot S = i \frac{\partial}{\partial \theta}. \quad (\text{A21})$$

$$\begin{aligned}S^2 &= \sum_K (V_K \cdot S)^2 + (\tan\theta - \cot\theta)(-iV_1 \cdot S) \\ &= \tan^2\theta (V_2 \cdot I)^2 + \cot^2\theta (V_3 \cdot I)^2 - \frac{\partial^2}{\partial \theta^2} - 2 \cot(2\theta) \frac{\partial}{\partial \theta}\end{aligned}$$

$$I \cdot S = \sum_K (V_K \cdot I)(V_K \cdot S) = -\tan\theta (V_3 \cdot I)(V_2 \cdot I) - \cot\theta (V_2 \cdot I)(V_3 \cdot I) + iV_1 \cdot I \frac{\partial}{\partial \theta}.$$

It follows that

$$H_0 = \frac{1}{2\mathcal{J}} I^2 + \frac{1}{2\mathcal{J}} \left[ \tan^2\theta I_\eta^2 + \cot^2\theta I_\zeta^2 - \frac{\partial^2}{\partial \theta^2} - 2 \cot(2\theta) \frac{\partial}{\partial \theta} \right] + \frac{\mathcal{J}_n - \mathcal{J}_p}{4\mathcal{J}_r \mathcal{J}_p} \left[ -\tan\theta I_\zeta I_\eta - \cot\theta I_\eta I_\zeta + i I_\xi \frac{\partial}{\partial \theta} \right]. \quad (\text{A23})$$

Using  $[(V_K \cdot I), (V_n \cdot I)] = -iV_K \times V_n \cdot I$ , implied by (A22) and  $[I_K, I_n] = i\epsilon_{Knr}I_r$ , the second bracket in  $H_0$  can also be rewritten as

$$\frac{\mathcal{J}_n - \mathcal{J}_p}{4\mathcal{J}_r \mathcal{J}_p} \left[ -\frac{1}{2}(\tan\theta + \cot\theta)(I_\zeta I_\eta + I_\eta I_\zeta) - \frac{i}{2}(\tan\theta - \cot\theta)I_\xi + i I_\xi \frac{\partial}{\partial \theta} \right]. \quad (\text{A24})$$

## APPENDIX B

As explained in the paper, we must require that the wave functions of our system satisfy

$$\begin{aligned}(\mathcal{O}_p F)(\zeta^{(p)}, \zeta^{(n)}) &= F(-\zeta^{(p)}, \zeta^{(n)}) = F(\zeta^{(p)}, \zeta^{(n)}), \\ (\mathcal{O}_n F)(\zeta^{(p)}, \zeta^{(n)}) &= F(\zeta^{(p)}, -\zeta^{(n)}) = F(\zeta^{(p)}, \zeta^{(n)}),\end{aligned}\quad (\text{B1})$$

Inserting (A19) into (A17) and also using our definition (A3) of the Euler angles, we could easily derive from (A16) the explicit form of the operators  $-iV_K \cdot I$  (angular momentum operators of a three dimensional rotator referred to the intrinsic frame) reported in many textbooks. This result, however, has not been used in the paper. It is, on the contrary, worth to note that from (A19) and (A20) the commutation relations  $[V_K \cdot I, (V_n)_r]$  and  $[V_K \cdot S, (V_n)_r]$   $[(V_n)_r = e_r \cdot V_n]$  can be derived. The latter are needed to transform to the  $(\theta, \alpha, \beta, \gamma)$  representation the operators  $I^{(p)2}, I^{(n)2}$  appearing in the Hamiltonian of the model. In fact, it is easy to see that

$$[-iV_K \cdot I, (V_n)_r] = [\dot{V}_n^{(K)}(\epsilon)]_r.$$

From (A19)

$$[V_K \cdot I, V_n] = -iV_K \times V_n, \quad (\text{A22})$$

from which all other commutators can be derived, since  $V_3 \cdot S, V_2 \cdot S$  are proportional to  $V_2 \cdot I, V_3 \cdot I$ , and, of course,  $V_1 \cdot S = i(\partial/\partial\theta)$  commutes with the  $V_K$ 's whose dependence is only on the Euler angles.

We have  $\sum_K (V_K \cdot I)^2 = I^2$  and

here we use the notation  $O_p, O_n$  instead of  $R_\xi^{(p)}(\pi), R_\xi^{(n)}(\pi)$ .

Since  $O_p O_n = O_n O_p$  and  $O_p^2 = O_n^2 = 1$ , we can impose the equivalent conditions

$$OF = O_p O_n F = F, \quad O_p F = F, \quad (B2)$$

and with the help of the unitary transformation  $V$  defined in (A7) and (A8), it is easy to find the action of the operators  $O$  and  $O_p$  on the wave functions in the  $(\theta, \alpha, \beta, \gamma)$  representation

$$(\bar{O}G)(\theta, \alpha, \beta, \gamma) = (VOV^{-1}G)(\theta, \alpha, \beta, \gamma) = G(\theta, \alpha', \beta', \gamma'),$$

where the transformed Euler angles  $(\alpha', \beta', \gamma')$  are defined by

$$\begin{aligned} R(\alpha', \beta', \gamma') &= R_{V_1(\alpha, \beta, \gamma)}(\pi) R(\alpha, \beta, \gamma) = R_{R(\alpha, \beta, \gamma) e_1}(\pi) R(\alpha, \beta, \gamma) \\ &= [R(\alpha, \beta, \gamma) R_{e_1}(\pi) R^{-1}(\alpha, \beta, \gamma)] R(\alpha, \beta, \gamma) = R(\alpha, \beta, \gamma) R_{e_1}(\pi) \end{aligned} \quad (B3)$$

and

$$(\bar{O}_p G)(\theta, \alpha, \beta, \gamma) = (VO_p V^{-1}G)(\theta, \alpha, \beta, \gamma) = G\left[\frac{\pi}{2} - \theta, \alpha'', \beta'', \gamma''\right],$$

where

$$\begin{aligned} R(\alpha'', \beta'', \gamma'') &= R_{V_3(\alpha, \beta, \gamma)}\left(\frac{3}{2}\pi\right) R_{V_2(\alpha, \beta, \gamma)}\left[\frac{\pi}{2}\right] R_{V_3(\alpha, \beta, \gamma)}\left(\frac{3}{2}\pi\right) R(\alpha, \beta, \gamma) = R_p(\alpha, \beta, \gamma) R(\alpha, \beta, \gamma) R_p, \\ R_p &= R_3\left(\frac{3}{2}\pi\right) R_2\left[\frac{\pi}{2}\right] R_3\left(\frac{3}{2}\pi\right). \end{aligned} \quad (B4)$$

We use here  $R(\alpha, \beta, \gamma)$  and  $V_K(\alpha, \beta, \gamma)$  as defined in (A3). Since the Hamiltonian of our model commutes with the total angular momentum  $I = I^{(p)} + I^{(n)}$ , its eigenfunctions must be of the form

$$\Psi(\theta, \alpha, \beta, \gamma) = \sum_K \mathcal{D}_{MK}^I(\alpha, \beta, \gamma) \phi_{IK}(\theta), \quad (B5)$$

where we suppressed the additional quantum number  $\sigma$  in  $\phi_{IK}$ , since it does not play any role here. We choose for the  $\mathcal{D}_{MK}^I$  functions the definition given in Ref. 9

$$\mathcal{D}_{MK}^I(\alpha, \beta, \gamma) = [\psi_{IM}, D^I(\alpha, \beta, \gamma) \psi_{IK}]^*,$$

where

$$D^I(\alpha, \beta, \gamma) = e^{-i\alpha I_3} e^{-i\beta I_2} e^{-i\gamma I_3}. \quad (B6)$$

Here  $D^I(R)$  is the spin- $I$  representation of the rotation  $R \in \text{SO}(3)$  and the  $\Psi_{IM}$  are standard basic vectors in the space of the said representation.

From (B6) it is easy to derive the equations

$$(I_i \mathcal{D}_{MK}^I)(\alpha, \beta, \gamma) = \sum_{M'} (\psi_{IM}, I_i \psi_{IM'})^* \mathcal{D}_{M'K}^I(\alpha, \beta, \gamma)$$

and

$$[(V_i \cdot I) \mathcal{D}_{MK}^I](\alpha, \beta, \gamma) = V_i(\alpha, \beta, \gamma) \cdot (I \mathcal{D}_{MK}^I)(\alpha, \beta, \gamma) = \sum_{K'} (\psi_{IK}, I_i \psi_{IK'}) \mathcal{D}_{MK'}^I(\alpha, \beta, \gamma), \quad (B7)$$

giving, respectively, the actions on the  $\mathcal{D}_{MK}^I$  of the fixed and intrinsic frame  $I$  components of the total momentum. The symmetry conditions on  $\Psi$  are

$$\bar{O}\Psi = \Psi, \quad O_p \Psi = \Psi.$$

Using (B5),

$$\begin{aligned} \sum_K \mathcal{D}_{MK}^I(\alpha, \beta, \gamma) \phi_{IK}(\theta) &= \Psi(\theta, \alpha, \beta, \gamma) = (\bar{O}\Psi)(\theta, \alpha, \beta, \gamma) = \Psi(\theta, \alpha', \beta', \gamma') = \sum_{K'} \mathcal{D}_{MK'}^I(\alpha', \beta', \gamma') \phi_{IK'}(\theta) \\ &= \sum_{K'} [\psi_{IM}, D^I(\alpha', \beta', \gamma') \psi_{IK'}]^* \phi_{IK'}(\theta) = \sum_{K'} [\psi_{IM}, D^I(\alpha, \beta, \gamma) D_\xi^I(\pi) \psi_{IK'}]^* \phi_{IK'}(\theta) \\ &= \sum_{KK'} [\psi_{IM}, D^I(\alpha, \beta, \gamma) \psi_{IK}]^* [\psi_{IK}, D_\xi^I(\pi) \psi_{IK'}]^* \phi_{IK'}(\theta), \end{aligned}$$

$$D_\xi^I(\pi) = e^{-i\pi I_\xi} = e^{-i\pi I_1}.$$

Hence,  $\bar{O}\Psi = \Psi$  is equivalent to

$$\phi_{IK}(\theta) = \sum_{K'} (\psi_{IK}, e^{-i\pi I_1} \psi_{IK'})^* \Phi_{IK'}(\theta). \quad (\text{B8})$$

Similarly, it is seen that  $\bar{O}_p \psi = \psi$  means

$$\Phi_{IK}(\theta) = \sum_{K'} (\psi_{IK}, e^{-i(3/2)\pi I_3} e^{-i(\pi/2)I_2} e^{-i(3/2)\pi I_3} \psi_{IK'})^* \Phi_{IK'} \left[ \frac{\pi}{2} - \theta \right]. \quad (\text{B9})$$

It is very easy to solve Eq. (B8). In fact,

$$\begin{aligned} (\psi_{IK}, e^{-i\pi I_1} \psi_{IK'}) &= (\psi_{IK}, e^{i(\pi/2)I_3} e^{-i\pi I_2} e^{-i(\pi/2)I_3} \psi_{IK'}) = e^{i(\pi/2)(K-K')} (\psi_{IK}, e^{-i\pi I_2} \psi_{IK'}) \\ &= e^{i(\pi/2)(K-K')} d_{KK'}^I(-\pi) = e^{i(\pi/2)(K-K')} (-1)^{I-K'} \delta_{K,-K'} = (-1)^I \delta_{K,-K'}, \end{aligned}$$

where we introduced the functions

$$d_{KK'}^I(\beta) = (\psi_{IK}, e^{i\beta I_2} \psi_{IK'}),$$

following Edmonds<sup>10</sup> and the results reported there

$$d_{KK'}^I(-\pi) = d_{KK'}^I(\pi) = (-1)^{I-K'} \delta_{K,-K'}, \quad (\text{B10})$$

for integer spin  $I$ . Equation (B8) becomes, therefore,

$$\Phi_{IK}(\theta) = (-1)^I \Phi_{I-K}(\theta). \quad (\text{B11})$$

Equation (B9) is easier to be solved when treated simultaneously with (B8). To begin with, we note that, exploiting the reality of the  $d_{KK'}^I(\beta)$  functions,<sup>10</sup> Eqs. (B8) and (B9) can be written

$$\phi_{IK}(\theta) = \sum_{K'} (\psi_{IK}, e^{-i\pi I_1} \psi_{IK'}) \phi_{IK'}(\theta), \quad (\text{B12})$$

$$\Phi_{IK}(\theta) = \sum_{K'} (\psi_{IK}, e^{i(3/2)\pi I_3} e^{-i(\pi/2)I_2} e^{i(3/2)\pi I_3} \psi_{IK'}) \Phi_{IK'} \left[ \frac{\pi}{2} - \theta \right].$$

Using the well-known relations

$$e^{-i\theta n \cdot I} e^{-im \cdot I} e^{i\theta n \cdot I} = e^{-iR_n(\theta)m \cdot I}$$

with  $R_n(\theta)$  given by (A1), and the fact that, for integer  $I$   $e^{i2\pi n \cdot I} = 1$ , Eqs. (B12) can be expressed more compactly as vector equations,

$$\begin{aligned} \Phi_I(\theta) &= e^{-i\pi I_1} \Phi_I(\theta), \\ \Phi_I(\theta) &= e^{-i(\pi/2)I_3} e^{-i(\pi/2)I_2} e^{-i(\pi/2)I_3} \Phi_I \left[ \frac{\pi}{2} - \theta \right] \\ &= e^{i(\pi/2)I_1} e^{-i\pi I_3} \Phi_I \left[ \frac{\pi}{2} - \theta \right] \\ &= e^{-i\pi I_2} e^{i(\pi/2)I_1} \Phi_I \left[ \frac{\pi}{2} - \theta \right]. \end{aligned} \quad (\text{B13})$$

These in turn can be recasted in the more tractable form

$$\begin{aligned} \chi_I(\theta) &= e^{-i\pi I_3} \chi_I(\theta), \\ \chi_I(\theta) &= e^{-i\pi I_2} e^{-i(\pi/2)I_3} \chi_I \left[ \frac{\pi}{2} - \theta \right], \end{aligned} \quad (\text{B14})$$

where

$$\chi_I(\theta) = e^{-i(\pi/2)I_2} \Phi_I(\theta). \quad (\text{B15})$$

From (B14) we infer that

$$\chi_{IK}(\theta) = e^{-i\pi K} \chi_{IK}(\theta)$$

or

$$\chi_{IK}(\theta) = 0$$

for odd  $K$  values, and

$$\chi_{IK}(\theta) = \sum_{K'} (-1)^{I-K'} \delta_{K,-K'} e^{-i(\pi/2)K'} \chi_{IK'} \left[ \frac{\pi}{2} - \theta \right],$$

otherwise. Since

$$\chi_{I,2n+1}(\theta) = 0 \forall n,$$

we can rewrite this as

$$\chi_{I,2n}(\theta) = (-1)^{I+n} \chi_{I,-2n} \left[ \frac{\pi}{2} - \theta \right].$$

Let us now have

$$\chi_I = \chi_I^{(1)} + \chi_I^{(-1)},$$

where

$$\chi_I^{(\epsilon)}(\theta) = \frac{1}{2} \left[ \chi_I(\theta) + \epsilon \chi_I \left[ \frac{\pi}{2} - \theta \right] \right]$$

so that

$$\chi_I^{(\epsilon)} \left[ \frac{\pi}{2} - \theta \right] = \epsilon \chi_I^{(\epsilon)}(\theta).$$

Substituting in the previous equations, we get the final form of the symmetry conditions on the vector  $\chi_I$ ,

$$\chi_{I,2n+I}^{(\epsilon)} = 0,$$

$$\chi_{I,2n}^{(\epsilon)} = \epsilon (-1)^{I+n} \chi_{I,-2n}^{(\epsilon)}.$$

It is then possible to parametrize the general solution, e.g., as follows:

$$\chi_{IK}(\theta) = 0, \quad K = 2n + 1,$$

$$\chi_{I0}(\theta) = C_{I0}(\theta),$$

$$\chi_{I,2n}(\theta) = a_n(\theta) + b_n(\theta),$$

$$n \geq 1,$$

$$\chi_{I,-2n}(\theta) = (-1)^{I+n} [a_n(\theta) - b_n(\theta)],$$

where  $a_n(\theta)$  [ $b_n(\theta)$ ] are arbitrary functions of  $\theta$  which are even (odd) under the transformation  $\theta \rightarrow (\pi/2) - \theta$ , whereas  $C_{I0}(\theta)$  is any function satisfying

$$C_{I0} \left[ \frac{\pi}{2} - \theta \right] = (-1)^I C_{I0}(\theta).$$

With the help of (B15) we recover

$$\Phi_I(\theta) = e^{i(\pi/2)I_2} \chi_I(\theta),$$

that is

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$$\Phi_{IK}(\theta) = d_{K0}^I \left[ \frac{\pi}{2} \right] C_{I0}(\theta) + \sum_{n \geq 1} \left\{ d_{K,2n}^I \left[ \frac{\pi}{2} \right] [a_n(\theta) + b_n(\theta)] + (-1)^{I+n} d_{K,-2n}^I \left[ \frac{\pi}{2} \right] [a_n(\theta) - b_n(\theta)] \right\}. \quad (B16)$$

We can derive from those results reported in Ref. 10, the following two relations, valid for integer spin  $I$ :

$$d_{-K,-K'}^I \left[ \frac{\pi}{2} \right] = (-1)^{I+K'} d_{KK'}^I \left[ \frac{\pi}{2} \right], \quad (B17)$$

$$d_{K,-K'}^I \left[ \frac{\pi}{2} \right] = (-1)^{I+K} d_{KK'}^I \left[ \frac{\pi}{2} \right]. \quad (B18)$$

Using (B17) in (B16) enables one to check that our solution of the symmetry conditions obeys (B11) as it must. On the other hand, using Eq. (B18), we can write

$$\Phi_{IK}(\theta) = d_{K0}^{I*} \left[ \frac{\pi}{2} \right] C_{I0}^* + \sum_{n \geq 1} d_{K,2n}^I \left[ \frac{\pi}{2} \right] \{ [1 + (-1)^{K+n}] a_n(\theta) + [1 - (-1)^{K+n}] b_n(\theta) \}. \quad (B19)$$

We specialize this formula to the values  $I=0, 1$ , and  $2$  needed in the paper. Recalling that

$$C_{I0} \left[ \frac{\pi}{2} - \theta \right] = (-1)^I C_{I0}(\theta),$$

we have

$$I=0: \phi_{00}(\theta) = d_{00}^0 \left[ \frac{\pi}{2} \right] C_{00}(\theta) = \phi_{00} \left[ \frac{\pi}{2} - \theta \right], \quad (B20)$$

$$I=1: \Phi_{1K}(\theta) = d_{K0}^1 \left[ \frac{\pi}{2} \right] C_{10}(\theta).$$

From (B17),

$$d_{00}^1 \left[ \frac{\pi}{2} \right] = 0,$$

$$d_{10}^1 \left[ \frac{\pi}{2} \right] = -d_{-10}^1 \left[ \frac{\pi}{2} \right],$$

with  $d_{10}^1(\pi/2)$  being different from 0 [see, e.g., Rose (Ref. 11)]. Hence

$$I=1: \phi_{11}(\theta) = -\Phi_{1-1}(\theta) = -\phi_{11} \left[ \frac{\pi}{2} - \theta \right]. \quad (B21)$$

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$$I=2: \phi_{22}(\theta) = d_{20}^2 \left[ \frac{\pi}{2} \right] C_{20}(\theta) + 2d_{22}^2 b_1(\theta),$$

$$\phi_{21}(\theta) = d_{10}^2 \left[ \frac{\pi}{2} \right] C_{20}(\theta) + 2d_{22}^2 \left[ \frac{\pi}{2} \right] a_1(\theta),$$

$$\phi_{20}(\theta) = d_{00}^2 \left[ \frac{\pi}{2} \right] C_{20}(\theta) + 2d_{02}^2 \left[ \frac{\pi}{2} \right] b_1(\theta).$$

From (B18),

$$d_{20}^2 \left[ \frac{\pi}{2} \right] = -d_{20}^2 \left[ \frac{\pi}{2} \right] = 0,$$

$$d_{02}^2 \left[ \frac{\pi}{2} \right] = d_{20}^2 \left[ \frac{\pi}{2} \right].$$

Let us use the explicit formula for the  $d^I$  functions given in Rose<sup>11</sup> (taking care of the difference in the definition used by Rose with respect to the ones used by us),

$$d_{22}^2 \left[ \frac{\pi}{2} \right] = -\frac{1}{2}, \quad d_{22}^2 \left[ \frac{\pi}{2} \right] = \frac{1}{4},$$

$$d_{20}^2 \left[ \frac{\pi}{2} \right] = \frac{1}{2} \sqrt{3/2}, \quad d_{00}^2 \left[ \frac{\pi}{2} \right] = -\frac{1}{2}.$$

We then obtain

$$\Phi_{22}(\theta) = -a_1(\theta) = \phi_{22} \left[ \frac{\pi}{2} - \theta \right], \quad (\text{B22})$$

and

$$\Phi_{22}(\theta) = \frac{1}{2} \sqrt{3/2} C_{20}(\theta) + \frac{1}{2} b_1(\theta),$$

$$\phi_{20}(\theta) = -\frac{1}{2} C_{20}(\theta) + \sqrt{3/2} b_1(\theta).$$

This shows that  $\phi_{22}$  and  $\phi_{20}$  are independent wave functions. Furthermore, since  $C_{20}(\theta)$  is even and  $b_1(\theta)$  is odd with respect to  $O \rightarrow (\pi/2) - \theta$ , we obtain

$$\phi_{22} \left[ \frac{\pi}{2} - \theta \right] = \frac{1}{2} \sqrt{3/2} C_{20}(\theta) - \frac{1}{2} b_1(\theta),$$

$$\phi_{20} \left[ \frac{\pi}{2} - \theta \right] = -\frac{1}{2} C_{20}(\theta) - \sqrt{3/2} b_1(\theta).$$

Finally, expressing  $C_{20}(\theta)$  and  $b_1(\theta)$  by means of  $\phi_{20}(\theta)$  and  $\phi_{22}(\theta)$ , we have

$$\phi_{22} \left[ \frac{\pi}{2} - \theta \right] = \frac{1}{2} \phi_{22}(\theta) - \frac{1}{2} \sqrt{3/2} \phi_{20}(\theta),$$

$$\phi_{20} \left[ \frac{\pi}{2} - \theta \right] = -\sqrt{3/2} \phi_{22}(\theta) - \frac{1}{2} \phi_{20}(\theta). \quad (\text{B23})$$

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