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# Exact expression for the projected energy

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**Abstract.** The angle integrated exact expression for the projected energy is derived from two different expansions of the rotation operator. In one, the spin matrix polynomial expansion method is used while in the other the disentangling theorem for angular momentum operator is used.

**Keywords.** Nuclear spectrum; variational method; angular momentum projection.

## 1. Introduction

The eigenvalue problem of a nuclear Hamiltonian with realistic interactions is a difficult one. In such a manybody problem one often aims at finding a good approximation to the exact solution. The straightforward method would be the diagonalization of the Hamiltonian ($H$) matrix in a given manybody basis states. The calculation of the $H$-matrix for anti-symmetric basis states of given angular momentum is not easy. Moreover, a prohibitively large basis set is required to study the low lying spectrum of $H$. This is because such a calculation amounts to the introduction of linear variational parameters in the trial wavefunction. It is well known that such variational wavefunction is not as effective as the one in which the dependence of the variational parameters is nonlinear. The projected Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) trial wavefunction can have such variational parameters describing the nuclear shape. This powerful method is used in almost all the microscopic calculations of nuclear energy levels and their properties. Besides the numerical calculations there has been no attempt to find the exact angular momentum ($J$) dependence of the energy expression obtained from this method. Based on the observation of numerical results, Warke and Gunye (1967), and Warke and Khadkikar (1968) had derived the approximate form of the projected energy $E(J)$ as a function of $J$. This work was criticized by McDonald (1970). In a recent paper by Warke (1974) the exact expression of $E(J)$ was derived. There we developed a method of angular momentum projection operator based on the Lanczos algorithm, In the present paper we derive the functional form of $E(J)$ starting from the usual well-known projection operator used in numerical calculations.

## 2. Derivation

In this paper we follow the spin matrix polynomial expansion method of an arbitrary function of the spin matrix $J_y$. Such an expansion was developed by Williams *et al* (1966) for fixed value $J$ of the spin. However, this expansion is valid even if the spin takes a set of values say $(0, 2, \ldots J_m)$. From the eigen-values of $J_y$, a complete set of polynomials $W_{2S+1}(J_y)$ and $J_y W_{2S+1}(J_y)$ are constructed as follows

$$W_{2S+1}(x) = (x - S) \ldots (x-1)\, x\, (x+1) \ldots (x+S);\; W_{-1}(x) = \frac{1}{x}.$$

The coefficients of expansion of a function can be calculated by evaluating the function at the successive zeros of the polynomials $W_{2S+1}(x)$. From this we obtain the expansion

$$\cos \beta J_y = \sum_0^{\infty} \frac{(-1)^n\, 2^n}{(2n)!} (1 - \cos \beta)^n\, J_y W_{2n-1}^{(J_y)}. \tag{1}$$

In a manybody variational calculation one uses a trial wave function $\phi(\beta, \triangle_P, \triangle_n, a_i)$, where the deformation parameter $\beta$, the neutron and proton pairing gaps $\triangle_n$ and $\triangle_P$ and $a_i$ are the variational parameters. Such a wavefunction in general is not an eigenfunction of the total angular momentum of all the nucleons. The required trial wave function $\Psi^J$ can easily be constructed from $\phi$ by using the projection operator

$$\Psi^J = \frac{(2J+1)}{8\pi^2} \int_0^{2\pi} d\alpha \int_0^{2\pi} d\gamma \int_0^{\pi} d\theta\, e^{-i\alpha J_z}\, e^{-i\theta J_y}\, e^{-i\gamma J_z}\, \phi_K \overset{*}{D}{}^J_{MK}(\alpha, \theta, \gamma,)$$

$$\equiv P^J_{MK}\phi_K. \tag{2}$$

With the axial symmetry restrictions on the nuclear shape variations, the angular momentum component on the nuclear symmetry axis is a constant of motion. We restrict our discussion to the case of even-even nuclei in which case the corresponding quantum number $K = 0$. The nuclear energy expression to be minimized is then given by

$$E_J(\beta, \triangle_P, \triangle_n, a_i) = \langle \Psi^J \mid H \mid \Psi^J \rangle / \langle \Psi^J \mid \Psi^J \rangle$$
$$= h_J / p_J. \tag{3}$$

where

$$\begin{pmatrix} h_J \\ p_J \end{pmatrix} = \int_0^{\pi} d^J_{00}(\theta) \langle \phi \mid \begin{pmatrix} H \\ I \end{pmatrix} e^{-i\theta J_y} \mid \phi \rangle \sin\theta\, d\theta. \tag{4}$$

and $I$ is an identity operator. In deriving the above expression for $E_J$ the axial symmetry of $\phi$ and the rotational and time invariance of $H$ are used. For even-even nuclei with axial symmetry it was proved by Warke and Gunye (1967) that $\phi$ has components corresponding to the even values of $J = 0, 2, \ldots J_m$. This allows one to replace $e^{-i\theta J_y}$ by $\cos \theta J_y$ in the integrant of eq. (4). As seen from the expansion of $\cos \beta J_y$ in eq. (1), the general integral to be evaluated is

$$\int_0^{\pi} d^J_{00}(\theta)\, (1 - \cos\theta)^n \sin\theta\, d\theta$$

$$= 2^{n+1} \int_0^1 y^n\, P_J(1 - 2y)\, dy \tag{5}$$

$$= \frac{2^{n+1}}{(n+1)}\, {}_3F_2\,(-J, J+1, n+1;\ 1, n+2;\ 1). \tag{6}$$

The function ${}_3F_2$ is the generalized hypergeometric series. It is to be noted that ${}_3F_2$ of the above arguments is a Saalschutsian series. Therefore, from Saalschutz's theorem (Bateman 1953)

$${}_3F_2\,(-J, J+1, n+1;\ 1, n+2\ ;\ 1) = \frac{(n-J+1, J)\,(1, J)}{(n+2, J)\,(-J, J)} \tag{7}$$

The appel symbol $(a, n)$ is defined as follows,

$$(a, 0) = 1 \text{ and } (a, n) = a\,(a+1)\ \ldots\ (a+n-1). \tag{8}$$

Using this result, it is easy to prove that

$$\int_0^{\pi} P_J\,(\cos\theta)\,(1-\cos\theta)^n \sin\theta d\theta = \frac{2^{n+1}}{(n+1)}\,\frac{(n-J+1, J)}{(n+2, J)}\,. \tag{9}$$

We also used the result that $J$ is an even integer. As expected this integral vanishes for $n < J$. Substituting this result in the expression for $h_J$ and $p_J$, we obtain the exact angle integrated expression for $E_J$

$$E_J = \Big[\sum_J^{Jm} \frac{(-1)^n\ 2^{2n}}{(2n)\,!}\ \frac{(n+1-J, J)}{(n+1)\,(n+2, J)}\,\langle \phi \mid HJ_y W_{2n-1}\,(J_y) \mid \phi \rangle\Big]\Big/$$

$$\Big[\sum_J^{Jm} \frac{(-1)^n\ 2^{2n}}{(2n)\,!}\ \frac{(n+1-J, J)}{(n+1)\,(n+2, J)}\,\langle \phi \mid J_y\, W_{2n-1}\,(J_y) \mid \phi \rangle\Big]. \tag{10}$$

The upper limit $J_m$ for the series is derived from the observation that $W_{2n-1}\,(J_y)$ vanishes for $n > J_m$ (The maximum value of $J$ contained in $\phi$) in the infinite series expansion of $\cos\theta J_y$. The lower limit $J$ on the series follows from the fact that $(n+1-J, J)$ vanishes for $n < J$.

Let us now use the disentangling theorem (Arecchi *et al* 1972) for the operator $e^{i\theta J_y}$ in eq. (4), instead of the expansion of $\cos\theta J_y$ in eq. (1).

$$e^{-i\theta J_y} = e^{-\theta\,[J_x + i J_y - (J_x - i J_y)]/2} \equiv \exp\,[-\theta\,(J_+ - J_-)/2]$$

$$= e^{tJ_+}\, e^{\log\,(1+t^2) J_z}\, e^{-tJ_-} \tag{11}$$

where

$$t = -\tan\,(\theta/2).$$

In order to carry out the integration in eq. (4), the following general expectation value is to be calculated first (the operator $O = H$ or $I$).

$$\langle \phi \mid O\, e^{-i\theta J_y} \mid \phi \rangle = \langle \phi \mid O\, e^{tJ_+}\, e^{\log\,(1+t^2)\, J_z}\, e^{-tJ_-} \mid \phi \rangle$$

$$= \sum_0^{Jm} \frac{(-1)^n}{(n\,!)^2}\ \sin^{2n}(\theta/2)\,\langle \phi \mid OJ_+^n\, J_-^n \mid \phi \rangle \tag{12}$$

In obtaining the last step, we used that the operator $O$ is invariant under rotations; the state vector $\phi$ has the projection quantum number zero and has the components up to a maximum angular momentum $J_m$. From eq. (12) and the integration result in eq. (9), we obtain the second expression for $E_J$ in eqs (3) and (4).

$$E_J = \Big[ \sum_J^{J_m} \frac{(-1)^n}{(n!)^2} \frac{(n-J+1, J)}{(n+1)(n+2, J)} \langle \phi \mid HJ_+^n J_-^n \mid \phi \rangle \Big] \Big/$$

$$\Big[ \sum_J^{J_m} \frac{(-1)^n}{(n!)^2} \frac{(n-J+1, J)}{(n+1)(n+2, J)} \langle \phi \mid J_+^n J_-^n \mid \phi \rangle \Big]. \tag{13}$$

## 3. Conclusion

The angle integrated exact expression for the projected energy is derived using two different expansions of the rotation operator. In one, the spin matrix polynomial expansion method is used, while in the other the disentangling theorem for angular momentum operator is used. Neither of the two expressions of $E_J$ so obtained have the same $J$ dependence as that derived in the earlier work. All the expressions for $E_J$ have different forms. This suggests that the construction of projection operator is not unique. This gives rise to the non-uniqueness in the $J$ dependence of $E_J$. The simplest projection operator, which would also work for the $K \neq 0$ intrinsic state $\phi_K$, can be taken as the polynomial in $J^2$ of degree $N$. It is assumed that there are $N$ components of $J = K, K+1, \ldots K+N-1$ in $\phi_K$. The $N$ unknown coefficients in this polynomial are to be found from the conditions that this polynomial projects out the component corresponding to the angular momentum $J$. It is expected that the $E_J$ so obtained would be similar to that derived from the Lanczos algorithm.

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