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Formal Aspects of Nuclear Moment-of-Inertia Theory*

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Projected Hartree-Fock states are used as a *representation* in calculating nuclear wave functions. The rotational energy is determined consistently through $J(J+1)/\langle J^2\rangle$, and the moment of inertia thus obtained is compared with the expressions of other authors. The formulas of Peierls and Yoccoz and Thouless and Valatin yield approximately the same results as ours, but all of these formulas exhibit discrepancies with the Inglis independent-particle cranking-model formula. We find that the spurious state $J_x|\phi\rangle$ plays a dominant role, in agreement with Banerjee, D'Oliveira, and Stephenson. Interesting observations are made for the case of the soluble $SU(3)$ model of Elliott.

I. INTRODUCTION

Much has been written about the cranking model,[1-5] and the resulting formulas for calculating nuclear moments of inertia, $\mathcal{I}$. Much has also been written on the projection method, or the Peierls-Yoccoz (PY) method,[6-10] which leads to very different formulas for the same parameter. In this work we study the relationship between these two methods and their corresponding formulas.

We find that, by a logical extension of the PY method, we can obtain a cranking-type formula for the rotational energy which is consistent to order $J(J+1)/\langle J^2\rangle$. At the same time, we see that the new formula provides approximately the same value of $\mathcal{I}$ as that obtained from the PY formula. We find that the spurious state,[4] $J_x|\phi\rangle$ ($|\phi\rangle$ is the Hartree-Fock ground state), plays a dominant role in determining the moment of inertia. This is in agreement with Banerjee, D'Oliveira, and Stephenson.[5] Under these circumstances, the *self-consistent* cranking formula (not the Inglis formula) and the PY formula give the same results, but the PY formula displays more explicitly the importance of the spurious state. This feature is obscure in the cranking formulas and lost completely in the independent-particle Inglis formula.

Before presenting our results, we briefly review, in Sec. II, the essential aspects of both the cranking and projection methods. This will serve to establish our notation and provide a reference for comparisons in later sections. In Sec. III, we discuss the extension of the PY technique, which allows us to develop the link between the cranking and projection methods. Finally in Sec. IV, we present the conclusions to be drawn from the results of Sec. III. In order to facilitate reading we have relegated several of the crucial proofs to Appendices at the end of the article.

II. REVIEW

We begin this brief review with a discussion of the cranking model. This work is generally associated with the names Inglis,[1] and Thouless and Valatin.[2] The cranking model is a semiclassical approach which assumes that the nucleus under investigation has a static deformed shape and that it is rotating with an unquantized angular velocity ω about a fixed axis, e.g., the x axis.

The time-independent Hamiltonian in the rest frame of the nucleus is

$$\hat{H}=H-\omega\hbar J_x\,, \tag{II.1}$$

and the wave function associated with $\hat{H}$, $|\phi_\omega\rangle$, is the intrinsic wave function. The total energy of the rotating system is then

$$E=\langle\phi_\omega|H|\phi_\omega\rangle/\langle\phi_\omega|\phi_\omega\rangle\,, \tag{II.2}$$

and for small ω this would have the form

$$E=E_0+\tfrac{1}{2}\mathcal{I}\omega^2\,. \tag{II.3}$$

Clearly, the moment of inertia may be extracted by determining the coefficient of $\frac{1}{2}\omega^2$ in the expression for the total energy.

One method[11] of obtaining a formula for $\mathcal{I}$ makes use of

$$E=\langle\phi_\omega|\hat{H}|\phi_\omega\rangle-\omega\frac{\partial}{\partial\omega}\langle\phi_\omega|\hat{H}|\phi_\omega\rangle\,. \tag{II.4}$$

One then takes the Hartree-Fock (HF) solution for H as a zero-order approximation to $|\phi_\omega\rangle$, and treats $\omega\hbar J_x$ [see (II.1)] as a perturbation in obtaining $\langle\phi_\omega|\hat{H}|\phi_\omega\rangle$. To lowest order this leads to

$$\mathcal{I}_{\rm GI}=2\hbar\sum\frac{|\langle\alpha|J_x|\phi_0\rangle|^2}{E_\alpha-E_\phi}\,, \tag{II.5}$$

where $|\phi_0\rangle$ is the HF ground-state solution for H and where $|\alpha\rangle$ and E_α are states and energies involving 1p-1h excited HF configurations; the subscript GI denotes this expression as the "generalized Inglis" formula.

In the following we consider the case that $|\phi_0\rangle$, the HF wave function, is symmetric about the z axis; that it has $J_z=0$; and that it has the following time-reversal symmetry,

$$e^{-iJ_y\pi}|\phi\rangle=|\phi\rangle\ . \tag{II.6}$$

It is convenient to define the matrix Γ as $(H-E_\phi)$ in the space of 1p-1h excited HF configurations, i.e.,

$$(\mathrm{ph}|\Gamma|\mathrm{p'h'})\equiv\langle\mathrm{ph}|(H-E_\phi)|\mathrm{p'h'}\rangle\ . \tag{II.7}$$

In the following we shall also use the symbolic notation,

$$(\mathrm{ph}|\Gamma J_x|\phi_0\rangle\equiv\sum_{\mathrm{p'h'}}(\mathrm{ph}|\Gamma|\mathrm{p'h'})\langle\mathrm{p'h'}|J_x|\phi_0\rangle\ . \tag{II.8}$$

Then, the expression for $\mathscr{I}$ in Eq. (II.5) may be concisely written as

$$\mathscr{I}_{\mathrm{GI}}=2\hbar^2\langle\phi_0|J_x\Gamma^{-1}J_x|\phi_0\rangle\ . \tag{II.9}$$

Under the assumption that H is an independent-particle Hamiltonian, Inglis obtained the celebrated formula,

$$\mathscr{I}_{\mathrm{I}}=2\hbar^2\sum_{\mathrm{ph}}\frac{|\langle\mathrm{p}|J_x|\mathrm{h}\rangle|^2}{\epsilon_p-\epsilon_h}\ . \tag{II.10}$$

This formula has also been used with HF solutions, where the ϵ_p and ϵ_h are taken to the eigenvalues of the HF Hamiltonian. (Note the distinction between using HF eigenvalues in the denominator and using Γ^{-1}.)

A more self-consistent treatment of the cranking model is due to Thouless and Valatin.[2,12] They set

$$|\phi_\omega\rangle=e^{iF}|\phi_0\rangle\ ,$$

where F is a one-body operator whose matrix elements are determined variationally from

$$\delta\frac{\langle\phi_\omega|\hat{H}|\phi_\omega\rangle}{\langle\phi_\omega|\phi_\omega\rangle}=0\ . \tag{II.11}$$

This leads to the Thouless-Valatin formula, which has the form

$$\mathscr{I}_{\mathrm{TV}}=2\hbar^2\langle\phi_0|J_x(\Gamma+\Lambda)^{-1}J_x|\phi_0\rangle\ , \tag{II.12}$$

where Γ is defined in (II.7) and where Λ represents the matrix elements of H between the HF ground state and 2p-2h excitations,

$$(\mathrm{ph}|\Lambda|\mathrm{p'h'})\equiv\langle\mathrm{ph,p'h'}|H|\phi_0\rangle\ . \tag{II.13}$$

By considering

$$\langle\mathrm{ph}|[H,J_x]|\phi_0\rangle=0\ , \tag{II.14}$$

it can be shown[5] that for axially symmetric $|\phi_0\rangle$,

$$\sum_{\mathrm{p'h'}}(\mathrm{ph}|\Gamma|\mathrm{p'h'})\langle\mathrm{p'h'}|J_x|\phi_0\rangle=\sum_{\mathrm{p'h'}}(\mathrm{ph}|\Lambda|\mathrm{p'h'})\langle\mathrm{p'h'}|J_x|\phi_0\rangle\ , \tag{II.15a}$$

or more briefly

$$\Gamma J_x|\phi_0\rangle=\Lambda J_x|\phi_0\rangle\ , \tag{II.15b}$$

a relationship to be used later.

Now we turn to the Peierls-Yoccoz,[6] or angular momentum projection,[8,10] method. Here, one tries to find an approximate wave function for the full Hamiltonian. Such a wave function must, of course, have J as a good quantum number. One starts with the HF ground state of H, $|\phi\rangle$, for which J is not a good quantum number, and does a Hill-Wheeler type of integral over the direction of the symmetry axis of $|\phi\rangle$, using as a weighting function $\mathfrak{D}^J_{M0}{}^*(\Omega)$,

$$|\psi^{JM}\rangle=\frac{2J+1}{8\pi^2}\int d\Omega\,\mathfrak{D}^J_{M0}{}^*(\Omega)R(\Omega)|\phi_0\rangle\ . \tag{II.16}$$

The integral goes over the three Euler angles α, β, and γ represented by Ω, with

$$R(\Omega)=e^{-iJ_z\alpha}e^{-iJ_y\beta}e^{-iJ_z\gamma}\ . \tag{II.17}$$

The integral in Eq. (II.16) may be summarized by P^J_{M0}, and it can be shown that P^J_{00} projects out of $|\phi_0\rangle$ the component having good angular momentum J.

The method for determining $\mathscr{I}$ involves finding

$$E^J=\frac{\langle\psi^{JM}|H|\psi^{JM}\rangle}{\langle\psi^{JM}|\psi^{JM}\rangle}=\frac{\langle\phi|HP^J|\phi\rangle}{\langle\phi|P^J|\phi\rangle}\ . \tag{II.18}$$

If the spectrum is rotational, we would expect

$$E^J=E^0+(\hbar^2/2\mathscr{I})J(J+1)+\dots\ . \tag{II.19}$$

Yoccoz[7] obtained an expression for $\mathscr{I}$ by evaluating E^J in the approximation of large nuclear deformations and large $\langle\phi|J^2|\phi\rangle$. The important features of this type of calculation are given in Appendix A. He obtained

$$\begin{aligned}E^J_{PY}&=E_\phi-\frac{\langle\phi|J_x(H-E_\phi)J_x|\phi\rangle}{\langle\phi|J_x{}^2|\phi\rangle}+\frac{J(J+1)}{2}\,\frac{\langle\phi|J_x(H-E_\phi)J_x|\phi\rangle}{\langle\phi|J_x{}^2|\phi\rangle^2}\ ,\\&=E_\phi-\frac{\hbar^2}{2\mathscr{I}_{\mathrm{PY}}}\langle J^2\rangle+\frac{\hbar^2}{2\mathscr{I}_{\mathrm{PY}}}J(J+1)\ ,\end{aligned} \tag{II.20}$$

from which the Peierls-Yoccoz formula for the moment of inertia, $\mathscr{I}_{\mathrm{PY}}$, may be extracted;

$$\mathscr{I}_{\mathrm{PY}}=\hbar^2\frac{\langle\phi|J_x{}^2|\phi\rangle^2}{\langle\phi|J_x\Gamma J_x|\phi\rangle}\ . \tag{II.21}$$

This formula has an appearance entirely different from the corresponding cranking formulas in Eqs. (II.9) and (II.12). It will be the purpose of Sec. III to reconcile this difference, and to provide a better understanding for all forms.

III. EXTENSION OF PROJECTION METHOD

We have extended the projection method in an attempt to improve that approach[2,13,14] and, at the same time, to find a link between it and the cranking methods. Our work is discussed in this section and related Appendices.

In the original projection approach one takes

$$|\psi^J\rangle \cong P^J|\phi\rangle, \tag{III.1}$$

where the subscripts on P^J_{M0} have been suppressed. We improve the wave function by considering

$$|\psi^J\rangle \cong P^J|\phi\rangle + |R^J\rangle . \tag{III.2}$$

We take the correction $|R^J\rangle$ to lie in the space spanned by the set of vectors

$$\{P^J|\gamma, J_z = 1\rangle\},$$

where the set of states $\{|\gamma, 1\rangle\}$ includes all 1p-1h excited configurations of the HF ground state consistent with

$$\langle R^J|P^J|\phi\rangle = 0 . \tag{III.3}$$

(Since $P^J|\gamma, -1\rangle \propto P^J|\gamma, +1\rangle$,[8] the space in which $|R^J\rangle$ lies also is the space spanned by $\{P^J|\gamma, -1\rangle\}$ and we could have as well considered that set of vectors.) Using the perturbation approach discussed below, we find the change in the energy E^J,

$$E^J = E_{\mathrm{PY}} + \Delta E^J_R, \tag{III.4}$$

which arises from the correction to the wave function. If we were to have included within $|R^J\rangle$ terms of the form $P^J|\gamma', J_z > 1\rangle$, these would not affect in lowest order the terms in ΔE^J which go as $J(J+1)$.

In the algebraic steps to be discussed below we assume that the ground state $|\phi\rangle$ is highly deformed and that

$$\langle\phi|J^2|\phi\rangle >> J(J+1). \tag{III.5}$$

This is required to allow us to evaluate angular integrals by considering only the contributions from very forward or backward angles. This assumption limits the validity of our results to states E^J, with relatively low J; but these states are, in fact, the only ones for which the concept of a J-independent moment of inertia is valid.

We evaluate ΔE^J_R in two forms which are quite different in appearance, but which we believe are equivalent in value. The difference between the two expressions lies in the representation we choose for the operator, π^J, which projects onto the space spanned by $\{P^J|\gamma, +1\rangle\}$. Using π^J we have

$$|\psi^J\rangle = P^J|\phi\rangle + \pi^J|\psi^J\rangle . \tag{III.6}$$

If we require that

$$\langle\phi|P^J(H - E^J)|\psi^J\rangle = 0 , \tag{III.7}$$

and use (III.6) in (III.7), we obtain

$$E^J = E^J_{\mathrm{PY}} + \frac{\langle\phi|P^J H\pi^J|\psi^J\rangle}{\langle\phi|P^J|\phi\rangle} , \tag{III.8}$$

where from (II.18)

$$E^J_{\mathrm{PY}} = \frac{\langle\phi|HP^J|\phi\rangle}{\langle\phi|P^J|\phi\rangle} .$$

We then find

$$\Delta E^J_R = \frac{\langle\phi|P^J H\pi^J|\psi^J\rangle}{\langle\phi|P^J|\phi\rangle} . \tag{III.9}$$

The two representations for π^J which we use are developed in Appendix B where we obtain the following:

(a) For the first form,

$$\pi^J_1 = \sum_\gamma \frac{P^J|\gamma, 1\rangle\langle\gamma, 1|P^J}{\langle\gamma, 1|P^J|\gamma, 1\rangle} , \tag{III.10}$$

where $\{|\gamma, 1\rangle\}$ includes all $J_z = 1$ states consisting of 1p-1h excited HF configurations with

$$\langle\gamma, 1|J_+|\phi\rangle = 0 , \tag{III.11}$$

$$\langle\gamma, 1|H|\gamma', 1\rangle = \delta_{\gamma\gamma'}\langle\gamma|H|\gamma\rangle . \tag{III.12}$$

(b) For the second form,

$$\pi^J_2 = \tfrac{1}{2}\sum_u \frac{P^J|u, 1\rangle\langle u, 1|P^J}{\langle u, 1|P^J|u, 1\rangle} , \tag{III.13}$$

where $\{|u, 1\rangle\}$ includes all $J_z = 1$ states consisting of 1p-1h, 2p-2h, and 3p-3h excited HF configurations with

$$\langle u, 1|J_+|\phi\rangle = 0 , \tag{III.14}$$

$$\langle u, 1|J_+J^2|\phi\rangle = 0 , \tag{III.15}$$

$$\langle u, 1|H|u', 1\rangle = \delta_{u,u'}\langle u|H|u\rangle . \tag{III.16}$$

We will suppress the $J_z = 1$ index in what follows. Comparing Eqs. (III.10) and (III.13) we find that the sum in the latter covers more states by including 2p-2h and 3p-3h configurations but that this increase in the number of terms is compensated for by the factor of $\frac{1}{2}$ which is justified in Appendix B.

Using these forms for π^J in Eq. (III.9), we find

$$\Delta E^J_{R_1} = \sum_\gamma \frac{\langle\phi|P^J H|\gamma\rangle\langle\gamma|P^J|\psi^J\rangle}{\langle\gamma|P^J|\gamma\rangle\langle\phi|P^J|\phi\rangle} ; \tag{III.17}$$

$$\Delta E^J_{R_2} = \tfrac{1}{2}\sum_\gamma \frac{\langle\phi|P^J H|u\rangle\langle u|P^J|\psi^J\rangle}{\langle u|P^J|u\rangle\langle\phi|P^J|\phi\rangle} . \tag{III.18}$$

To evaluate $\langle\gamma|P^J|\psi^J\rangle$, we require

$$\langle\gamma|P^J(H - E^J)|\psi^J\rangle = 0 , \tag{III.19}$$

which provides

$$\langle\gamma|P^J HP^J|\phi\rangle + \langle\gamma|P^J(H-E^J)|R^J\rangle = 0 . \qquad \text{(III.20)}$$

We now assume H is nearly diagonal in $P^J|\gamma\rangle$, so that

$$\langle\gamma|P^J(H-E^J)|R^J\rangle \cong \frac{\langle\gamma|P^J(H-E^J)P^J|\gamma\rangle\langle\gamma|P^J|\psi^J\rangle}{\langle\gamma|P^J|\gamma\rangle} . \qquad \text{(III.21)}$$

Combining Eq. (III.21) with (III.20),

$$\langle\gamma|P^J|\psi^J\rangle \cong -\frac{\langle\gamma|HP^J|\phi\rangle}{(\langle\gamma|HP^J|\gamma\rangle / \langle\gamma|P^J|\gamma\rangle - E^J)} , \qquad \text{(III.22)}$$

so that

$$\Delta E^J_{R_1} \cong -\sum_\gamma \frac{\langle\phi|P^J H|\gamma\rangle\langle\gamma|HP^J|\phi\rangle}{\langle\phi|P^J|\phi\rangle\langle\gamma|P^J|\gamma\rangle\,(\langle\gamma|HP^J|\gamma\rangle / \langle\gamma|P^J|\gamma\rangle - E^J_{\mathrm{PY}})} . \qquad \text{(III.23)}$$

In a completely analogous manner

$$\Delta E^J_{R_2} \cong -\tfrac{1}{2}\sum_u \frac{\langle\phi|P^J H|u\rangle\langle u|HP^J|\phi\rangle}{\langle\phi|P^J|\phi\rangle\langle u|P^J|u\rangle\,(\langle u|HP^J|u\rangle / \langle u|P^J|u\rangle - E^J_{\mathrm{PY}})} . \qquad \text{(III.24)}$$

In the remainder of this section we evaluate the factors of which ΔE^J_R is comprised, using various approximations. We sketch this development in some detail for $\Delta E^J_{R_1}$, treating each factor in turn. We can then follow the same lines in obtaining $\Delta E^J_{R_2}$.

A. Evaluation of $\Delta E^J_{R_1}$ and $\mathcal{I}_1$

Consider first the factors $\langle\phi|P^J|\phi\rangle$ and $\langle\gamma|P^J|\gamma\rangle$. We have

$$\langle\phi|P^J|\phi\rangle = (2J+1)\int_0^{\pi/2} \langle\phi|e^{-iJ_y\beta}|\phi\rangle d^J_{00}(\beta)\sin\beta d\beta , \qquad \text{(III.25)}$$

$$\langle\gamma|P^J|\gamma\rangle = \frac{2J+1}{2}\int_0^{\pi} \langle\gamma|e^{-iJ_y\beta}|\gamma\rangle d^J_{11}(\beta)\sin\beta d\beta . \qquad \text{(III.26)}$$

Using the approximations outlined in Appendix A, Eqs. (A6)–(A9), we obtain

$$\langle\phi|P^J|\phi\rangle \cong \frac{2J+1}{\langle J_y^2\rangle}\left[1-\frac{J(J+1)}{\langle J^2\rangle}\right] . \qquad \text{(III.27)}$$

Using similar approximations for $\langle\gamma|P^J|\gamma\rangle$, we have, to lowest order in $1/\langle J^2\rangle$,

$$\langle\gamma|P^J|\gamma\rangle \cong \frac{2J+1}{2\langle J_y^2\rangle} \cong \tfrac{1}{2}\langle\phi|P^J|\phi\rangle . \qquad \text{(III.28)}$$

Therefore,

$$\langle\phi|P^J|\phi\rangle\langle\gamma|P^J|\gamma\rangle \cong \tfrac{1}{2}\langle\phi|P^J|\phi\rangle^2 . \qquad \text{(III.29)}$$

Consider next the energy denominator,

$$\text{Denom.} = \frac{\langle\gamma|HP^J|\gamma\rangle}{\langle\gamma|P^J|\gamma\rangle} - E^J_{\mathrm{PY}} . \qquad \text{(III.30)}$$

In analogy with the Peierls-Yoccoz development shown in Appendix A, we take

$$\frac{\langle\gamma|HP^J|\gamma\rangle}{\langle\gamma|P^J|\gamma\rangle} = E_\gamma - \frac{\hbar^2}{2\mathcal{I}_\gamma}\langle J^2\rangle + \frac{\hbar^2}{2\mathcal{I}_\gamma}\Big[J(J+1)-1\Big] , \qquad \text{(III.31)}$$

which gives

$$\text{Denom.} = (E_\gamma - E_\phi) + \left(\frac{\hbar^2}{2\mathcal{I}_\gamma} - \frac{\hbar^2}{2\mathcal{I}_\phi}\right) \times\Big[-\langle J^2\rangle + J(J+1)\Big] - \frac{\hbar^2}{2\mathcal{I}_\gamma} . \qquad \text{(III.32)}$$

Assuming $\mathcal{I}_\gamma \approx \mathcal{I}_\phi$, we obtain

$$\text{Denom.} = E_\gamma - E_\phi - \frac{\hbar^2}{2\mathcal{I}} = \langle\gamma|H - E_\phi - \frac{\hbar^2}{2\mathcal{I}}|\gamma\rangle . \qquad \text{(III.33a)}$$

In what follows, we ignore $\frac{\hbar^2}{2\mathcal{I}}$ relative to $E_\gamma - E_\phi$, to obtain

$$\text{Denom.} = \langle\gamma|H - E_\phi|\gamma\rangle . \qquad \text{(III.33b)}$$

Finally, consider $\langle\gamma|HP^J|\phi\rangle$. We take

$$\langle\gamma|HP^J|\phi\rangle = \sum_\lambda \langle\gamma|H|\lambda\rangle\langle\lambda|P^J|\phi\rangle , \qquad \text{(III.34)}$$

where $\{|\lambda\rangle\}$ is a complete set of states. We have

$$\langle\lambda|P^J|\phi\rangle = (2J+1)\int_0^{\pi/2} \langle\lambda|e^{-iJ_y\beta}|\phi\rangle d^J_{10}(\beta)\sin\beta d\beta , \qquad \text{(III.35)}$$

which we evaluate by making small-angle approximations[8,13] similar to those presented in Appendix A, i.e.,

$$\langle\lambda|e^{-iJ_y\beta}|\phi\rangle \cong -\langle\lambda|\tfrac{1}{2}J_+|\phi\rangle\langle\phi|e^{-iJ_y\beta}|\phi\rangle\,\beta ; \qquad \text{(III.36)}$$

$$d^J_{10}(\beta) \cong -\tfrac{1}{2}[J(J+1)]^{1/2}\beta . \qquad \text{(III.37)}$$

Putting Eqs. (III.36) and (III.37) into (III.35) and considering (III.27), we obtain

$$\langle\lambda|P^J|\phi\rangle = \langle\lambda|J_+|\phi\rangle \frac{[J(J+1)]^{1/2}}{\langle J^2\rangle} \langle\phi|P^J|\phi\rangle . \tag{III.38}$$

Putting (III.38) into (III.34),

$$\langle\gamma|HP^J|\phi\rangle = \frac{[J(J+1)]^{1/2}}{\langle J^2\rangle} \langle\gamma|HJ_+|\phi\rangle\langle\phi|P^J|\phi\rangle . \tag{III.39}$$

Since we have chosen $|\gamma\rangle$ such that

$$\langle\gamma|J_+|\phi\rangle = 0 ,$$

we are at liberty to take

$$\langle\gamma|HJ_+|\phi\rangle = \langle\gamma|(H-E_\phi)J_+|\phi\rangle . \tag{III.40}$$

Combining all of the factors to form $\Delta E^J_{R_1}$, we have

$$\Delta E^J_{R_1} = -2\frac{J(J+1)}{\langle J^2\rangle^2} \times \sum_\gamma \frac{\langle\phi|J_-(H-E_\phi)|\gamma\rangle\langle\gamma|(H-E_\phi)J_+|\phi\rangle}{\langle\gamma|H-E_\phi|\gamma\rangle} . \tag{III.41}$$

In order to carry out the sum over γ in Eq. (III.41), we put

$$\frac{\langle\gamma|(H-E_\phi)J_+|\phi\rangle}{\langle\gamma|(H-E_\phi)|\gamma\rangle}$$

into a different form. We have defined the operator Γ in Eq. (II.7) as $H-E_\phi$ in the space of 1p-1h excited HF configurations, and Γ^{-1} as the inverse of Γ. Considering the condition (III.11),

$$\langle\gamma|J_+|\phi\rangle = 0 ,$$

we find

$$\langle\gamma|\Gamma 1^+_{\text{ph}}\Gamma^{-1}J_+|\phi\rangle = 0 , \tag{III.42}$$

where 1^+_{ph} is the unit operator in the space of 1p-1h configurations,

$$1^+_{\text{ph}} = \sum_\gamma |\gamma\rangle\langle\gamma| + \frac{J_+|\phi\rangle\langle\phi|J_-}{\langle J^2\rangle} . \tag{III.43}$$

Combining (III.42) and (III.43) and considering (III.12), we obtain

$$\frac{\langle\gamma|\Gamma J_+|\phi\rangle}{\langle\gamma|\Gamma|\gamma\rangle} = -\frac{\langle\gamma|\Gamma^{-1}J_+|\phi\rangle\langle J^2\rangle}{\langle\phi|J_-\Gamma^{-1}J_+|\phi\rangle} . \tag{III.44}$$

Putting Eq. (III.44) into (III.41), we obtain

$$\Delta E^J_{R_1} = \frac{2J(J+1)}{\langle J^2\rangle} \sum_\gamma \frac{\langle\phi|J_-\Gamma|\gamma\rangle\langle\gamma|\Gamma^{-1}J_+|\phi\rangle}{\langle\phi|J_-\Gamma^{-1}J_+|\phi\rangle} . \tag{III.45}$$

Summing over γ and using Eq. (III.43), we obtain

$$\Delta E^J_{R_1} = 2J(J+1)\left(\frac{1}{\langle\phi|J_-\Gamma^{-1}J_+|\phi\rangle} - \frac{\langle\phi|J_-\Gamma J_+|\phi\rangle}{\langle J^2\rangle^2}\right) , \tag{III.45a}$$

or equivalently

$$\Delta E^J_{R_1} = J(J+1)\left(\frac{1}{\langle\phi|J_x\Gamma^{-1}J_x|\phi\rangle} - \frac{\langle\phi|J_x\Gamma J_x|\phi\rangle}{\langle J_x{}^2\rangle^2}\right) . \tag{III.45b}$$

Combining $\Delta E^J_{R_1}$ with E^J_{PY}, we obtain for the inertial parameter

$$\frac{\hbar^2}{2\mathcal{I}_1} = \left(\frac{1}{\langle\phi|J_x\Gamma^{-1}J_x|\phi\rangle} - \frac{\langle\phi|J_x\Gamma J_x|\phi\rangle}{2\langle J_x{}^2\rangle^2}\right) . \tag{III.46}$$

This expression is neither of the cranking form nor the projection form, but rather a combination of both.

B. Evaluation of $\Delta E^J_{R_2}$ and $\mathcal{I}_2$

The difference between $\Delta E^J_{R_1}$ and $\Delta E^J_{R_2}$, as given in Eqs. (III.23) and (III.24), is that in the latter, 2p-2h and 3p-3h configurations are included in the summation while the entire sum is multiplied by $\frac{1}{2}$. We may evaluate $\Delta E^J_{R_2}$ exactly as was done in the case $\Delta E^J_{R_1}$, and we obtain

$$\Delta E^J_{R_2} = -\frac{J(J+1)}{\langle J^2\rangle} \times \sum_u \frac{\langle\phi|J_-(H-E_\phi)|u\rangle\langle u|(H-E_\phi)J_+|\phi\rangle}{\langle u|(H-E_\phi)|u\rangle} . \tag{III.47}$$

We use a technique analogous to that used for $\Delta E^J_{R_1}$ for reexpressing

$$\frac{\langle u|(H-E_\phi)J_+|\phi\rangle}{\langle u|H-E_\phi|u\rangle} .$$

Here we consider

$$\langle u|J_+|\phi\rangle = 0 \tag{III.48a}$$

and

$$\langle u|QJ_+J^2|\phi\rangle = 0 , \tag{III.48b}$$

where

$$Q = 1 - \frac{J_+|\phi\rangle\langle\phi|J_-}{\langle J^2\rangle} . \tag{III.48c}$$

Let us define the operator $\tilde{\Gamma}$ as $H-E_\phi$ in the space of 1p-1h, 2p-2h, and 3p-3h excitations of the HF ground state. Let 1^+_3 be the unit operator in this space,

$$1^+_3 = \sum_u |u\rangle\langle u| + \frac{J_+|\phi\rangle\langle\phi|J_-}{\langle J^2\rangle} + \frac{QJ_+J^2|\phi\rangle\langle\phi|J^2J_-Q}{\langle\phi|J^2J_-QJ_+J^2|\phi\rangle} , \tag{III.49}$$

and let $\tilde{\Gamma}^{-1}$ be the inverse of $\tilde{\Gamma}$. Then from Eqs. (III.48) and (III.49) we obtain

$$\Delta E^J_{K_2} = J(J+1)\left[\frac{1}{\langle\phi|J_-\tilde{\Gamma}^{-1}J_+|\phi\rangle(1+\delta)} - \frac{\langle\phi|J_-\Gamma J_+|\phi\rangle}{\langle J^2\rangle^2}\right], \tag{III.50}$$

where

$$\delta = \frac{|\langle\phi|J^2J_-Q\tilde{\Gamma}^{-1}J_+|\phi\rangle|^2}{\langle\phi|J_-\tilde{\Gamma}^{-1}J_+|\phi\rangle\langle\phi|J^2J_-Q\tilde{\Gamma}^{-1}QJ_+J^2|\phi\rangle}\ . \tag{III.51}$$

We assume $\delta \ll 1$, and so obtain

$$\Delta E^J_{K_2} = J(J+1)\left(\frac{1}{2\langle\phi|J_x\tilde{\Gamma}^{-1}J_x|\phi\rangle} - \frac{\langle\phi|J_x\Gamma J_x|\phi\rangle}{2\langle J_x{}^2\rangle^2}\right)\ . \tag{III.52}$$

Combining $\Delta E^J_{K_2}$ with E^J_{PY} we obtain

$$\frac{\hbar^2}{2\mathcal{I}_2} = \frac{1}{2\langle\phi|J_x\tilde{\Gamma}^{-1}J_x|\phi\rangle}\ . \tag{III.53}$$

This expression is indeed of the cranking form, with

$$\mathcal{I}_2 = \hbar^2\langle\phi|J_x\tilde{\Gamma}^{-1}J_x|\phi\rangle\ . \tag{III.54}$$

It is instructive to equate the results for $\Delta E^J_{K_1}$ and $\Delta E^J_{K_2}$. This leads to

$$\frac{\hbar^2}{2\mathcal{I}_{\mathrm{PY}}} - \frac{\hbar^2}{2\mathcal{I}_2} = \frac{1}{\langle\phi|J_x\Gamma^{-1}J_x|\phi\rangle} - \frac{1}{\langle\phi|J_x\tilde{\Gamma}^{-1}J_x|\phi\rangle}\ . \tag{III.55}$$

Consider now

$$\langle\phi|J_x\tilde{\Gamma}^{-1}J_x|\phi\rangle = \sum_\alpha \frac{|\langle\phi|J_x|\alpha\rangle|^2}{E_\alpha - E_\phi}\ . \tag{III.56}$$

The dominant contribution to this sum over α comes from the low-lying states of $\tilde{\Gamma}$ and the states which are predominantly composed of 1p-1h configurations, because of the overlap $|\langle\phi|J_x|\alpha\rangle|^2$. It seems reasonable to assume that these states will correspond very closely to the low-lying states of Γ. In that case

$$\langle\phi|J_x\tilde{\Gamma}^{-1}J_x|\phi\rangle \cong \langle\phi|J_x\Gamma^{-1}J_x|\phi\rangle\ . \tag{III.57}$$

We shall assume Eq. (III.57) and investigate its consequences in the following section.

IV. CONCLUSIONS

We have extended the projection method by the addition of a term $|R^J\rangle$ to $P^J|\phi\rangle$ so that the resultant rotational energy is consistent to order $J(J+1)/\langle J^2\rangle$. The moment of inertia is given by Eq. (III.54), which we now denote by

$$\mathcal{I}_{\mathrm{FW}} = \hbar^2\langle\phi|J_x\tilde{\Gamma}^{-1}J_x|\phi\rangle\ . \tag{IV.1}$$

This has the appearance of a cranking form. Under the assumption of Eq. (III.57) we have

$$\mathcal{I}_{\mathrm{FW}} \cong \hbar^2\langle\phi|J_x\Gamma^{-1}J_x|\phi\rangle\ , \tag{IV.2}$$

which should be compared with the generalized Inglis cranking formula

$$\mathcal{I}_{\mathrm{GI}} = 2\hbar^2\langle\phi|J_x\Gamma^{-1}J_x|\phi\rangle\ . \tag{IV.3}$$

It is clear that the two formulas differ by a factor of 2. This will be discussed below.

Under the assumption of Eq. (III.57) we have

$$\mathcal{I}_{\mathrm{PY}} \approx \mathcal{I}_{\mathrm{FW}}\ . \tag{IV.4}$$

We thus find that the value of $\mathcal{I}_{\mathrm{FW}}$ is about equal to the value of $\mathcal{I}_{\mathrm{PY}}$, even though the terms added to the wave function have radically changed the form of the expression.

From $\mathcal{I}_{\mathrm{PY}} \approx \mathcal{I}_{\mathrm{FW}}$, we find that $J_x|\phi\rangle$ is approximately an eigenfunction of Γ. This is discussed in Appendix C. A similar result was obtained by Banerjee, D'Oliveira, and Stephenson[5] from a completely different point of view. We make two remarks here concerning $J_x|\phi\rangle$. First, it is the collective state which is said to be "spurious" in the Tamm-Dancoff approximation.[4] Second, the eigenvalues $\langle\phi|J_x\Gamma J_x|\phi\rangle/\langle J_x{}^2\rangle$ are found by Banerjee, D'Oliveira, and Stephenson[5] to be lower than the smallest independent-particle energy difference of $\epsilon_p - \epsilon_h$ in the corresponding nuclei.

We noted above that our formula differed from the generalized Inglis formula by a factor of 2. We now wish to compare our formula with the self-consistent cranking formula of Thouless and Valatin,

$$\mathcal{I}_{\mathrm{TV}} = 2\hbar^2\langle\phi|J_x(\Gamma+\Lambda)^{-1}J_x|\phi\rangle\ . \tag{IV.5}$$

We have stated above in Eq. (II.15) that

$$\Gamma J_x|\phi\rangle = \Lambda J_x|\phi\rangle\ .$$

If $J_x|\phi\rangle$ is an eigenstate of Γ, then

$$\mathcal{I}_{\mathrm{TV}} \cong 2\hbar^2\langle\phi|J_x(2\Gamma)^{-1}J_x|\phi\rangle \cong \hbar^2\langle\phi|J_x\Gamma^{-1}J_x|\phi\rangle\ . \tag{IV.6}$$

This is in agreement with our result.

The Inglis independent-particle cranking formula,

$$\mathcal{I}_{\mathrm{I}} = 2\hbar^2\sum_{ph}\frac{|\langle\phi|J_x|ph\rangle|^2}{\epsilon_p - \epsilon_h}\ , \tag{IV.7}$$

would seem to be faulty on two counts. First, the factor of 2 tends to overestimate $\mathcal{I}$. Second, the particle-hole energy denominator ignores the low-lying collective state $J_x|\phi\rangle$ and tends to underestimate $\mathcal{I}$. These two effects, however, are in opposite directions and tend to cancel. It is shown in Appendix D that for the case of a two-body potential of the form

$$V=\sum_{\substack{\lambda\text{ even}\\ \mu}} \tfrac{1}{2}V_{0\lambda}(-)^{\mu}Q_{\lambda\mu}Q_{\lambda-\mu}\,, \tag{IV.8}$$

these two effects cancel identically if we can ignore exchange terms in the potential. Then

$$\tfrac{1}{2}\mathscr{I}_{\rm GI}\cong\mathscr{I}_{\rm I}\cong\mathscr{I}_{\rm PY}\cong\mathscr{I}_{\rm TV}\cong\mathscr{I}_{\rm FW}\,. \tag{IV.9}$$

Such a situation occurs for the case of the Elliott quadrupole-quadrupole force.[15] With this force the exact solution is

$$\mathscr{I}_{\rm exact}=\frac{1}{3|V_0|}\,, \tag{IV.10}$$

and ignoring exchange it is shown in Appendix D that

$$\mathscr{I}_{\rm I}=\mathscr{I}_{\rm PY}=\frac{1}{3|V_0|}\,. \tag{IV.11}$$

It is possible that the relatively good fits to the experimental moments of inertia in the rare-earth region, obtained from the independent-quasiparticle analog of the Inglis formula,[16] may also owe their success to this cancellation.

The cranking model and projection method give similar results (for low J and large $\langle J^2\rangle$) provided the cranking method is used self-consistently. This last refinement can change results by a factor of 2. Since it seems that $J_x|\phi\rangle$ is in fact nearly an eigenfunction of Γ, the sum over states in the Thouless-Valatin cranking formula is dominated by this one collective state. Because of this, the Peierls-Yoccoz form appears more straightforward than the cranking-model form.

It seems appropriate that the collective state $J_x|\phi\rangle$ should be important in determining the collective parameter $\mathscr{I}$, since one generally argues that this state must be removed in calculating excitation spectra, as it represents some motion of the nucleus as a whole.[4]

APPENDIX A. DEVELOPMENT OF THE PY MOMENT OF INERTIA

We start with

$$E^J=\frac{\langle\phi|HP^J|\phi\rangle}{\langle\phi|P^J|\phi\rangle}\,, \tag{A1}$$

where

$$E_\phi=\langle\phi|H|\phi\rangle\,. \tag{A2}$$

The J-dependent terms are evaluated by considering

$$\frac{\langle\phi|(H-E_\phi)P^J|\phi\rangle}{\langle\phi|P^J|\phi\rangle}=\sum_\lambda\langle\phi|(H-E_\phi)|\lambda\rangle\frac{\langle\lambda|P^J|\phi\rangle}{\langle\phi|P^J|\phi\rangle}\,. \tag{A3}$$

From the definition of P^J, we have

$$\langle\lambda|P^J|\phi\rangle=(2J+1)\int_0^{\pi/2}d\beta\langle\lambda|e^{-iJ_y\beta}|\phi\rangle d^J_{00}(\beta)\sin\beta\,, \tag{A4}$$

$$\langle\phi|P^J|\phi\rangle=(2J+1)\int_0^{\pi/2}d\beta\langle\phi|e^{-iJ_y\beta}|\phi\rangle d^J_{00}(\beta)\sin\beta\,. \tag{A5}$$

Because of the symmetry of $|\phi\rangle$ the integral need only be taken over the range $0\leqslant\beta\leqslant\pi/2$. With highly deformed nuclei, for which

$$\langle J_x{}^2\rangle=\langle J_y{}^2\rangle=\tfrac{1}{2}\langle J^2\rangle>>1\,, \tag{A6}$$

one takes[8,13]

$$\langle\phi|e^{-iJ_y\beta}|\phi\rangle\cong e^{-1/2\langle J_y{}^2\rangle\beta^2}\,, \tag{A7}$$

$$\langle\lambda|e^{-iJ_y\beta}|\phi\rangle\cong-\tfrac{1}{2}\langle\lambda|J_y{}^2|\phi\rangle\beta^2e^{-1/2\langle J_y{}^2\rangle\beta^2}\,. \tag{A8}$$

Due to Eq. (A6) the largest contributions to the integrals of Eqs. (A4) and (A5) come from $\beta\approx0$, and for low J we need consider only the small-angle expansion,

$$d^J_{00}(\beta)\sim1-\tfrac{1}{4}J(J+1)\beta^2\,. \tag{A9}$$

Inserting Eqs. (A7)–(A9) into (A4) and (A5) one obtains

$$E^J=E_\phi-\frac{\langle\phi|J_y{}^2(H-E_\phi)|\phi\rangle}{\langle\phi|J_y{}^2|\phi\rangle}+J(J+1)\frac{\langle\phi|J_y{}^2(H-E_\phi)|\phi\rangle}{2\langle\phi|J_y{}^2|\phi\rangle^2}\,. \tag{A10}$$

In (A10), $J_x{}^2$ or $\frac{1}{2}J^2$ may interchange with $J_y{}^2$.

APPENDIX B. π^J OPERATORS

1. Development of π_1^J

We assume the HF ground state $|\phi\rangle$ is such that

$$\langle\phi|J^2|\phi\rangle>>1\,. \tag{B1}$$

Since all the particles contribute to the diagonal elements of J^2, we assume the 1p-1h excitation of the ground state will have essentially the same diagonal matrix elements,

$$\langle\phi|J^2|\phi\rangle\cong\langle{\rm ph}|J^2|{\rm ph}\rangle\,. \tag{B2}$$

We also assume that, for all state $|\gamma\rangle$ consisting of $J_z=1$ mixtures of 1p-1h configurations (with the exception of the collective state $J_+|\phi\rangle$),

$$\langle\gamma|J^2|\gamma\rangle\approx\langle\phi|J^2|\phi\rangle>>1\,. \tag{B3}$$

With this assumption it can be shown that[13]

$$\langle\gamma|P^J|\gamma\rangle \cong \frac{2J+1}{\langle J^2\rangle} \cong \langle\gamma'|P^J|\gamma'\rangle\ , \tag{B4}$$

$$\langle\gamma|P^J|\gamma'\rangle \cong -\frac{2J+1}{\langle J^2\rangle^2}\ \langle\gamma|J^2|\gamma'\rangle\ , \tag{B5}$$

$$\langle\gamma|P^J|\phi\rangle = \frac{2J+1}{\langle J^2\rangle}\,[J(J+1)]^{1/2}\langle\gamma|J_+|\phi\rangle\ . \tag{B6}$$

To insure $\langle\gamma|P^J|\phi\rangle = 0$, we take $\langle\gamma|J_+|\phi\rangle = 0$.

Let $\{|\kappa\rangle\}$ span the space of 1p-1h HF excitations which is orthogonal to $J_+|\phi\rangle$. Choose this set such that

$$\langle\kappa|J^2|\kappa'\rangle = \delta_{\kappa,\kappa'}\langle\kappa|J^2|\kappa\rangle\ . \tag{B7}$$

Then from Eq. (B5), for $\kappa\neq\kappa'$,

$$\langle\kappa|P^J|\kappa'\rangle \approx 0\ . \tag{B8}$$

Therefore, to the extent of our approximations the set of vectors $\{P^J|\kappa\rangle\}$ is orthogonal, and consequently

$$\pi_1^J = \sum \frac{P^J|\kappa\rangle\langle\kappa|P^J}{\langle\kappa|P^J|\kappa\rangle}\ . \tag{B9}$$

Using Eq. (B4) we then find

$$\pi_1^J = \sum \frac{P^J|\gamma\rangle\langle\gamma|P^J}{\langle\gamma|P^J|\gamma\rangle}\ , \tag{B10}$$

where $\{|\gamma\rangle\}$ is any orthogonal set of states spanning the same space as $\{|\kappa\rangle\}$. In particular, one may take the set $\{|\gamma\rangle\}$ such that

$$\langle\gamma|H|\gamma'\rangle = \delta_{\gamma,\gamma'}\langle\gamma|H|\gamma\rangle\ . \tag{B11}$$

2. Development of π_2^J

Consider the state $P^J J^2|\gamma\rangle$. Then

$$P^J J^2|\gamma\rangle = J(J+1)P^J|\gamma\rangle\ , \tag{B12}$$

$$P^J J^2|\gamma\rangle = \sum_{\gamma'} P^J|\gamma'\rangle\langle\gamma'|J^2|\gamma\rangle + \sum_n P^J|n\rangle\langle n|J^2|\gamma\rangle\ , \tag{B13}$$

where $\{|\gamma'\rangle\}$ is a complete set of states spanning the space of 1p-1h ($J_z = 1$) excitations of the HF ground state, and $\{|n\rangle\}$ is a complete set of states spanning 2p-2h and 3p-3h ($J_z = 1$) excitations. The latter are reached by the two-body operator J^2. Combining Eqs. (B12) and (B13) we obtain

$$[J(J+1) - \langle\gamma|J^2|\gamma\rangle]P^J|\gamma\rangle = \sum_{\gamma\neq\gamma'} P^J|\gamma'\rangle\langle\gamma'|J^2|\gamma\rangle + \sum_n P^J|n\rangle\langle n|J^2|\gamma\rangle\ . \tag{B14}$$

Then assuming $J(J+1)/\langle\gamma|J^2|\gamma\rangle \ll 1$,

$$P^J|\gamma\rangle \cong -\sum_{\gamma'\neq\gamma} P^J|\gamma'\rangle\frac{\langle\gamma'|J^2|\gamma\rangle}{\langle\gamma|J^2|\gamma\rangle} - \sum_n P^J|n\rangle\frac{\langle n|J^2|\gamma\rangle}{\langle\gamma|P^J|\gamma\rangle}\ . \tag{B15}$$

Using the following expressions for the matrix element of P^J,

$$\langle\gamma|P^J|\gamma\rangle \cong \frac{2J+1}{\langle J^2\rangle} \cong \langle n|P^J|n\rangle\ , \tag{B16}$$

$$\langle n|P^J|\gamma\rangle \cong -\langle\gamma|P^J|\gamma\rangle\,\frac{\langle n|J^2|\gamma\rangle}{\langle\gamma|J^2|\gamma^2\rangle}\ , \tag{B17}$$

$$\langle\gamma'|P^J|\gamma\rangle \cong -\langle\gamma|P^J|\gamma\rangle\frac{\langle\gamma'|J^2|\gamma\rangle}{\langle\gamma|J^2|\gamma\rangle}\ , \tag{B18}$$

and assuming

$$\langle\gamma|J^2|\gamma\rangle \cong \langle J^2\rangle \cong \langle n|J^2|n\rangle\ , \tag{B19}$$

we obtain from Eq. (B15)

$$P^J|\gamma\rangle \cong \sum_{\gamma'\neq\gamma} P^J|\gamma'\rangle\frac{\langle\gamma'|P^J|\gamma\rangle}{\langle\gamma'|P^J|\gamma'\rangle} + \sum_n P^J|n\rangle\frac{\langle n|P^J|\gamma\rangle}{\langle n|P^J|n\rangle}\ . \tag{B20}$$

Finally, including γ in the sum over γ' in Eq. (B20), we obtain

$$P^J|\gamma\rangle = \tfrac{1}{2}\left(\sum_{\gamma'} P^J|\gamma'\rangle\frac{\langle\gamma'|P^J|\gamma\rangle}{\langle\gamma'|P^J|\gamma'\rangle} + \sum P^J|n\rangle\frac{\langle n|P^J|\gamma\rangle}{\langle n|P^J|n\rangle}\right)\ . \tag{B21}$$

If we wish to restrict $|\gamma\rangle$ to states such that $\langle\gamma|P^J|\phi\rangle = 0$, we may choose for the states $\{|\gamma\rangle\}$ those 1p-1h states orthogonal to $J_+|\phi\rangle$ and orthogonal to the 1p-1h component of $J_+J^2|\phi\rangle$, and for the states $\{|n\rangle\}$ those 2p-2h and 3p-3h states orthogonal to the corresponding components of $J_+J^2|\phi\rangle$. Let $\{|u\rangle\}$ be any orthogonal set of vectors spanning the space of all 1p-1h, 2p-2h, and 3p-3h ($J_z = 1$) states orthogonal to $J_+|\phi\rangle$ and $J_+J^2|\phi\rangle$. Then, assuming

$$\langle u|P^J|u\rangle \cong \langle\gamma|P^J|\gamma\rangle \cong \langle n|P^J|n\rangle\ , \tag{B22}$$

we obtain from (B21)

$$\pi_2^J = \tfrac{1}{2}\sum_u \frac{P^J|u\rangle\langle u|P^J}{\langle u|P^J|u\rangle}\ . \tag{B23}$$

In particular, we can choose for the set of states $\{|u\rangle\}$ one such that

$$\langle u|H|u'\rangle = \delta_{uu'}\langle u|H|u\rangle\ . \tag{B24}$$

APPENDIX C. EIGENFUNCTION OF Γ

We prove here that

$$\frac{\langle\phi|J_x\Gamma J_x|\phi\rangle}{\langle\phi|J_x{}^2|\phi\rangle^2} = \frac{1}{\langle\phi|J_x\Gamma^{-1}J_x|\phi\rangle} \tag{C1}$$

implies that $J_x|\phi\rangle$ is an eigenstate of Γ. Equation (C1) may be written

$$\langle\phi|J_x\Gamma J_x|\phi\rangle\langle\phi|J_x\Gamma^{-1}J_x|\phi\rangle = |\langle\phi|J_x{}^2|\phi\rangle|^2 . \quad \text{(C2)}$$

For convenience let us write $J_x|\phi\rangle$ as $|\alpha\rangle$. Then (C2) becomes

$$\langle\alpha|\Gamma|\alpha\rangle\langle\alpha|\Gamma^{-1}|\alpha\rangle - |\langle\alpha|\alpha\rangle|^2 = 0 . \quad \text{(C3)}$$

Assuming Γ is Hermitian we obtain

$$\Gamma = \sum_i |\lambda_i\rangle\langle\lambda_i|E_i , \quad \text{(C4)}$$

where $E_i > 0$ and $\{|\lambda_i\rangle\}$ is a complete set of vectors. Putting (C4) in (C3),

$$\tfrac{1}{2}\sum_{i\neq j} |\langle\alpha|\lambda_i\rangle|^2|\langle\alpha|\lambda_j\rangle|^2\left[\frac{E_i}{E_j}+\frac{E_j}{E_i}-2\right] = 0 , \quad \text{(C5a)}$$

$$\tfrac{1}{2}\sum_{i\neq j} |\langle\alpha|\lambda_i\rangle|^2|\langle\alpha|\lambda_j\rangle|^2\left[\frac{(E_i-E_j)^2}{E_iE_j}\right] = 0 . \quad \text{(C5b)}$$

All the terms are positive. Therefore if $|\langle\alpha|\lambda_0\rangle|^2 \neq 0$, then $|\langle\alpha|\lambda_i\rangle|^2 = 0$ for all $i \neq 0$, and thus

$$|\alpha\rangle \equiv J_x|\phi\rangle = |\lambda_0\rangle . \quad \text{(C6)}$$

APPENDIX D. INDEPENDENT-PARTICLE APPROXIMATION AND $SU(3)$ WAVE FUNCTIONS

We have defined the operators Γ and Λ in the body of the paper [Eq. (II.7) and Eq. (II.13)] and we have stated that

$$\Gamma J_x|\phi\rangle = \Lambda J_x|\phi\rangle . \quad \text{(D1)}$$

We now define Γ_0 and Γ_1 such that

$$\Gamma = \Gamma_0 + \Gamma_1 , \quad \text{(D2)}$$

$$(\mathrm{ph}|\Gamma_0|\mathrm{p'h'}) = \langle\mathrm{ph}|(H_0 - E)|\mathrm{p'h'}\rangle . \quad \text{(D3)}$$

$$(\mathrm{ph}|\Gamma_1|\mathrm{p'h'}) = \langle\mathrm{PH}|V^{(2)}|\mathrm{p'h'}\rangle , \quad \text{(D4)}$$

where H_0 is an independent particle Hamiltonian, and $V^{(2)}$ a two-body interaction. From Eqs. (D1) and (D2) we have

$$\Gamma_0 J_x|\phi\rangle = (\Lambda - \Gamma_1)J_x|\phi\rangle . \quad \text{(D5)}$$

We shall prove here that with $V^{(2)}$ of the following tensor form,

$$V^{(2)} = \tfrac{1}{2}V_0 \sum_{\substack{\lambda\ \mathrm{even}\\ \mu}} (-)^\mu Q_{\lambda\mu}Q_{\lambda-\mu} , \quad \text{(D6)}$$

one obtains

$$(\Lambda - \Gamma_1)J_x|\phi\rangle = 2\Lambda J_x|\phi\rangle , \quad \text{(D7)}$$

when exchange terms are ignored. With Eqs. (D1) and (D2) one then obtains

$$\Gamma_0 J_x|\phi\rangle = 2\Gamma J_x|\phi\rangle . \quad \text{(D8)}$$

For the potential given in Eq. (D6)

$$(\mathrm{ph}|\Gamma_1|\mathrm{p'h'}) = V_0 \sum_{\mu,\lambda_e} (-)^\mu\langle\mathrm{ph}|Q_{\lambda\mu}|\phi\rangle\langle\phi|Q_{\lambda-\mu}|\mathrm{p'h'}\rangle , \quad \text{(D9)}$$

$$(\mathrm{ph}|\Lambda|\mathrm{p'h'}) = V_0 \sum_{\mu,\lambda_e} (-)^\mu\langle\mathrm{ph}|Q_{\lambda\mu}|\phi\rangle\langle\mathrm{p'h'}|Q_{\lambda-\mu}|\phi\rangle , \quad \text{(D10)}$$

and

$$\sum_{\mathrm{p'h'}} (\mathrm{ph}|\Gamma_1|\mathrm{p'h'})\langle\mathrm{p'h'}|J_+|\phi\rangle = V_0 \sum_{\mu,\lambda_e} (-)^\mu\langle\mathrm{ph}|Q_{\lambda\mu}|\phi\rangle\langle\phi|Q_{\lambda-\mu}J_+|\phi\rangle = (\mathrm{ph}|\Gamma_1 J_+|\phi\rangle , \quad \text{(D11)}$$

$$\sum_{\mathrm{p'h'}} \langle\phi|J_+|\mathrm{p'h'}\rangle(\mathrm{ph}|\Lambda|\mathrm{p'h'}) = V_0 \sum_{\mu,\lambda_e} (-)^\mu\langle\mathrm{ph}|Q_{\lambda\mu}|\phi\rangle\langle\phi|J_+Q_{\lambda-\mu}|\phi\rangle = \langle\phi|J_+\Lambda|\mathrm{ph}) . \quad \text{(D12)}$$

Now, consider the tensor operator

$$W_{LM} = \sum_\mu (\lambda - \mu 1 + 1|LM)(Q_{\lambda-\mu}J_+) .$$

For axially symmetric ($J_z = 0$) states $|\phi\rangle$, $\langle\phi|W_{LM}|\phi\rangle$ vanishes unless $M = 0$ and L is even. Considering this, we find

$$(\mathrm{ph}|\Gamma_1 J_+|\phi\rangle = (-)^{\lambda+1}\langle\phi|J_+\Lambda|\mathrm{ph}) , \quad \text{(D13a)}$$

$$(\mathrm{ph}|\Gamma_1 J_-|\phi\rangle = (-)^{\lambda+1}\langle\phi|J_-\Lambda|\mathrm{ph}) , \quad \text{(D13b)}$$

and thus

$$(\mathrm{ph}|\Gamma_1 J_x|\phi\rangle = (-)^{\lambda+1}\langle\phi|J_x\Lambda|\mathrm{ph}) = (-)^{\lambda+1}(\mathrm{ph}|\Lambda J_x|\phi\rangle , \quad \text{(D14)}$$

or

$$(\Lambda - \Gamma_1)J_x|\phi\rangle = [1 + (-)^\lambda]\Lambda J_x|\phi\rangle . \quad \text{(D15)}$$

For λ even

$$(\Lambda - \Gamma_1)J_x|\phi\rangle = 2\Lambda J_x|\phi\rangle . \quad \text{(D16)}$$

This proves that for potentials of the form given in Eq. (D7)

$$\Gamma_0 J_x|\phi\rangle = 2\Gamma J_x|\phi\rangle . \quad \text{(D17)}$$

We now consider in detail the case of the quadrupole-quadrupole interaction

$$V^{(2)} = -\tfrac{1}{2}|V_0| \sum_{\substack{\mu\\ i\neq j}} (-)^\mu Q_{2\mu}(i)Q_{2-\mu}(j) , \quad \text{(D18)}$$

for which an exact expression for the moment of inertia is[15]

$$\mathcal{I} = \hbar^2/3|V_0| . \quad \text{(D19)}$$

For the intrinsic wave function associated with the quadrupole-quadrupole force let us take the $SU(3)$ wave function of maximum weight[15] $\phi(\lambda\mu)$ ($\mu = 0$ for the case of axial symmetry).

We now calculate the moment of inertia using the independent-particle Inglis formula

$$\mathcal{I}_{\mathrm{I}} = 2\hbar^2 \sum_i \frac{|\langle i|L_x|\phi(\lambda 0)\rangle|^2}{E_i - E_\phi} . \quad \text{(D20)}$$

In choosing the independent-particle states $|i\rangle$ we consider the states reached by[15]

$$L_x|\phi(\lambda 0)\rangle = \sum_L{}' a_y^+(i)\,a_z(i)|\phi(\lambda 0)\rangle \,, \qquad \text{(D21)}$$

and take as our basis

$$|i\rangle = N_i a_y^+(i) a_z(i)|\phi(\lambda 0)\rangle \,. \qquad \text{(D22)}$$

To normalize the states $|i\rangle$ we must have

$$N_i = 1/(n_{z_i} - n_{y_i})^{1/2} \,, \qquad \text{(D23)}$$

where n_{z_i} and n_{y_i} are the number of z and y quanta in the ith single-particle level of $\phi(\lambda 0)$.

For the independent-particle energy denominator we consider[15]

$$H_0 = \sum_i [h_0(i) - |V_0|2\lambda Q_{20}(i)] \,; \qquad \text{(D24a)}$$

$$(i|\Gamma_0|i') = \delta_{i,i'}\langle i|H_0 - E_\phi|i\rangle \,. \qquad \text{(D24b)}$$

This gives

$$E_i - E_\phi = \langle i|H_0|i\rangle - \langle\phi|H_0|\phi\rangle = 6\lambda|V_0| \,, \qquad \text{(D25)}$$

for all i.

Next consider the numerator in Eq. (D20), for which we have

$$\langle i|L_x|\phi(\lambda 0)\rangle = (n_{z_i} - n_{y_i})^{1/2} \,. \qquad \text{(D26)}$$

Combining (D25) and (D26) in (D20) we obtain

$$\mathscr{I}_{\rm I} = 2\hbar^2 \sum_i \frac{(n_{z_i} - n_{y_i})}{6\lambda|V_0|} \,, \qquad \text{(D27)}$$

but $\sum_i (n_{z_i} - n_{y_i}) = \lambda$, so

$$\mathscr{I}_{\rm I} = \hbar^2/3|V_0| \,. \qquad \text{(D28)}$$

Now let us consider the full operator Γ which involves two-body interactions as well as Γ_0. From Eq. (D9) we have

$$(i|\Gamma_1|i') = -|V_0|\sum_\mu (-)^\mu \langle i|Q_{2\mu}|\phi\rangle\langle\phi|Q_{2-\mu}|i'\rangle \,, \qquad \text{(D29)}$$

but[15]

$$Q_{2+1}|\phi(\lambda 0)\rangle = \sqrt{\tfrac{3}{2}}\,L_+|\phi(\lambda 0)\rangle \,, \qquad \text{(D30a)}$$

$$\langle\phi(\lambda 0)|Q_{2-1} = -\sqrt{\tfrac{3}{2}}\,\langle\phi(\lambda 0)|L_- \,, \qquad \text{(D30b)}$$

therefore

$$(i|\Gamma_1|i') = -3|V_0|\langle i|L_x|\phi(\lambda 0)\rangle\langle\phi(\lambda 0)|L_x|i'\rangle \,, \qquad \text{(D31)}$$

and using Eq. (D26)

$$(i|\Gamma_1|i') = -3|V_0|(n_{z_i} - n_{y_i})^{1/2}(n_{z_{i'}} - n_{y_{i'}})^{1/2} \,. \qquad \text{(D32)}$$

For convenience let

$$n_{z_i} - n_{y_i} = \lambda_i \,, \quad \sum_i \lambda_i = \lambda \,. \qquad \text{(D33)}$$

Then with Eq. (D32) we can write

$$(i|\Gamma|i') = 6|V_0|\lambda\delta_{i,i'} - 3|V_0|\sqrt{\lambda_i}\,\sqrt{\lambda_{i'}} \,. \qquad \text{(D34)}$$

To find the collective eigenstate of Γ, we use the techniques of the schematic model[4] and consider

$$\sum_{i'} (i|\Gamma|i')C_{i'}^\alpha = \epsilon^\alpha C_i^\alpha \,,$$

or

$$6|V_0|\lambda C_i^\alpha - 3|V_0|\sqrt{\lambda_i}\,\left(\sum C_{i'}^\alpha \sqrt{\lambda_{i'}}\right) = \epsilon^\alpha C_i^\alpha \,. \qquad \text{(D35)}$$

Multiplying by $\sqrt{\lambda_i}$ and summing over i we find

$$6|V_0|\lambda\left(\sum C_i^\alpha\sqrt{\lambda_i}\right) - 3|V_0|\sum_i \lambda_i\left(\sum C_i^\alpha\sqrt{\lambda_i}\right) = \epsilon^\alpha\left(\sum C_i^\alpha\sqrt{\lambda_i}\right). \qquad \text{(D36)}$$

This leads to one energy, ϵ,

$$\epsilon = 3|V_0|\lambda \,, \qquad \text{(D37a)}$$

with

$$C_i = \sqrt{\lambda_i/\lambda} \,. \qquad \text{(D37b)}$$

The eigenstate associated with this energy is

$$|\epsilon\rangle = \frac{1}{\sqrt{\lambda}}\sum_i \sqrt{\lambda_i}\,|i\rangle \,, \qquad \text{(D38a)}$$

$$= \frac{1}{\sqrt{\lambda}}\,L_x|\phi(\lambda 0)\rangle \,. \qquad \text{(D38b)}$$

Thus $L_x|\phi(\lambda 0)\rangle$ is shown to be an eigenstate of Γ, and furthermore we have shown

$$\Gamma L_x|\phi\rangle = (3V_0\lambda)L_x|\phi\rangle \,, \qquad \text{(D39)}$$

which indeed gives

$$\Gamma L_x|\phi\rangle = \tfrac{1}{2}\Gamma_0 L_x|\phi\rangle \,. \qquad \text{(D40)}$$

Since

$$\langle\epsilon|\epsilon\rangle = 1 \,,$$

we have

$$\langle\phi|L_x{}^2|\phi\rangle = \lambda \,. \qquad \text{(D41)}$$

Finally using Eq. (D39) and Eq. (D41) to evaluate the Peierls-Yoccoz formula for the moment of inertia, we have

$$\mathscr{I}_{\rm PY} = \hbar^2 \frac{\langle\phi|L_x{}^2|\phi\rangle^2}{\langle\phi|L_x\Gamma L_x|\phi\rangle} = \frac{\lambda^2\hbar^2}{3|V_0|\lambda^2} = \frac{\hbar^2}{3|V_0|} \,. \qquad \text{(D42)}$$

We have thus shown for this model case that

$$\mathscr{I}_{\rm exact} = \mathscr{I}_{\rm I} = \mathscr{I}_{\rm PY} = \mathscr{I}_{\rm FW} . \qquad \text{(D43)}$$

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Higher-Order Corrections to Internal Conversion*

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Higher-order corrections to internal conversion and γ-ray emission involving atomic electrons have been calculated. Experimental anomalies in low-energy $E2$ L-subshell ratios are shown to be substantially explained by these calculations.

The development of high-resolution β spectrometers in recent years has allowed accurate comparisons between theoretical and experimental internal-conversion coefficients. In particular, the measurement of L-shell ratios can attain an accuracy of 2–3%. The low-energy $2^+ \to 0^+$ transitions observed in deformed nuclei allow one to systematically study the internal conversion of a single multipole. Extensive measurements of these $E2$ transitions have been made in many laboratories.[1] The L_I/L_{II} ratio was regularly observed to be some 5% higher than predicted by theory; whereas the L_{II}/L_{III} ratio was in good agreement (3%) with the theoretical ratio. Although there are discrepancies between the earlier tabulations of theoretical internal-conversion coefficients,[2] the predicted $E2$ L-shell ratios are in good enough agreement to indicate an experimental anomaly. In addition, independent calculations of internal-conversion coefficients confirm the existence of an experimental anomaly the same size.[3-6]

"Penetration effects" which lead to large deviations from theoretical conversion coefficients are known to occur in highly retarded transitions.[7] These effects are due to nuclear-structure-dependent terms not included in a tabulation of theoretical conversion coefficients. They are expected to be negligible for fast transitions such as the collective $E2$ transitions in deformed nuclei. We have estimated the magnitude of penetration effects in these well-understood $2^+ \to 0^+$ transitions and found that they change the tabulated conversion coefficients by less than 0.5%. Matese has investigated the effect of atomic wave-function distortion due to the static nuclear quadrupole moment and has concluded that the internal-conversion coefficient is changed to an insignificant extent.[8]

At the present time, all calculations of internal-conversion coefficients only include terms to the lowest order in the fine-structure constant. In the