Determination of Nuclear Rotational Parameters*

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The methods of extracting nuclear rotational parameters are critically reviewed. An external consistency condition is proposed, as a necessary condition for the validity of such methods.

I. INTRODUCTION

IT is useful, when treating the question of rotational (and collective) spectra and their "microscopic" origin, to review briefly the hierarchy of problems of which it is part.

It is observed experimentally that some nuclear systems—in a few rather well-defined regions—have low-lying rotational spectra. This is manifested both by the typical $I(I+1)$ energy-level rule and by the large enhancement of the intraband electric-quadrupole-transition probabilities. That a complicated many-body system will—in selected cases—have such a simple and neat behavior may, indeed, seem a puzzling accident. To fully understand this phenomenon, one has to know exactly the Hamiltonians describing the nuclear systems, and to find their pertinent eigenenergies and eigenfunctions. This, in fact, is the ultimate solution to nuclear structure in general, inasmuch as any level in any nucleus—with its related properties—could be traced back, quantitatively, to a common origin. This ultimate solution, however, cannot be achieved. First, the exact form of the Hamiltonian is not known. Second, the techniques of many-body theory and the capabilities of present-day digital computers are totally inadequate for exact numerical solutions.

Thus, one has to be satisfied with substitute Hamiltonians, often taken on an *ad hoc* basis, and with treating them by various approximative methods. It is, usually, when the derivation of exact eigenenergies is completely out of question, that one has to resort to the rotational (or—in general—collective) description of motion.

Two, basically different questions now arise. First, under what conditions will a rotational spectrum emerge? Second, assuming that such a spectrum actually exists, how does one determine its quantitative characteristic, namely, the moment of inertia $\mathcal{J}$, or the rotation parameter $A=\hbar^2/2\mathcal{J}$? Both questions have to be answered, preferably without recourse to explicit solutions of the many-body Hamiltonian.

To explain the occurrence of rotational behavior, we make some assumptions about the nature of the low-lying energy states of the system. (In a few cases, where actual calculations could be carried out, these assumptions appear to be well founded.) We assume that the nucleus has a permanent deformation from sphericity, and that this deformation is rigidly retained in time. We further assume that an independent-particle motion takes place in the average field described by this deformed shape, so that we may represent the nucleus by a determinantal-product wave function. Such a wave function, however, will not have well-defined angular momentum. Rather, it will be a superposition of states with different angular momenta. These states can, in fact, be projected out of the determinantal wave function, and be properly normalized. We believe that they represent the various members of the rotational band.

We believe, therefore, in the existence of an "intrinsic" state (as this determinantal wave function is often referred to) which represents, in an internally correlated manner, all the members of a rotational band simultaneously.

It is extremely important to note, at this point, that the notion of an "intrinsic" state is totally independent of that of a product wave function. The quantitative information concerning the band is inherent in this intrinsic state. It can, so we argue, be extracted from it without actually performing the projection of angular momentum. In Sec. II we give a concise review of the cranking approach. In Sec. III we propose an external-consistency condition, that this approach (or any other theory that tries to get rotational parameters) should obey. In Sec. IV a specific numerical case is presented, where that condition is violated, and an attempt is made to understand why this is so. In Sec. V, an alternative variational approach is discussed which does obey the Sec. III condition, and some modifications of it are suggested.

II. "CRANKING" APPROACH TO ROTATIONAL MOTION

A definite procedure to obtain explicitly an intrinsic state to represent the rotational band is provided by the theory and philosophy of the Hartree-Fock theory,[1] borrowed from atomic physics.

Given a Hamiltonian, in second-quantization notation

$$H=\sum_{\alpha,\beta}\langle\alpha|K|\beta\rangle a_\alpha^\dagger a_\beta + \tfrac{1}{4}\sum_{\alpha,\beta,\gamma,\delta}\langle\alpha\beta|V_A|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma, \quad (1)$$

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[1] For a general review of the subject see, for example, M. Baranger, in *Cargèse Lectures in Theoretical Physics* (W. A. Benjamin, Inc., New York, 1963).

where K is a one-body operator, and V_A an antisymmetrized two-body operator, we seek the determinantal wave function ϕ such that

$$\langle\phi|H|\phi\rangle=\text{minimum} \tag{2a}$$

or

$$\delta\langle\phi|H|\phi\rangle=\langle\delta\phi|H|\phi\rangle=0. \tag{2b}$$

This variational principle is known to lead to the following self-consistency problem. A one-body (nonlocal) Hamiltonian h, and a set $\{\lambda\}$ of wave functions (equaling in number the number of particles in the system) are sought, such that

$$h=\sum_{\alpha,\beta}\{\langle\alpha|K|\beta\rangle+\sum_{\lambda}\langle\alpha\lambda|V_A|\beta\lambda\rangle\}a_\alpha^\dagger a_\beta \tag{3a}$$

and

$$h|\lambda\rangle=e_\lambda|\lambda\rangle \tag{4a}$$

hold simultaneously. ϕ is then the antisymmetrized product wave function of the set $\{\lambda\}$. An alternative formulation may be followed by defining the one-body projection operator

$$\rho=\sum_{\lambda}a_\lambda^\dagger a_\lambda. \tag{5}$$

The self-consistency equations are then

$$h_1=K_1+\mathrm{Tr}_2V_{12}\rho_2 \tag{3b}$$

and

$$[h,\rho]=0. \tag{4b}$$

In Eq. (3b) the subscripts refer to the particle in whose space the operators operate. The Hartree-Fock Hamiltonian h gives rise to a complete representation, spanning the nonoccupied states as well. This representation is considered to be of relatively great importance for performing perturbation calculations on the system.

It is the stability of the solution ϕ against small variations which is believed by many authors[2–4] to be the prime indication of the existence of a rotational spectrum, provided this solution is not spherically symmetric. This stability, in turn, may be inferred from the magnitude of the energy gap between the occupied and the nonoccupied single-particle states.

The prevailing methods of deriving a quantitative expression for the moment of inertia stem from this approach.

The function ϕ, and hence the operators ρ and h, will not necessarily retain all the symmetry properties of the many-body Hamiltonian H. In the description of the ground-state rotational band of an even-even nucleus, ϕ, ρ, and h have only axial symmetry. If the axis of symmetry is chosen to be the z axis, it is easy to see that

$$\langle\phi|J_x|\phi\rangle=0. \tag{6a}$$

We now investigate the response of the system to a rotation around the x axis, which is perpendicular to the axis of symmetry. To do this, the variational problem is solved with the additional subsidiary condition

$$\langle\phi|J_x|\phi\rangle=\eta, \tag{6b}$$

using a Lagrange multiplier ω. The modified solution ϕ_ω will give rise to an increment in the energy, which is attributed to the effect of rotation around the x axis with angular velocity ω. Thus

$$\langle\phi_\omega|H|\phi_\omega\rangle-\langle\phi|H|\phi\rangle\equiv\tfrac{1}{2}\mathcal{I}\omega^2. \tag{7}$$

To express $\mathcal{I}$ in terms of the microscopic structure of the Hamiltonian H, a detailed analysis of the variational problem must be carried out (see Appendix A). Depending on what approximation to this problem one makes, different expressions for $\mathcal{I}$ come out. Merely replacing h by $h-\omega J_x$ gives rise to Inglis's cranking formula[5]:

$$\mathcal{I}=2\hbar^2\sum_{\sigma,\mu}\frac{|\langle\sigma|J_x|\mu\rangle|^2}{e_\sigma-e_\mu}. \tag{8}$$

Including also diagonal elements of the $\mathrm{Tr}_2\rho_2V_{12}$ term, one gets the Thouless-Valatin expression[6]

$$\mathcal{I}=2\hbar^2\sum_{\sigma,\mu}\frac{|\langle\sigma|J_x|\mu\rangle|^2}{e_\sigma-e_\mu-\langle\sigma\mu|V_A|\sigma\mu\rangle}. \tag{9}$$

In both expressions, σ runs over nonoccupied and μ over occupied single-particle states of the unperturbed Hartree-Fock representation.

In practical cases, the formulas may differ very appreciably from one another, and they may both provide a poor approximation to the sought-for infinitesimal energy increment. As one clearly sees, this will depend in a crucial way on the form and properties of the two-body interaction.

III. EXTERNAL CONSISTENCY CONDITION ON MICROSCOPIC DERIVATION OF ROTATIONAL PARAMETERS

From a conceptual point of view the "cranking" formula, mentioned in the last section, is a *recipe* which gives, for a given Hamiltonian, a value for a rotational parameter $A=\hbar^2/2\mathcal{I}$. The same holds true for any other approach, which may vary in detail and technique but tries to achieve the same end.

That H will at all have a low-lying rotational spectrum is not tested, but assumed. Clearly, if H does not have this expected rotational behavior, the whole discussion is meaningless. But when it does, as we assume it to, the validity or invalidity of the "cranking"—or any other approach—becomes a *mathematical* proposition. To investigate this question without actual re-

[2] R. S. Nataf, Nucl. Phys. **2**, 492 (1957).
[3] D. J. Thouless, Nucl. Phys. **22**, 225 (1960).
[4] R. E. Peierls and D. J. Thouless, Nucl. Phys. **38**, 154 (1962).
[5] D. R. Inglis, Rev. Mod. Phys. **25**, 390 (1953).
[6] D. J. Thouless and J. G. Valatin, Nucl. Phys. **31**, 211 (1962).

course to a solution of H, we propose an *external-consistency criterion.*

Let us symbolically describe by the relation

$$\hbar^2/2\mathcal{I}=A=\mathcal{R}[H] \tag{10}$$

any procedure which extracts the parameter A from the Hamiltonian H. According to our basic assumption, the system described by H has a low-lying rotational band, with energies

$$E_I=AI(I+1)=\mathcal{R}[H]I(I+1). \tag{11}$$

We may now consider the Hamiltonian

$$H(\alpha)=H+\alpha J^2. \tag{12}$$

If H has the spectrum (11), $H(\alpha)$ will clearly also have a rotational spectrum

$$E_I(\alpha)=AI(I+1)+\alpha I(I+1). \tag{13}$$

Applying the "recipe" under consideration to $H(\alpha)$, we obtain

$$E_I(\alpha)=A(\alpha)I(I+1)=\mathcal{R}[H+\alpha\mathbf{J}^2]I(I+1). \tag{14}$$

Equating (13) and (14), we impose a criterion on $\mathcal{R}$

$$\mathcal{R}[H+\alpha\mathbf{J}^2]=\mathcal{R}[H]+\alpha. \tag{15}$$

In a less stringent way, we may demand

$$\left.\frac{\partial A(\alpha)}{\partial\alpha}\right|_{\alpha=0}\approx 1. \tag{16}$$

The condition thus imposed is clearly only a *necessary* condition for the validity of $\mathcal{R}$. It is by no means sufficient. However, if it is violated by a certain "recipe" in some particular case, it means that whatever agreement such "recipe" achieves, it necessarily is to be deemed accidental *in that particular case.*

Let us begin by investigating the cranking approach in particular. To do this we have to determine the behavior of the self-consistency problem under the simultaneous perturbations $\alpha\mathbf{J}^2$ and $-\omega J_x$.

Let ϕ be the Hartree-Fock solution to the unperturbed problem: ϕ^α to $H+\alpha J^2$, ϕ_ω to $H-\omega J_x$, $\phi_\omega{}^\alpha$ to $H+\alpha J^2-\omega J_x$. We can expand these functions up to second order in α and ω, thereby defining the various functions appearing in the expansion. Thus

$$\begin{aligned}
&\phi^\alpha\equiv\phi+\alpha\phi^{(1)}+\alpha^2\phi^{(2)},\\
&\phi_\omega\equiv\phi+\omega X^{(1)}+\omega^2X^{(2)},\\
&\phi_\omega{}^\alpha\equiv\phi+\alpha\phi^{(1)}+\alpha^2\phi^{(2)}+\omega X^{(1)}+\omega^2X^{(2)}+\alpha\omega\psi^{(2)}.
\end{aligned} \tag{17}$$

It can be easily shown that higher-order terms are not necessary for the verification of the external criterion (16).

We now note that

$$\begin{aligned}
&\langle\phi^\alpha|\phi^\alpha\rangle=1+O(\alpha^2),\\
&\langle\phi_\omega|\phi_\omega\rangle=1+O(\omega^2),\\
&\langle\phi_\omega{}^\alpha|\phi_\omega{}^\alpha\rangle=1+O(\{\alpha,\omega\}^2),\\
&\langle\phi|J_x|\phi\rangle=\langle\phi^\alpha|J_x|\phi\rangle=\langle\phi^\alpha|J_x|\phi^\alpha\rangle=0.
\end{aligned} \tag{18}$$

The moment of inertia $\mathcal{I}$ is extracted from the functions in Eq. (17):

$$\langle\phi_\omega|J_x|\phi_\omega\rangle=2\omega\langle\phi|J_x|X^{(1)}\rangle+O(\omega^2)\equiv\mathcal{I}_0\omega \tag{19}$$

and

$$\begin{aligned}
\langle\phi_\omega{}^\alpha|J_x|\phi_\omega{}^\alpha\rangle=&\,2\omega\langle\phi|J_x|X^{(1)}\rangle+2\omega\alpha\langle\phi|J_x|\psi^{(2)}\rangle\\
&+2\omega\alpha\langle\phi^{(1)}|J_x|X^{(1)}\rangle\equiv\mathcal{I}_\alpha\omega.
\end{aligned} \tag{20}$$

Thus, one obtains

$$\mathcal{I}_0=2\langle\phi|J_x|X^{(1)}\rangle, \tag{21}$$

$$\mathcal{I}_\alpha=\mathcal{I}_0+2\alpha\{\langle\phi|J_x|\psi^{(2)}\rangle+\langle\phi^{(1)}|J_x|X^{(1)}\rangle\}, \tag{22}$$

or

$$\left.\frac{\partial\mathcal{I}_\alpha}{\partial\alpha}\right|_{\alpha=0}=2\{\langle\phi|J_x|\psi^{(2)}\rangle+\langle\phi^{(1)}|J_x|X^{(1)}\rangle\}. \tag{23}$$

The criterion may be expressed, therefore, as

$$\left.\frac{\partial\mathcal{I}_\alpha}{\partial\alpha}\right|_{\alpha=0}=-2\mathcal{I}_0{}^2 \tag{24}$$

or

$$\langle\phi|J_x|\psi^{(2)}\rangle+\langle\phi^{(1)}|J_x|X^{(1)}\rangle=-4|\langle\phi|J_x|X^{(1)}\rangle|^2. \tag{25}$$

The relationship to be fulfilled may be conveniently reexpressed in terms of J^2 expectation values. This is done by explicitly using the fact that $\phi_\omega{}^\alpha$ is a variational solution to a problem of the general nature given by Eq. (2b). As particular applications we write

$$\begin{aligned}
\langle\phi^{(1)}+2\alpha\phi^{(2)}+\omega\psi^{(2)}|H+\alpha J^2-\omega J_x|\phi+\alpha\phi^{(1)}+\alpha^2\phi^{(2)}\\
+\omega X^{(1)}+\omega^2X^{(2)}+\alpha\omega\psi^{(2)}\rangle=0,
\end{aligned} \tag{26a}$$

$$\begin{aligned}
\langle X^{(1)}+2\omega X^{(2)}+\alpha\psi^{(2)}|H+\alpha J^2-\omega J_x|\phi+\alpha\phi^{(1)}+\alpha^2\phi^{(2)}\\
+\omega X^{(1)}+\omega^2X^{(2)}+\alpha\omega\psi^{(2)}\rangle=0.
\end{aligned} \tag{26b}$$

Equating the coefficients of ω in (26a) or of α in (26b), one obtains

$$\langle\psi^{(2)}|H|\phi\rangle=0, \tag{27}$$

reflecting the fact that $\psi^{(2)}$ can be obtained from ϕ by a linear combination of one-particle promotion operators. Writing the coefficients of ω^2 in (26a) and of $\alpha\omega$ in (26b), we get, respectively,

$$\begin{aligned}
\langle\phi^{(1)}|H|X^{(2)}\rangle-\langle\phi^{(1)}|J_x|X^{(1)}\rangle+\langle\psi^{(2)}|H|X^{(1)}\rangle\\
-\langle\psi^{(2)}|J_x|\phi\rangle=0,
\end{aligned} \tag{28}$$

$$\begin{aligned}
2\langle X^{(1)}|H|\psi^{(2)}\rangle+\langle X^{(1)}|J^2|X^{(1)}\rangle\\
-\langle\phi^{(1)}|J_x|X^{(1)}\rangle+2\langle X^{(2)}|H|\phi^{(1)}\rangle\\
+2\langle X^{(2)}|J^2|\phi\rangle-\langle\psi^{(2)}|J_x|\phi\rangle=0.
\end{aligned} \tag{29}$$

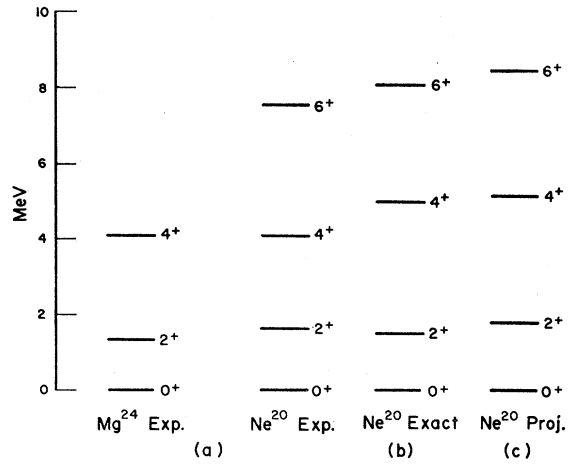

FIG. 1. (a) The experimental sequence of levels in Mg^{24} and Ne^{20}, belonging to the ground-state rotational band. (b) An exact diagonalization result [T. Inoue, T. Sebe, H. Haqwara, and A. Arima, Nucl. Phys. **59**, 1 (1964). Also, B. French (private communication).] for the Hamiltonian (33), with the lowest 0^+ state matched to the Ne^{20} ground state. (c) Results of projecting good J from the Hartree-Fock determinantal state, displaying the very good approximation to the calculated exact spectrum.

Upon multiplying (28) by 2 and subtracting from (29), the matrix elements involving the Hamiltonian are seen to drop out and one obtains the equality

$$\langle\phi|J_x|\psi^{(2)}\rangle+\langle\phi^{(1)}|J_x|X^{(1)}\rangle=-\langle X^{(1)}|J^2|X^{(1)}\rangle -2\langle X^{(2)}|J^2|\phi\rangle. \quad (30)$$

Upon substitution of (30) into (25), the criterion becomes

$$\langle X^{(1)}|J^2|X^{(1)}\rangle+2\langle X^{(2)}|J^2|\phi\rangle=4|\langle\phi|J_x|X^{(1)}\rangle|^2. \quad (31)$$

The merit of this expression is that it involves only the first- and second-order perturbative contributions, due to the perturbative J_x alone. J_x being a one-body operator, the problem lends itself more easily to detailed microscopic analysis in terms of the one- and two-body parts of the Hamiltonian.

The perturbation of the self-consistency equations, up to second order in ω, is treated in the Appendix. The complexity of the treatment bars one from making rigorous statements as to what characteristics in the Hamiltonian are essential for the fulfillment of the condition of external consistency, by the cranking approach.

In the next section, a numerical example is treated by the cranking approach, providing a case where the criterion is not met. It should be stressed again that this does not necessarily imply any general weakness of the approach. Rather, it demonstrates its inapplicability in the treated example.

IV. NUMERICAL EXAMPLE

As a numerical example of the application of the considerations of the last sections, we take up the s-d shell and, in particular, the nuclei Ne^{20} and Mg^{24}, which have been treated in great detail elsewhere.[7]

The Hamiltonian of the system, defined over the subspace of the $2s_{1/2}$, $1d_{5/2}$, and $1d_{3/2}$ orbits, is composed of a one-body part, with single-particle energies

$$e(d_{3/2})=0, \quad e(s_{1/2})=-4.2 \text{ MeV}, \quad e(d_{5/2})=-7.0 \text{ MeV}, \quad (32)$$

and of a two-body Yukawa potential, with a Rosenfeld-type spin-isospin mixture[8]

$$V_0\frac{\tau_1\cdot\tau_2}{3}(0.3+0.7\sigma_1\cdot\sigma_2)\frac{e^{-r_{12}/a}}{r_{12}/a}. \quad (33)$$

The range parameter a is taken as 1.37×10^{-13} cm; the basic states are eigenstates of a harmonic oscillator with length parameter $b=1.65\times10^{-13}$ cm; the over-all strength of the potential V_0 is 50 MeV; and V_{TS}, as can be verified, has the eigenvalues $V_{00}=9/5$, $V_{01}=-1$, $V_{10}=-3/5$, $V_{11}=1/3$.

In order to achieve a clear and systematic presentation of the relevant argumentation, we give a series of statements and observations.

(a) The low-lying experimental spectrum of both Ne^{20} and Mg^{24} displays clear rotational characteristics. This is evidenced both in the energy spectrum [see Fig. 1(a)] and in the $E2$ transition probabilities. This feature explains why an effort to treat these nuclei in the microscopic-rotational framework was made at all.

(b) In the case of Ne^{20}, the Hamiltonian (33) can be diagonalized exactly, although with a certain amount of toil. The results of this exact diagonalization do bear a

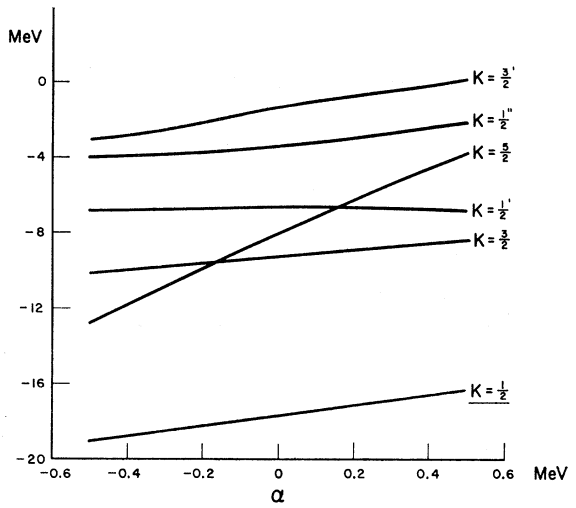

FIG. 2. The Hartree-Fock single-particle energy levels in the case of Ne^{20}, for the Hamiltonian[33] with a term αJ^2 added to it, as a function of α. The occupied level is underlined.

[7] For example, W. H. Bassichis, C. A. Levinson, and I. Kelson, Phys. Rev. **136**, B380 (1964).

[8] L. Rosenfeld, *Nuclear Forces* (North-Holland Publishing Company, Amsterdam, 1948), p. 233.

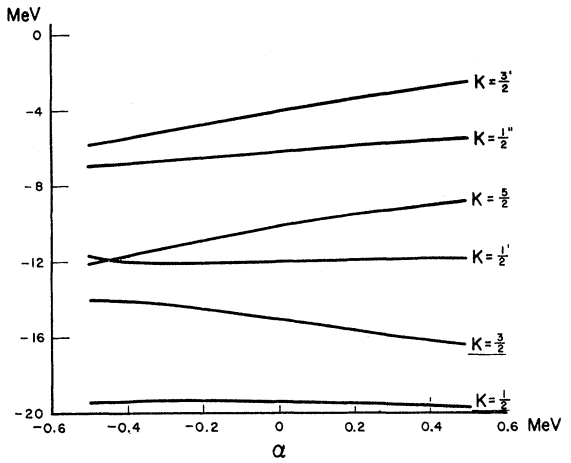

FIG. 3. The Hartree-Fock single-particle energy levels, in the case of Mg^{24}, for the Hamiltonian[33] with a term αJ^2 added to it, as a function of α. The occupied levels are underlined. The fact that the axial-symmetry approximation is poor is reflected in the small energy gap between occupied and unoccupied levels.

great similarity to the experimental spectrum, and in fact, by slight changes of the parameters in (33) this agreement can be made perfect. This is gratifying indeed, but has *no direct bearing* on our present problem. We are dealing with a purely mathematical proposition which has to do with the model Hamiltonian, whether or not it agrees with experiment. The essential point is that our basic assumption about the existence of a low-lying rotational spectrum of a particular Hamiltonian can, in this case at least, be actually checked and shown to be true [Fig. 1(b)].

(c) The Hartree-Fock (HF) Hamiltonian, possessing only axial symmetry, and derived from our model Hamiltonian, does indeed have the general characteristics we originally assumed it to have. (This is so for Ne^{20}; for Mg^{24} the axial-symmetry condition does *not* seem to be justified.[9]) Namely; (1) There is a large energy gap between the occupied and nonoccupied single-particle states, which implies relatively high energetic stability against particle promotion. Figure 2 (for Ne^{20}) and Fig. 3 (for Mg^{24}) give the HF Hamiltonian for $H+\alpha J^2$ as a function of α. (2) The single-particle wave functions are similar to those obtained by solving for a particle in a deformed-harmonic-oscillator local potential (Nilsson wave functions[10]). (See Table I.)

(d) The Hartree-Fock determinantal ground-state wave function does provide, upon projection, a good description of the various members of the rotational band. The energies of the projected angular-momentum components are shown in Fig. 1(c), where the similarity to the results of the exact diagonalization is readily apparent. The overlap between the exact and the projected wave functions is also very high.

[9] J. Bar-Touv and I. Kelson, Phys. Rev. **138**, B1035 (1965).
[10] S. G. Nilsson, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. **29**, No. 16 (1955).

(e) Having thus confirmed that all the necessary conditions for the application of the cranking approach indeed exist, we may proceed to calculate the moment-of-inertia parameter A as a function of α. The exact value, as well as the Inglis formula [Eq. (8)] and the Thouless-Valatin formula [Eq. (9)] values, are plotted and compared to the actual relevant parameter of the model Hamiltonian. They are shown in Fig. 4, which is based on Fig. 2.

One clearly sees that the Thouless-Valatin (as expected) is a better approximation to Eq. (21) than Inglis's formula is. Paradoxically, the less rigorous formula provides in this case, *for* $\alpha=0$, a better approximation to the actual value of A. Had one merely concerned oneself with the present situation, one would have had a real puzzle, in particular, when recalling the historical fact that Thouless and Valatin's formula was suggested to correct for inadequacies of Inglis's expression in other regions.

However, we see upon examination that both expressions, as well as the exact one which they approximate, totally fail to fulfill the criterion of Sec. III. They are very slowly varying functions of α, instead of going up linearly with it at a 45° slope.

Therefore, *in this case*, the success or failure of the cranking approach appears to be accidental. This, in fact, will always be the case, unless the external consistency criterion is specifically met.

It may be argued that the failure of the cranking approach in the case of Ne^{20} is due to the small number of particles in the variational treatment. In that case one might suspect the results, because of the fluctuations in the expectation value of J_x^2. However, a similar treatment of Si^{28} (which has three times as many nucleons outside the O^{16} core) reveals that the criterion is badly violated there, too. The calculated value of $\partial A/\partial\alpha$ is 0.08 instead of approximately 1. Also the inclusion of the 16 particles of the core does not seem to change the results much, essentially because the operators $J_\pm$ do

TABLE I. The components of different j, in decreasing order, for the Hartree-Fock single-particle levels resulting from the Hamiltonian (33), for Ne^{20} and Mg^{24}, compared with the corresponding Nilsson levels, for $\eta=2$.

	Ne^{20}	Mg^{24}	Nilsson ($\eta=2$)
$k=1/2$	0.819	0.848	0.879
	−0.380	−0.251	−0.198
	0.429	0.466	0.410
$k=3/2$	0.997	0.974	0.992
	−0.080	−0.226	−0.125
$k=5/2$	1.000	1.000	1.000
$k=1/2'$	0.552	0.467	0.413
	0.321	0.770	0.424
	−0.769	−0.435	−0.806
$k=1/2''$	0.155	−0.249	−0.061
	0.867	0.587	0.895
	0.473	0.770	0.440
$k=3/2'$	0.080	0.226	0.125
	0.997	0.974	0.992

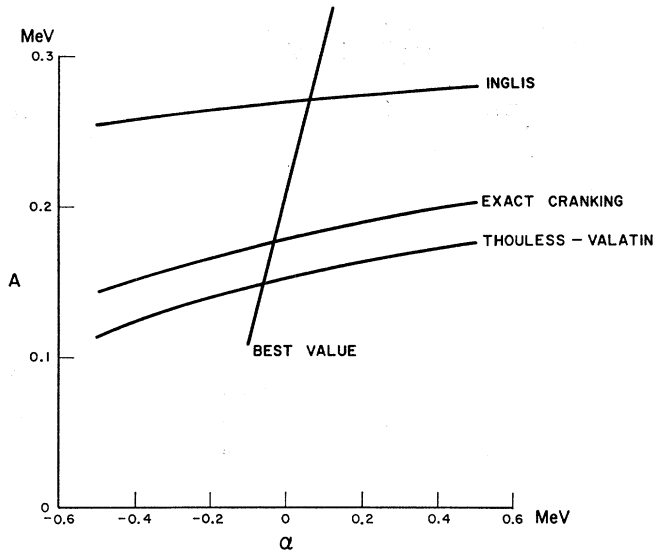

FIG. 4. The exact cranked moment-of-inertia parameter, as well as the Inglis and the Thouess and Vallatin formulas for Ne^{20}, for the Hamiltonian $H+\alpha J^2$, as a function of α. The best value indicates the actual value to be used, and the slope of its curve is the one imposed by the external consistency condition.

not change the principal quantum number of the nucleons.

V. ALTERNATIVE VARIATIONAL APPROACHES

A different approach, also of a variational nature, for determining the moment-of-inertia parameter, was suggested by Skyrme,[11] and also employed by Levinson.[12] This approach centers on two familiar assumptions: first, that the various members of the rotational band can be projected from a single intrinsic state; second, that this intrinsic state is precisely the Hartree-Fock determinantal ground state ϕ_A of the intrinsic Hamiltonian $H-AJ^2$. Clearly, if both assumptions were rigorously true, then, for the true moment-of-inertia parameter A, we would have

$$(H-AJ^2)\phi_A=0. \tag{34}$$

This ideal situation is, however, nonexistent. One hopes, though, that the actual state of affairs is close enough to it so that (34) may serve as a guiding principle. Designating by ϕ_β the Hartree-Fock determinantal solution of $H-\beta J^2$, where β is a variable parameter, one has in general

$$(H-\beta J^2)\phi_\beta=\chi_\beta. \tag{35}$$

The length $I^2=\langle\chi_\beta|\chi_\beta\rangle$, as a function of β, is then subjected to the requirement that it is as small as possible. The value β where this occurs is identified as the proper A of the Hamiltonian H. It was also shown[12] that the length I_A provides an estimate of the dispersion of the actual projected eigenvalues from a true rotational band.

It is easy to see that this prescription (doing first a self-consistency problem for fixed β, and then varying β) satisfies automatically the external-consistency condition, formulated in Sec. III. Clearly, if we replace H by $H+\alpha J^2$, the minimum of $\langle\chi_\beta|\chi_\beta\rangle$ will shift from A to $A+\alpha$. Moreover, the method has the great merit of not only providing a meaningful value for A, but also giving a quantitative estimate of how good a rotational spectrum the intrinsic state is generating. This estimate is contained both in the absolute magnitude of I_A, as well as in the sharpness with which this minimum is attained. Figure 5(a), which is reproduced from Ref. 12, illustrates the results of applying this method to Ne^{20}, using the same Hamiltonian as in the previous section. At the same time, Fig. 5(b), demonstrates the failure of this variational prescription for Mg^{24}. The curve of I^2 lies very high and does not display a clear-cut minimum. This, we presume, is closely related to the fact that the axially symmetric determinantal wave function, used in this treatment of Mg^{24}, is improper for this purpose. The intrinsic state is much more likely to be axially asymmetric, thus giving rise to other states of the rotational bands (corresponding to an additional $K=2$ band) upon projection. In the framework of axial symmetry, the axially asymmetric determinant can be expressed as a particle-hole expansion series about an axially symmetric determinant. It therefore seems, in this framework, that the failure of the Skyrme variational approach for Mg^{24} is due to the fact that the sought intrinsic state is of a rather complicated nature. In other words, we are justified in conceiving the existence of such an intrinsic state, but unjustified in attributing to it the very simple form of an axially symmetric determinant. Incidentally, to account for the large enhancement of electric quadrupole transitions within a band, one similarly requires only the existence of an intrinsic state, while its detailed character is of secondary importance. An extension of the set of wave functions over which the intrinsic states are varied may therefore be significant. Of course, the extended set in

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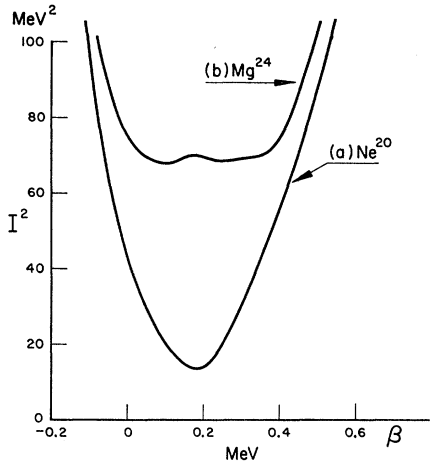

FIG. 5. The "remnant" curves as a function of β, for Ne^{20} and Mg^{24}, displaying the drastic difference of behavior in the two cases.

the case of Mg^{24} is still of a determinantal nature, but it is indicative of the possibilities in more general extension. In particular, one might expect this to be useful in treating nuclei which are not good rotators. This, incidentally, could provide a solution to the *s-d* shell dilemma discussed in the previous section.

Relaxing the condition that the intrinsic state be a single-particle determinant may thus open various possibilities for modification and improvement. Moreover, the interaction with the vibrational modes of motion may be better treated. Such possibilities, and related aspects, will be pursued and reported on elsewhere.

This relaxation may also be of importance to a modified application of a cranking-type approach. In its present form, the "cranked" moment of inertia seems to represent the response of the system, not so much to physical rotations, as to the artificial requirement of strictly independent-particle motion. Consequently, the wider the class of states available for the description of the intrinsic state, the better the cranking approach will describe the response to rotations.

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APPENDIX A

Let the Hamiltonian H be composed of a one-body and a two-body part

$$H=K+V. \tag{A1}$$

The perturbation $-\omega Jx$, which is a one-body operator, is added to (A1), and the self-consistency conditions are

$$h_1=K_1-\omega Jx_1+\mathrm{Tr}_2\rho_2 V_{12} \tag{A2}$$

and

$$[h,\rho]=0. \tag{A3}$$

The suffixes, where they appear, refer to the space on which the corresponding operator operates. We now expand, up to second order,

$$h=h^{(0)}+\omega h^{(1)}+\omega^2 h^{(2)}, \tag{A4}$$

$$\rho=\rho^{(0)}+\omega\rho^{(1)}+\omega^2\rho^{(2)}, \tag{A5}$$

and compare in (A2) and (A3) corresponding powers of ω. Thus the zeroth order yields the equations for the unperturbed consistency problem, presumably solved:

$$h_1^{(0)}=K_1+\mathrm{Tr}_2\rho_2^{(0)}V_{12}, \tag{A6}$$

$$[h^{(0)},\rho^{(0)}]=0. \tag{A7}$$

The first order yields

$$h_1^{(1)}=-Jx_1+\mathrm{Tr}_2\rho_2^{(1)}V_{12}, \tag{A8}$$

$$[h^{(0)},\rho^{(1)}]+[h^{(1)},\rho^{(0)}]=0, \tag{A9}$$

and the second order yields

$$h_1^{(2)}=\mathrm{Tr}_2\rho_2^{(2)}V_{12}, \tag{A10}$$

$$[h^{(0)},\rho^{(2)}]+[h^{(1)},\rho^{(1)}]+[h^{(2)},\rho^{(0)}]=0. \tag{A11}$$

First Order

To solve for the first-order perturbation equations, we substitute (A8) into (A9), getting

$$[h_1^{(0)},\rho_1^{(1)}]-[Jx_1,\rho_1^{(0)}]+[\mathrm{Tr}_2\rho_2^{(1)}V_{12},\rho_1^{(0)}]=0. \tag{A12}$$

Taking matrix elements of (A12) between states α,β of the unperturbed Hartree-Fock representation, and designating by u_α the occupation number of the state (1 if occupied, 0 if unoccupied), we get

$$(\epsilon_\alpha^0-\epsilon_\beta^0)\langle\alpha|\rho^{(1)}|\beta\rangle-(u_\beta-u_\alpha)\langle\alpha|Jx|\beta\rangle +(u_\beta-u_\alpha)\langle\alpha_1|\mathrm{Tr}_2\rho_2^{(1)}V_{12}|\beta_1\rangle=0, \tag{A13}$$

where ϵ_α^0, ϵ_β^0 are the unperturbed Hartree-Fock energies. But,

$$\langle\alpha_1|\mathrm{Tr}_2\rho_2^{(1)}V_{12}|\beta\rangle=\sum_\gamma\langle\alpha_1\gamma_2|\rho_2^{(1)}V_{12}\beta_1\gamma_2\rangle =\sum_\gamma\sum_\delta\langle\alpha\delta|V|\beta\gamma\rangle\langle\gamma|\rho^{(1)}|\delta\rangle. \tag{A14}$$

We get a set of linear equations for the matrix elements of $\rho^{(1)}$, of the form

$$\mathcal{A}_{\alpha\beta}{}^{\gamma\delta}\rho_{\gamma\delta}{}^{(1)}=\mathcal{C}_{\alpha\beta}, \tag{A15}$$

where

$$\mathcal{A}_{\alpha\beta}{}^{\gamma\delta}=(u_\beta-u_\alpha)\langle\alpha\delta|V|\beta\gamma\rangle+(\epsilon_\alpha^0-\epsilon_\beta^0)\delta_{\alpha\gamma}\delta_{\beta\delta} \tag{A16}$$

and

$$\mathcal{C}_{\alpha\beta}=(u_\beta-u_\alpha)\langle\alpha|Jx|\beta\rangle. \tag{A17}$$

Second Order

In a similar way, we substitute (A10) into (A11), obtaining

$$[h_1^{(0)},\rho_1^{(2)}]-[Jx_1,\rho_1^{(1)}]+[\mathrm{Tr}_2\rho_2^{(1)}V_{12},\rho_1^{(1)}] +[\mathrm{Tr}_2\rho_2^{(2)}V_{12},\rho_1^{(0)}]=0. \tag{A18}$$

Taking matrix elements for the various terms, one has

$$\langle\alpha|[h^{(0)}\,\rho^{(2)}]|\beta\rangle=(\epsilon_\alpha{}^0-\epsilon_\beta{}^0)\langle\alpha|\rho^{(2)}|\beta\rangle\,, \quad \text{(A19)}$$

$$\langle\alpha|[J_x,\rho^{(1)}]|\beta\rangle=\sum_\gamma\{\langle\alpha|J_x|\gamma\rangle\langle\gamma|\rho^{(1)}|\beta\rangle - \langle\alpha|\rho^{(1)}|\gamma\rangle\langle\gamma|J_x|\beta\rangle\}\,, \quad \text{(A20)}$$

$$\begin{aligned}\langle\alpha|[\mathrm{Tr}_2\rho_2{}^{(1)}V_{12},\rho_1{}^{(1)}]|\beta\rangle &=\sum_\gamma\{\langle\gamma|\rho^{(1)}|\beta\rangle\sum_\delta\langle\alpha_1\delta_2|\rho_2{}^{(1)}V_{12}|\gamma_1\delta_2\rangle \\ &\quad -\langle\alpha|\rho^{(1)}|\gamma\rangle\sum_\delta\langle\alpha_1\delta_2|\rho_2{}^{(1)}V_{12}|\beta_1\delta_2\rangle\} \\ &=\sum_{\gamma,\delta,\eta}\langle\delta|\rho^{(1)}|\eta\rangle\{\langle\gamma|\rho^{(1)}|\beta\rangle\langle\alpha\eta|V|\gamma\delta\rangle \\ &\quad -\langle\alpha|\rho^{(1)}|\gamma\rangle\langle\gamma\eta|V|\beta\delta\rangle\}\,, \quad \text{(A21)}\end{aligned}$$

$$\langle\alpha|[\mathrm{Tr}_2\rho_2{}^{(2)}V_{12},\rho_1{}^{(0)}]|\beta\rangle=(u_\beta-u_\alpha)\times\sum_{\gamma\delta}\langle\alpha\delta|V|\beta\gamma\rangle\langle\gamma|\rho^{(2)}|\delta\rangle\,. \quad \text{(A22)}$$

Thus, the matrix elements $\rho_{\gamma\delta}{}^{(2)}$ of $\rho^{(2)}$ are subject to the set of linear equations

$$\mathcal{B}_{\alpha\beta}{}^{\gamma\delta}\rho_{\gamma\delta}{}^{(2)}=\mathcal{D}_{\alpha\beta}\,, \quad \text{(A23)}$$

where

$$\mathcal{B}_{\alpha\beta}{}^{\gamma\delta}=\mathcal{A}_{\alpha\beta}{}^{\gamma\delta} \quad \text{(A24)}$$

and

$$\mathcal{D}_{\alpha\beta}=\sum_\gamma\{\langle\alpha|J_x|\gamma\rangle\langle\gamma|\rho^{(1)}|\beta\rangle-\langle\alpha|\rho^{(1)}|\gamma\rangle\langle\gamma|J_x|\beta\rangle\} -\sum_\gamma\sum_{\delta,\eta}\langle\delta|\rho^{(1)}|\eta\rangle\{\langle\gamma|\rho^{(1)}|\beta\rangle\langle\alpha\eta|V|\gamma\delta\rangle -\langle\alpha|\rho^{(1)}|\gamma\rangle\langle\gamma\eta|V|\beta\delta\rangle\}\,. \quad \text{(A25)}$$

The Thouless-Valatin formula is obtained when one restricts oneself to the lowest order in ω and neglects the off-diagonal elements of A:

$$\mathcal{A}_{\alpha\beta}{}^{\gamma\delta}\rightarrow\mathcal{A}_{\alpha\beta}{}^{\gamma\delta}\delta_{\alpha\gamma}\delta_{\beta\delta}\,.$$

The Inglis formula is obtained when one neglects not only the off-diagonal terms, but the two-body matrix elements in the diagonal terms as well.

In the case where the space of allowed single-particle orbits is truncated, the problem of finding $\rho^{(1)}$ and $\rho^{(2)}$ becomes finite. It can be solved with exactitude numerically. The only operation of any complexity is the inversion of the matrix $\mathcal{A}$ which appears both in the $\rho^{(1)}$ and $\rho^{(2)}$ equations.

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Scattering of Alpha Particles by Oxygen. I. Bombarding Energy Range 5.8 to 10.0 MeV*

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Absolute differential cross sections for the elastic scattering of α particles by O^{16} have been measured as a function of bombarding energy in the range 5.8–10.0 MeV. Measurements were made at center-of-mass angles of 90.0°, 109.9°, 114.0°, 125.3°, 131.4°, 140.8°, 149.4°, 154.0°, 158.8°, and 163.8°. Detailed angular distributions have been measured at 6.97, 8.63, and 9.92 MeV (lab). Sixteen resonances have been observed corresponding to energy levels in Ne^{20} at 9.50, 9.99, 10.30, 10.49, 10.55, ~10.7, 10.83, (10.93), 11.03, 11.29, ~11.6, (11.89), 11.99, 12.27, 12.39, and 12.58 MeV (c.m.). Spin and parity assignments have been made for six of these levels, tentative assignments are suggested for seven, and two or more possible assignments are given for two levels. Phase shifts have been extracted from the angular distribution data at 6.97, 8.63, and 9.92 MeV (lab). New rotational bands in Ne^{20} are suggested by the data and previously reported bands have been extended. Information about the levels in Ne^{20} is compared with that obtained in previous studies of other nuclear reactions. The correspondence with the results of an $O^{16}(\alpha,\gamma)Ne^{20}$ investigation is generally good. The set of Ne^{20} levels found in this work is somewhat different from the set determined by the $C^{12}(C^{12},\alpha)Ne^{20}$ reaction experiments, and this difference is discussed.

I. INTRODUCTION

THE elastic scattering of α particles by O^{16} has been studied from 0.94- to 4.0-MeV bombarding energy by Cameron[1] and from 3.7–6.5 MeV by McDermott *et al.*[2] In these experiments the data were analyzed to yield the spins, parities, and other level parameters of a number of states in the compound nucleus Ne^{20} between 5.48 and 9.93 MeV (c.m.). Prior to both of these experiments, Ferguson and Walker[3] had elastically scattered α's from O^{16} using α particles from RaC′, and observed resonances at bombarding energies of 5.5 and 6.5 MeV.

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