Variation after projection calculations for high-spin states — Zao-Chun Gao

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Overview

- Projection is a powerful technique that has long been used in various fields of physics.
- The projected wave functions can be as close as possible to the corresponding eigenfunctions obtained by the shell model.
- Such variation of the projected wave function is generally called as variation after projection (VAP).
- The VAP methods are expected to be applicable in large model space where full shell model calculation can not be performed presently or in the near future.

For angular momentum projection(AMP), it is believed that all the AMP states should be used to construct the VAP wave function.
If one uses n reference states to construct the VAP wave function with spin J, then the number of included projected states is $n(2J+1)$ (this number will be large in the calculation of high-spin states).
Too many projected states may increase the complexity of the VAP calculation. Actually, large number of projected states may increase the possibility of redundant projected states and may damage the stability of the VAP iteration.

Purpose

In this Letter, an improvement is made that only n projected states are adopted to construct the VAP wave function with arbibtrary spin J.
For simplicity, the reference states used in the present VAP are Slater determinants, so that the particle number projection can be omitted.

For a given J and M, one can project $|\Phi\rangle$ onto $2J+1$ different projected states, $P^J_{MK}|\Phi\rangle$, with $K = -J, -J+1, \cdots, J$. The nuclear wave function can be expressed like:

$$|\Psi_{JM\alpha}\rangle = \sum_{K=-J}^{J} f_K^{J\alpha} P^J_{MK}|\Phi\rangle \tag{1}$$

The coefficients $f_K^{J\alpha}$ and energy E^J_α can be determined by solving the Hill-Wheeler equation:

$$\sum_{K'=-J}^{J} (H^J_{KK'} - E^J_\alpha N^J_{KK'}) f_{K'}^{J\alpha} = 0 \tag{2}$$

with

$$H^J_{KK'} = \langle\Phi|\hat{H}P^J_{KK'}|\Phi\rangle, N^J_{KK'} = \langle\Phi|P^J_{KK'}|\Phi\rangle \tag{3}$$

The coefficients satisfy the normalization condition.

$$\sum_{K,K'=-J}^{J} f_K^{J\alpha *} N^J_{KK'} f_{K'}^{J\alpha} = 1 \tag{4}$$

To solve the HW equation, the first step is the diagonalization of N^J

$$\sum_{K'=-J}^{J} N^J_{KK'} R^k_{K'} = n_k R^k_K \tag{5}$$

Then one can establish a new set of orthonormal basis states

$$|\psi^J_k\rangle = \frac{1}{\sqrt{n_k}} \sum_{K=-J}^{J} R^k_K P^J_{MK} |\Phi\rangle \tag{6}$$

The HW equation can be transformed into a normal eigenvalue equation

$$\sum_{k'=1}^{2J+1} [\langle\psi^J_k|\hat{H}|\psi^J_{k'}\rangle - E^J_\alpha \delta_{kk'}] u^{J\alpha}_{k'} = 0 \tag{7}$$

coefficients $f^{J\alpha}_K$ are obtained from

$$f^{J\alpha}_K = \sum_{2J+1}^{k=1} \frac{R^k_K u^{J\alpha}_k}{\sqrt{n_k}} \tag{8}$$

Practically, we need to introduce a cutoff parameter $\epsilon > 0$ and only those $|\psi\rangle$ states with $n_k > \epsilon$ are taken to form the nuclear wave function.

To ensuring the VAP stability, the nuclear wave function can be simplified as

$$|\Psi_{JM}(K)\rangle = \frac{P^J_{MK}|\Phi\rangle}{\sqrt{\langle\Phi|P^J_{KK}|\Phi\rangle}} \tag{9}$$

where, K can be randomly chosen but should satisfy $\langle\Phi|P^J_{KK}|\Phi\rangle \neq 0$. K is put into bracket since it is not a good quantum number.
The energy then become

$$E^J(K) = \langle\Psi_{JM}(K)|\hat{H}|\Psi_{JM}(K)\rangle \tag{10}$$

The lowest $J^\pi = 2^+$ and 7^+ energies in ^{24}Mg

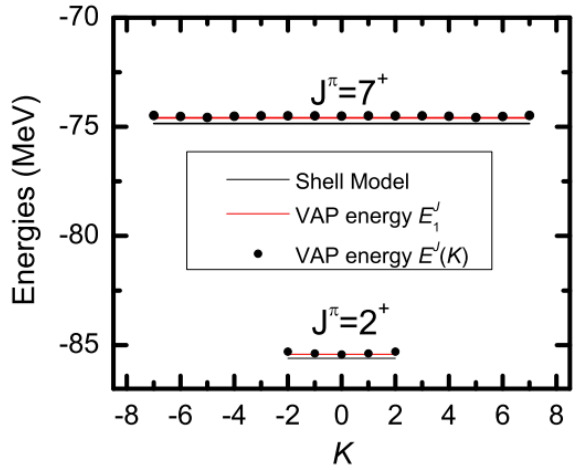

Fig. 1. Calculated VAP energies, E_1^J (red lines) and $E^J(K)$(filled dots), for the yrast 2^+ and 7^+ states in ^{24}Mg, with wave functions Eq. (1) and Eq. (8), respectively. The corresponding exact shell model energies are shown as black lines. The USDB interaction is adopted.

All energies $E^J(K)$ converge to the same level, which wave function should be unique, thus one should have

$$|\langle \Psi_{JM}(K)|\Psi_{JM}(K')\rangle| \approx 1 \qquad (11)$$

To improve the VAP approximation, Eq. (9) should be generalized by including more SDs, and the new form of VAP wave function can be written as

$$|\Psi_{JM\alpha}(K)\rangle = \sum_{i=1}^{n} f_i^{J\alpha} P_{MK}^{J} |\Phi_i\rangle \tag{12}$$

Also, the HW equation

$$\sum_{i'=1}^{n} (H_{ii'}^{J} - E_{\alpha}^{J} N_{ii'}^{J}) f_{i'}^{J\alpha} = 0 \tag{13}$$

with $H_{ii'}^{J} = \langle \Phi_i | \hat{H} P_{KK}^{J} | \Phi_{i'} \rangle$ and $N_{ii'}^{J} = \langle \Phi_i | P_{KK}^{J} | \Phi_{i'} \rangle$

Some problems with the projected basis.

- The norm N_{ii}^{J} could become vary tiny;
- The possibility of large overlap among the projected basis states.

To ensure the stability of VAP iteration, two constraint terms are attached to the energy sum

$$Q = \sum_{\alpha=1}^{m} E_{\alpha}^{J} + \chi_1 \sum_{i=1}^{n} \frac{1}{N_{ii}^{J}} + \frac{\chi_2}{2} \sum_{i,j=1;i\neq j}^{n} \frac{N_{ij}^{J} N_{ji}^{J}}{N_{ii}^{J} N_{jj}^{J}} \tag{14}$$

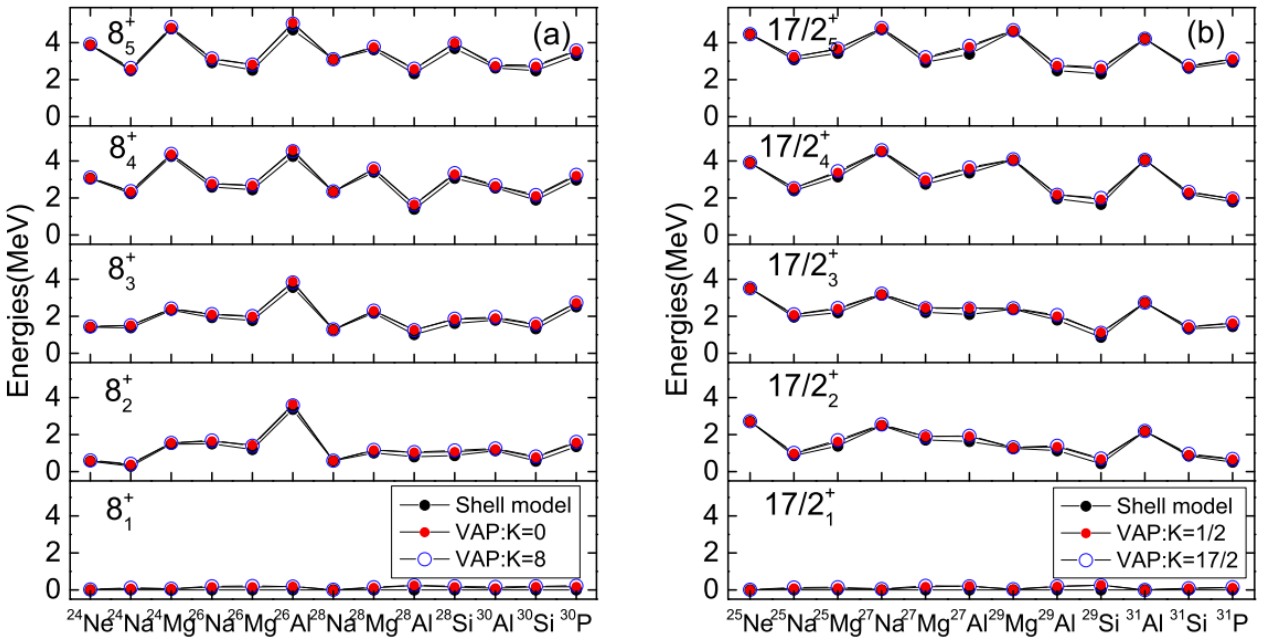

Fig. 2. Calculated lowest five $J^\pi = 8^+$ energies in some *sd* shell nuclei with the Shell model and the VAP, respectively. The five panels from low to high show the energies from the yrast 8_1^+ ones to the forth excited 8_5^+ ones, respectively. VAP:$K = 0$ and VAP:$K = 8$ refer to the results of the VAP calculations with $|\Psi_{JM\alpha}(K = 0)\rangle$ and $|\Psi_{JM\alpha}(K = 8)\rangle$, respectively. For each nucleus, all calculated energies are shifted by the same quantity so that the yrast SM energy is zero (see the lowest panel). The USDB interaction is adopted.

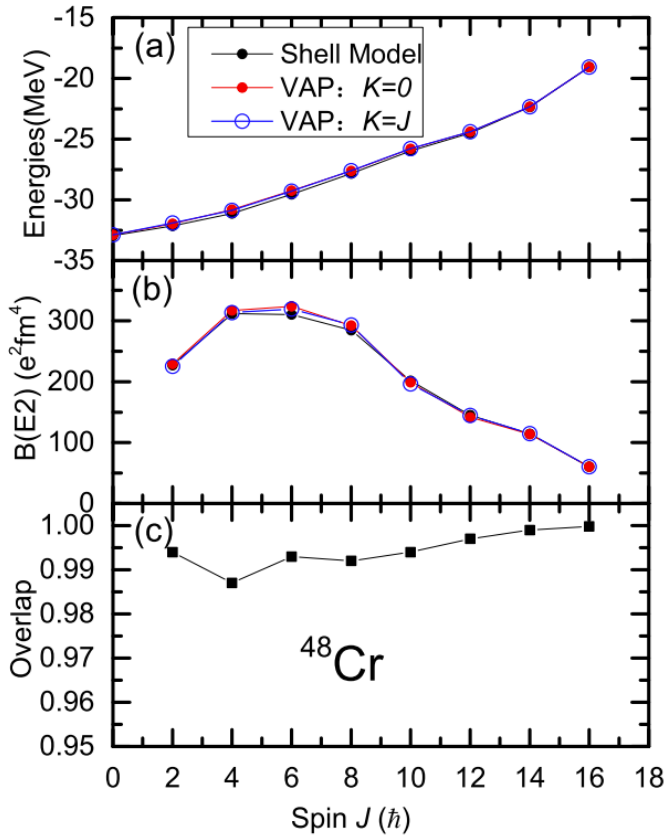

Fig. 3. Calculated results of the yrast states in ^{48}Cr with the VAP and the shell model. (a) The calculated energies. (b) The B(E2) values from the wave functions corresponding to (a). (c) The values of the overlap, $|\langle\Psi_{JM1}(K=0)|\Psi_{JM1}(K=J)\rangle|$. The KB3 interaction is adopted.