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Skyrme, Peierls-Yoccoz, and statistical approximations for the inertia parameter

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Angular momentum operator identities are used to show that Skyrme's expression can be written using the y component of angular momentum only. It is shown that the Gaussian approximation for the matrix element of $J_y{}^4$ leads to the Peierls-Yoccoz expression. A new approximation based on the theory of probability is introduced. The numerical calculations for the $2s$-$1d$ shell nuclei show that the inverse of the inertia parameter using the statistical approximation is much closer to Skyrme's value than the one given by the Peierls-Yoccoz approximation.

[NUCLEAR STRUCTURE Approximations for nuclear inertia parameter.]

It is well known that the low-lying spectra of many even-even nuclei belonging to $2s$-$1d$ shell and the rare-earth region exhibit rotational features.[1] In the theoretical study of such nuclei one constructs a deformed intrinsic wave function using one of the many variational techniques like Hartree-Fock, constrained Hartree-Fock, or energy minimization using Nilsson's deformed single particle wave functions. Once an intrinsic rotational wave function $|\Phi\rangle$ has been generated then it is used to extract the rotational parameters like the inertia parameter $\mathcal{J}$ and the bandhead E_0. A scheme which is used quite often for this purpose is the one given by Skyrme.[2] We recall that the energy E_J of a level having a good angular momentum J, using Skyrme's procedure is given by the following expression[2,3]

$$E_J = E_0 + AJ(J+1)\,, \tag{1}$$

where E_0 and the inverse inertia parameter A are given by

$$A = \frac{\langle HJ^2\rangle - \langle H\rangle\langle J^2\rangle}{\langle J^4\rangle - \langle J^2\rangle^2}\,, \tag{2a}$$

$$E_0 = \langle H\rangle - A\langle J^2\rangle\,. \tag{2b}$$

In the above the bracket sign, $\langle\Omega\rangle$ denotes the matrix element of the operator Ω with respect to the intrinsic wave function $|\Phi\rangle$. We see from expression (2a) that Skyrme's approximation involves the matrix elements of the square of total angular momentum operator. As shown by Peierls and Yoccoz[4] one can also derive an expression for the parameter A, using Hill-Wheeler integral,[5] which involves only the y component of angular momentum.

The purpose of the present work is to show that angular momentum operator identities can be used to express Skyrme's expression in terms of y component of angular momentum only. Further, if one uses the Gaussian approximation[1] for the matrix element of $J_y{}^4$, then Skyrme's expression becomes the same as that given by Peierls and Yoccoz. We also suggest a statistical approximation to calculate the matrix of $J_y{}^4$. As will be shown later, it provides a much better approximation than the Peierls-Yoccoz approximation. Let us consider the ground state band in even-even nuclei for which the projection quantum number $K=0$ and $J=0, 2, 4, \ldots$. Expression (2a) can then be written as

$$A = \frac{\langle (H - \langle H\rangle)J_y{}^2\rangle}{\langle J_y{}^4\rangle + \langle J_x{}^2 J_y{}^2\rangle - 2\langle J_y{}^2\rangle^2}\,. \tag{3}$$

Using the following operator identity,[6]

$$\exp(-i\mu J_x)\exp(-i\nu J_y) = \exp(-i\alpha J_z)\exp(-i\beta J_y)\exp(-i\gamma J_z)\,, \tag{4a}$$

where

$$\cos^2\tfrac{1}{2}\beta = \cos^2\tfrac{1}{2}\mu\cos^2\tfrac{1}{2}\nu + \sin^2\tfrac{1}{2}\mu\sin^2\tfrac{1}{2}\nu\,, \tag{4b}$$

$$\exp[i(\alpha+\gamma)] = (\cos\tfrac{1}{2}\mu\cos\tfrac{1}{2}\nu + i\sin\tfrac{1}{2}\mu\sin\tfrac{1}{2}\nu) \times (\cos\tfrac{1}{2}\mu\cos\tfrac{1}{2}\nu - i\sin\tfrac{1}{2}\mu\sin\nu)^{-1}\,, \tag{4c}$$

$$\exp[-i(\alpha-\gamma)] = (\cos\tfrac{1}{2}\mu\sin\tfrac{1}{2}\nu + i\sin\tfrac{1}{2}\mu\cos\tfrac{1}{2}\nu) \times (\cos\tfrac{1}{2}\mu\sin\tfrac{1}{2}\nu - i\sin\tfrac{1}{2}\mu\cos\tfrac{1}{2}\nu)^{-1}\,, \tag{4d}$$

it can be easily shown that for the intrinsic wave function $|\Phi\rangle$ which has $K=0$, the following relation holds

$$\langle J_x{}^2 J_y{}^2\rangle = \tfrac{1}{3}\langle J_y{}^4\rangle + \tfrac{2}{3}\langle J_y{}^2\rangle\,. \tag{5}$$

Thus Skyrme's expression for A can be written only in terms of y component of angular momentum as

$$A = \frac{3}{2}\,\frac{\langle (H - \langle H\rangle)J_y{}^2\rangle}{2\langle J_y{}^4\rangle + \langle J_y{}^2\rangle - 3\langle J_y{}^2\rangle^2}\,. \tag{6}$$

If we now put the Gaussian approximation[1]

$$\langle J_y^4\rangle = 3\langle J_y^2\rangle^2 , \tag{7}$$

in expression (6) we get

$$A_G = \frac{3}{2}\,\frac{\langle (H-\langle H\rangle)J_y^2\rangle}{3\langle J_y^2\rangle^2 + \langle J_y^2\rangle} . \tag{8}$$

Since for the validity of Gaussian approximation $\langle J_y^2\rangle$ must be large, expression (8) reduces to the Peierls-Yoccoz expression,

$$A_{\mathrm{P-Y}} = \frac{1}{2}\,\frac{\langle (H-\langle H\rangle)J_y^2\rangle}{\langle J_y^2\rangle^2} . \tag{9}$$

Comparing expressions (2) and (9) we find that in Peierls-Yoccoz (P-Y) approximation one has to calculate the matrix of J_y^2 rather than J_y^4. The operator J_y^4 is more involved than J_y^2 since it needs the evaluation of three and four body operators. However, it turns out that the accuracy of P-Y expression is not very high and it is because of this reason that one either uses[1,3] Skyrme's expression[2] or an alternative expression given by Inglis[7] and also by Thouless and Valatin,[8] which is called the cranking model expression. As is well known, the cranking expression needs the complete knowledge of the unoccupied single-particle orbits also and thus is not very convenient to use where only $|\Phi\rangle$ is given.

The question then arises whether we can derive an expression which involves only J_y^2 but has better accuracy than P-Y expression.

Perhaps one could first try to construct a pseudo Hamiltonian of the form $a+bJ_y^2$ and determine a, b by minimizing $\langle\Phi|(H-a-bJ_y^2)^2|\Phi\rangle$ as is done in obtaining Skyrme's expression.[2] If we carry out this minimization and then use the Gaussian approximation[1] for J_y^4, then we find that even though we have obtained an expression for A which involves only J_y^2, the value of this A turns out to be exactly half of that given by P-Y expression and is thus much poorer rather than better compared with $A_{\mathrm{P-Y}}$.

We now give a different approach based on statistical theory to achieve our goal. It can easily be shown that $\langle J_y^4\rangle$ can be exactly written as

$$\langle J_y^4\rangle = -\tfrac{1}{2}\langle J_y^2\rangle + \tfrac{3}{2}\alpha\langle J_y^2\rangle^2 , \tag{10}$$

where

$$\alpha = \frac{\langle J^4\rangle}{\langle J^2\rangle^2} . \tag{11}$$

Explicitly α can be written as

$$\alpha = \frac{\sum a_J^2[J(J+1)]^2}{[\sum a_J^2 J(J+1)]^2} , \tag{12}$$

where a_J are the expansion coefficients

$$|\Phi\rangle = \sum a_J \psi_J . \tag{13}$$

Writing $a_J^2 = \overline{a^2} + \delta a_J^2$, where $\overline{a^2}$ is the average value of a_J^2 and δa_J^2 is the fluctuation, the normalization condition $\sum a_J^2 = 1$, gives $\overline{a^2} = N^{-1}$ where N is the number of J states. Ignoring the fluctuation and keeping the leading term in expression (12) gives $\overline{\alpha} = \frac{9}{5}$. Using expression (6) and (10) we get the following expression for A using statistical approximation

$$A_{\mathrm{st}} = \frac{5}{8}\,\frac{\langle (H-\langle H\rangle)J_y^2\rangle}{\langle J_y^2\rangle^2} . \tag{14}$$

We would now like to see how the expressions $A_{\mathrm{P-Y}}$ and A_{st} compare with the expression given by Skyrme. For this purpose we use the deformed Hartree-Fock wave functions for the nuclei ^{12}C, ^{20}Ne, ^{28}Si, and ^{36}Ar which are tabulated by Ripka.[1] The values of the various parameters A for these nuclei are shown in Table I. In Table I we have also shown the values of the parameter A which are obtained using the first two values of E_J which are obtained by exact projection.[1] We find from Table I that the values of the parameter A using statistical approximation are better than the ones obtained using P-Y approximation. To check the validity of statistical approximation further we have also calculated the values of A not shown in

TABLE I. Values of the inverse inertia parameter given by exact projection of the first two levels, Skyrme, Peierls-Yoccoz, and statistical approximations for $2s$-$1d$ shell nuclei.

	Inverse of the inertia parameter A			
Nucleus	First two levels	Skyrme	Peierls-Yoccoz	Statistical
^{12}C	0.54	0.55	0.46	0.58
^{20}Ne	0.20	0.17	0.14	0.18
^{28}Si	0.12	0.10	0.08	0.10
^{36}Ar	0.19	0.16	0.15	0.19

Table I using the Hartree-Fock wave functions of Stamp and Spencer.[9] These calculations are carried out using a different two body interaction and the projected spectra is obtained for the two nuclei ^{20}Ne and ^{28}Si. We find that again the values of A calculated using statistical approximation are much closer to Skyrme's values than the ones given by P-Y approximation.

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