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New projection method and generalized rotational spectrum

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Lanczos's algorithm for the matrix eigenproblem is used to project out angular momentum (J) components from a given deformed intrinsic wave function, containing N different values of J. Using this method, it is proved that the low-lying energy spectrum of a nucleus obtained by using the wave functions projected from a deformed intrinsic state (Hartree-Fock, Hartree-Fock-Bogoliubov, or random-phase approximation) has a general form suggested by Bohr and Mottelson in their macroscopic approach,

$$E(J) = E(\beta) + \sum_{1}^{N-1} A_n(\beta) J^n (J+1)^n .$$

Expressions for $E(\beta)$ and $A_n(\beta)$ are derived. The first iteration gives Skyrme's formula for the nuclear moment of inertia. The above analytic form of $E(J)$ is exploited to deduce certain conclusions about the nature of the projected energy as a function of J.

As early as 1958 it was realized that the results of shell-model calculations can be reproduced using the projection method.[1] The projection method[2] has been preferred over the shell-model approach to study the low-lying energy levels of many-nucleon systems because of the prohibitively large dimension of the eigenvalue problem in the latter approach. A new computational method, based on Lanczos's algorithm for the matrix eigenvalue problem has recently been proposed for the shell-model calculations.[3] This method is very efficient to calculate few low-lying eigenvalues with a minimum of additional useless information. However, the serious disadvantage of the method is that it just provides numbers and no physical insight. The problem of understanding nuclear structure depends on finding good approximations for the eigenvalues and the corresponding eigenfunctions of a many-nucleon Hamiltonian H. Our discussion here is limited to open shell nuclei. We can assume that the effective interaction between nucleons in a nucleus is already known from the Brueckner-Bethe-Goldstone theory. Since our interest here is to study only the low-lying states of H, one can use the powerful variational methods which have either the Hartree-Fock (HF), Hartree-Fock-Boguliubov (HFB), or ground state of random-phase-approximation (RPA) form of the wave function. The rotational symmetry of H makes it very difficult to carry out such a variational calculation. Therefore, one often finds a variational solution of a lower symmetry first (such as axial symmetry). The approximate variational solution of H is then obtained by projecting the appropriate angular momentum J from it. This is used to calculate the approximate eigenvalues $E(J)$ of H.[4]

Irrespective of the wide popularity of this approach, no effort has been made to investigate analytically the general features of the projected spectrum. With certain assumptions, based on the observation of numerical results, we[5] tried to find the approximate form of $E(J)$ as a function of J. These assumptions have been criticised by MacDonald.[6] In this paper, our aim is to investigate how closely the projected spectrum resembles a rotational spectrum. The failure of the earlier attempts to answer this question was partly due to the use of the well-known projection operators. The recent new forms of the projection operators[7] are also not suitable for our purpose. Therefore, we propose another new method to project out N different angular momentum components from a deformed intrinsic wave function. This method is based on the Lanczos algorithm[8] for the matrix eigenvalue problem.

Let φ_0 be the deformed intrinsic wave function obtained from either the HF, HFB, or RPA approach. In order to use Lanczos's algorithm for the matrix eigenvalue problem, let us define the orthonormal set of wave functions φ_i ($i = 0, 1, \ldots, N$) by the follwoing set of equations

$$\begin{aligned}
\underline{J}^2\varphi_0 &= J_{00}\varphi_0 + J_{10}\varphi_1 ,\\
\underline{J}^2\varphi_i &= J_{i-1\,i}\varphi_{i-1} + J_{ii}\varphi_i + J_{i+1\,i}\varphi_{i+1} ,\\
\underline{J}^2\varphi_{N-1} &= J_{N-2\,N-1}\varphi_{N-2} + J_{N-1\,N-1}\varphi_{N-1} .
\end{aligned} \tag{1}$$

Let us assume that the intrinsic state φ_0 has N components of different values of J. This would imply that there are only N independent sets of functions φ_i and that $\underline{J}^2\varphi_N = 0$. In Eq. (1),

$$J_{ij} = J_{ji} = \langle \varphi_i | \underline{J}^2 | \varphi_j \rangle .$$

The matrix J_{ij} in Eq. (1) can easily be diagonalized in this basis set of functions. Using the known eigenvalues $\lambda_J = J(J+1)$, the eigenfunctions of $\underline{J}^2$ can easily be found from Eq. (1):

$$\varphi(J) = \sum_{n=0}^{N-1} x_n \varphi_n ,$$

where $x_0 = 1$ and

$$x_n = (-1)^n D_n[\lambda_J]/[J_{10}J_{21}\cdots J_{n\,n-1}] \quad \text{for } n \geq 1 . \tag{2}$$

The polynomial $D_n[\lambda_J]$ in λ_J is the leading principal minor of order n of the determinant

$$D_N[\lambda_J] = |J_{ij} - \lambda_J \delta_{ij}| . \tag{3}$$

The operator which projects out a component of given J from φ_0 is

$$P(J) = 1 + \sum_{1}^{N-1} D_n[\lambda_J]\mathfrak{D}_n[\underline{J}^+\underline{J}^-]/[J_{10}J_{21}\cdots J_{nn-1}]^2 . \tag{4}$$

The normalization of the projected wave function $\varphi(J)$ is such that $\langle\varphi_0|\varphi(J)\rangle = \langle\varphi_0|P(J)|\varphi_0\rangle = 1$. The operators $\mathfrak{D}_n$'s are defined in terms of $\mathfrak{D}_n[\lambda_J]$ with the replacement of λ_J by $\underline{J}^+\underline{J}^-$. In what follows below, let us assume that φ_0 has an axial symmetry with the quantum number $K = 0$. Since $\underline{J}^2$ does not break this symmetry, all the φ_i's are eigenfunctions of $\underline{J}_z$ with eigenvalue zero. This implies that

$$\underline{J}^2\varphi_i = \underline{J}^+\underline{J}^-\varphi_i = \underline{J}^-\underline{J}^+\varphi_i . \tag{5}$$

From Eqs. (1) and (4) it can be seen that

$$\begin{aligned} &J_{ii} = \langle\varphi_i|\underline{J}^+\underline{J}^-|\varphi_i\rangle , \\ &J_{01} = J_{10} = \langle\varphi_0(\underline{J}^+\underline{J}^- - J_{00})^2|\varphi_0\rangle^{1/2} , \\ &J_{i\,i+1} = J_{i+1\,i} = [\langle\varphi_i|(\underline{J}^+\underline{J}^- - J_{ii})^2|\varphi_i\rangle - J_{i\,i-1}]^{1/2} \\ &\qquad \text{for } 1 \leq i \leq N-1 . \end{aligned} \tag{6}$$

These relations are useful in the evaluation of J_{ij}. The approximate eigenvalue $E(J)$ of H obtained from $\varphi(J)$ is

$$E(J) = \frac{\langle\varphi(J)|H|\varphi(J)\rangle}{\langle\varphi(J)|\varphi(J)\rangle} = \frac{\langle\varphi_0|H|\varphi(J)\rangle}{\langle\varphi_0|\varphi(J)\rangle} . \tag{7}$$

Equation (7) follows from the fact that H commutes with $\underline{J}^2$. Using Eqs. (2) and (4), the expression for $E(J)$ takes the following form

$$E(J) = \langle\varphi_0|H|\varphi_0\rangle + \sum_{1}^{N-1} \frac{D_n[\lambda_J]\langle\varphi_0|H\mathfrak{D}_n[\underline{J}^+\underline{J}^-]|\varphi_0\rangle}{[J_{10}J_{21}\cdots J_{nn-1}]^2} . \tag{8}$$

At this stage, it may be worth pointing out that keeping only the first iteration in Eq. (8),

$$E(J) = \langle\varphi_0|H|\varphi_0\rangle + \frac{[J(J+1) - J_{00}]\langle\varphi_0|H(\underline{J}^+\underline{J}^- - J_{00})|\varphi_0\rangle}{\langle\varphi_0|(\underline{J}^+\underline{J}^- - J_{00})^2|\varphi_0\rangle} . \tag{9}$$

The moment of inertia $\mathcal{I}$, defined by the coefficient of $J(J+1)$ in Eq. (9) to be equal to $\hbar^2/2\mathcal{I}$ is identical with Skyrme's formula.[9] The approximate projected energy $E(J)$ in Eq. (9) is the same as that obtained by Das Gupta and Van Ginneken[10] using the conventional projection operator.

The J dependence of $E(J)$ in Eq. (8) arises only from the determinants $D_n[\lambda_J]$. Expanding these determinants one obtains

$$E(J) = E(\beta) + \sum_{1}^{N-1} A_n(\beta) J^n (J+1)^n . \tag{10}$$

In Eq. (10)

$$E(\beta) = \langle\varphi_0|H|\varphi_0\rangle + \sum_{1}^{N-1} \frac{D_n(\beta)\langle\varphi_0|H\mathfrak{D}_n[\underline{J}^+\underline{J}^-]|\varphi_0\rangle}{[J_{10}J_{21}\cdots J_{nn-1}]^2} \tag{11}$$

and

$$A_n(\beta) = \frac{1}{n!}\sum_{p=n}^{N-1}\left[\frac{\partial^n}{\partial x^n} D_p[x]\right]_{x=0} \frac{\langle\varphi_0|H\mathfrak{D}_p[\underline{J}^+\underline{J}^-]|\varphi_0\rangle}{[J_{10}J_{21}\cdots J_{nn-1}]^2} , \tag{12}$$

where

$$D_n(\beta) = D_n[\lambda_J = 0] = J\begin{pmatrix} & J_{01} & J_{12} & \cdots & J_{n-1\,n} \\ J_{00} & J_{11} & J_{22} & \cdots & J_{nn} \\ & J_{01} & J_{12} & \cdots & J_{n-1\,n} \end{pmatrix} = J(0,n) . \tag{13}$$

The central line in the bracket indicates the diagonal element of a $n\times n$ tridiagonal determinant $D_n(\beta)$, and the upper and the lower diagonal elements are given by the upper and the lower lines, respectively. For later use, we supplement the definition of $J(0,n)$ in Eq. (13) with

$$J(t,p) = 1 \quad \text{for } t > p \quad \text{and} \quad D_0[\lambda] = 1 .$$

The Bohr-Mottelson Hamiltonian[11] for the description of a nuclear collective motion which would give the same energy as $E(J)$ in Eq. (10) is

$$H_{BM} = E(\beta) + \sum_{1}^{N-1} A_n(\beta)\underline{J}^{2n} . \tag{14}$$

Following Baranger and Kumar,[12] one has to carry out the constrained HF or HFB calculations in order to obtain $E(\beta)$ and $A_n(\beta)$ as a function of deformation parameter β. As one is treating β quasi-static, one has to add to H_{BM} in Eq. (14) the kinetic

energy arising from the rate of change of β. In order to perform variation after projection, the minimization of $E(J)$ with respect to β can be carried out from Eq. (10), using the known functions of $E(\beta)$ and $A_n(\beta)$.

For a tridiagonal matrix $D_p[x]$,

$$\frac{\partial^n}{\partial x^n} D_p[x] = (-1)^n n! \sum d_{p-n,ii}(x) . \tag{15}$$

In the above equation $d_{p-n,ii}$ represents a principal minor of order $p-n$ in $D_p[x]$. The sum runs over all such minors of order $p-n$. The minor $d_{0,ii}$ is defined to be unity. It can be proved[8] that the principal minor of $J(0,p)$ obtained by dropping $(i_1 i_1)$, $(i_2 i_2)\cdots$ to $(i_n i_n)$ rows and columns is the following product:

$$d^{(0)}_{p-n,ii} = J(0,i_1-1)J(i_1+1,i_2-1)\cdots J(i_n+1,p) . \tag{16}$$

In obtaining Eq. (16), it is assumed that $0 \leq i_1 < i_2 < i_3 \cdots < i_n \leq p$. The ordering of i_r's does not change the value of $d_{p-n,ii}$. The sum in Eq. (15) is to be taken over all the sequences $(i_1, i_2, i_3, \ldots, i_n)$ satisfying this ordering. From Eqs. (12), (15), and (16) it follows that

$$A_n(\beta) = (-1)^n \sum_{p=n}^{N-1} \frac{\langle \varphi_0 | H \mathfrak{D}_p[\underline{J}^+ \underline{J}^-] | \varphi_0 \rangle}{[J_{10} J_{21} \cdots J_{p\,p-1}]^2} \left[\sum_{0 \leq i_1 < i_2 \cdots < i_n \leq p} J(0,i_1-1)J(i_1+1,i_2-1)\cdots J(i_n+1,p) \right] . \tag{17}$$

The zeros of the determinant $D_N[\lambda]$ are the values of λ_J corresponding to $J = 0, 2, 4, \ldots$. Since $\lambda_J \geq 0$, it follows from the variational principle that

$$J(i,j) \geq 0 . \tag{18}$$

From the Sturm sequence property,[8] $S(\lambda_J)$, the number of agreements in sign of consecutive members of the sequence

$$S = \{ D_0[\lambda_J], D_1[\lambda_J], \cdots, D_n[\lambda_J] \} \tag{19}$$

is the number of zeros of $D_N[\lambda]$ which are strictly greater than λ_J. Since $\lambda_J = 0$ is the minimum zero of $D_N[\lambda]$ (all other zeros are >0, and $D_0 = 1$, it follows from the Sturm sequence property that

$$D_n[\lambda = 0] = D_n(\beta) > 0 \quad \text{for all } n \leq N-1 . \tag{20}$$

There are only $N-2$ zeros of $D_N[\lambda]$ which are greater than λ_2 (the zero of $D_N[\lambda]$ corresponding to $J = 2$). Therefore, only $N-2$ consecutive pairs of the sequence in Eq. (19) have the same sign. This could happen only if all the $D_N[\lambda_2]$ for $n > N_1 (< N)$ change sign from positive to negative. It is also to be noticed that $D_n[\lambda_2]$ for $n < N_1$ have now the smaller positive values than $D_n[0]$,

$$0 < D_n[\lambda_2] < D_n[0] = D_n(\beta) \quad \text{for } n < N_1 . \tag{21}$$

From the separation property[8] of the roots of $D_n[\lambda]$, one expects N_1 to be nearer to $N-1$. Continuing this argument, one can say that
(a) there are more and more consecutive pairs of opposite sign in the sequence in Eq. (19) as J is increased and that the changes in sign are expected to start from the end of the sequence.

The lower members of the sequence which have not changed their original sign even once are becoming smaller in magnitude with increasing J.

Bohr and Mottelson[11] were the first to find that the low-lying energy levels of a well deformed nucleus, in the macroscopic model, has a form similar to that in Eq. (10). They also predicted that for such nuclei A_n's alternate in sign with n. The analysis of Sood[13] later showed that very good agreement between the experimental spectra of many well deformed nuclei and the generalized Bohr-Mottelson formula can be obtained only with alternating signs of A_n.

From Eqs. (8), (11), (17)–(21) and comment (a), it is easy to prove that for the wave function φ_0 and the Hamiltonian H for which $\langle \varphi_0 | H \mathfrak{D}_n[\underline{J}^+ \underline{J}^-] | \varphi_0 \rangle < 0$ for all n, the projected energy $E(J=0) < \langle \varphi_0 | H | \varphi_0 \rangle$, $E(J \neq 0) > E(J=0)$ and the coefficients $A_n(\beta)$ alternate in sign.

In the projection method, it will be almost impossible to extract the nature of $E(J)$ without assuming any structure of the Hamiltonian H and the intrinsic wave function φ_0. In the case of even-even nuclei, we assume the following general properties of H and φ_0,
(b) all the $E(J)$'s are negative, and are of the same order of magnitude.
(c) $a_J{}^2$, the probability of $\varphi(J)$ contained in φ_0, is much smaller for $J > 2$ than that for $J \leq 2$.

It follows from Eq. (18) that the square bracket in Eq. (17) is a positive quantity. The denominator in the same equation is clearly a positive definite quantity. Expanding φ_0 in the orthonormal set of functions $\varphi(J)$, we obtain

$$\langle \varphi_0 | H \mathfrak{D}_p[\underline{J}^+ \underline{J}^-] | \varphi_0 \rangle = \sum_{J=0\,(\text{even})}^{N-1} a_J{}^2 D_p[\lambda_J] E(J)$$

$$\approx a_0{}^2 D_p[0] E(0) + a_2{}^2 D_p[\lambda_2] E(2) . \tag{22}$$

The last step in Eq. (22) follows from (c). From Eq. (21), $D_p[0]$ is positive for all $p \leq N-1$ and from comment (a) $D_p[\lambda_2]$ is expected to be positive and less than $D_p[0]$ at least for $p < N_1 \approx N-1$. From this discussion and assumption (b), we conclude from Eq. (22) that

$$\langle \varphi_0 | H \mathfrak{D}_p[\underline{J}^+ \underline{J}^-] | \varphi_0 \rangle \leq 0 \quad \text{at least for } p < N_1 \approx N-1 . \tag{23}$$

Thus from Eqs. (17) and (23) A_n's will alternate in sign at least for a few lowest values of n for which the main contribution to A_n comes from $p < N_1$. The rest of the contribution is expected to be small both due to cancellation of the sum over $p > N_1$ as $\langle \varphi_0 | H \mathfrak{D}_p[\underline{J}^+ \underline{J}^-] | \varphi_0 \rangle$ then alternates in sign, and due to their relatively smaller values. From Eqs. (11), (20), and (23), it follows that $E(0) = E(\beta) < \langle \varphi_0 | H | \varphi_0 \rangle$. Similarly, from Eqs. (8), (11), (21), and (23) and comment (a) one obtains $E(0) < E(2)$. From comment (a) one may also expect that for larger values of J, $E(J) > E(2)$. These results are found to be true in all the calculations carried out so far using the projection method.

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