BULGARIAN JOURNAL OF PHYSICS
volume 17 1990 number 4

2100

A PRACTICAL THREE-DIMENSIONAL ANGULAR MOMENTUM PROJECTION AND THE "ENERGY VS DISPERSION" PROBLEM

V. I. Dimitrov and B. Slavov

Sofia University, Faculty of Physics, 5A A. Ivanov blvd, Sofia 1126, Bulgaria

Abstract. A practical procedure for restoration of the rotational symmetry of an arbitrary deformed intrinsic Slater determinant is developed in order to test the previous suggestion [3] that the state of minimal dispersion might be a better candidate for projecting out the components of good symmetry, rather than the one of minimal energy. Its application to the case of ^{28}Si in the $1s$-$0d$ single particle basis using a modified Wildenthal force does not confirm the above suggestion. The results indicate the importance of releasing the axial symmetry requirement for the intrinsic state.

Резюме. Предложена процедура для восстановления ротационной инвариантности произвольно деформированного Слэттеровского определителя с целью проверки предположения [3], что состояние минимальной дисперсии является лучшим для выделения проецированием компоненты желанной симметрии, чем состояние минимальной энергии. Ее применение к ядру ^{28}Si в $1s$—$0d$ одночастичном базисе, используя модифицированное взаимодействие Вильденталя, не подтверждает это предположение. Результаты указывают на важность снятия ограничения об аксиальной симметричности внутреннего состояния.

Although the techniques for the restoration of the rotational symmetry are, in principle, known for a long time [1], there does not exist a clear-cut prescription as to which is the optimal way of treating triaxial states. Efforts for optimizing the two main methods used in detailed applications, the integral representation of the projection operator

$$\widehat{P}_{JK}=\frac{(2J+1)}{8\pi^2}\int d\Omega \overset{*}{D}{}^{J}_{KK}(\Omega)\widehat{R}(\Omega) \tag{1}$$

and the shift operator representation

$$\hat{P}_{JK}=(2J+1)\,\frac{(J+sK)!}{(J-sK)!}\sum_{m=0}^{\infty}\frac{(-)^m}{m!(2J+m+1)!}\,\hat{J}^{J+m-sK}\hat{J}^{J+m+sK} \tag{2}$$

with $s=\pm 1$, have been reported [2] for the case of axially symmetric intrinsic states. One of the purposes of this communication is to develop an optimal finite sum representation of the Hill-Wheeler projection operator (1) such that no further improvement is possible without imposing symmetry restrictions on the intrinsic state that is to be projected. The second goal is to apply this technique to check the assumption that in realistic systems the state of minimal energy variance (dispersion) would give better results upon angular momentum projection, compared to the state of minimal energy (i. e. the Hartree-Fock solution). The last assumption is based on the results of [3] in a schematic model as well as on realistic applications in simpler cases [4]. Last but not the least, one can get a feeling how important the restriction to axially symmetric intrinsic states is.

Consider a basis built by orthonormal N-particle shell-model configurations $\{|IK\sigma\rangle\}$, where IK are the spin and its third component, and σ summarizes the rest quantum numbers not relevant for our discussion. Any N-particle Slater determinant $|\Phi\rangle$ can be expanded in this basis

$$|\Phi\rangle=\sum_{IK\sigma} g_{IK\sigma}|IK\sigma\rangle. \tag{3}$$

When no symmetry restrictions are imposed on $|\Phi\rangle$, the expansion (3) contains in general all I-s and K-s to which N particles can be coupled in the chosen single particle basis.

Now, let us address to the restoration of the axial symmetry first. Construct the operator $\widehat{Q}_M(\psi):=\frac{1}{2}(e^{iM\psi}\widehat{R}_z(\psi)+\text{h. c.})$, where $\widehat{R}_z(\psi)$ is a rotation on angle ψ along the z-axis. Obviously,

$$\widehat{Q}_M(\psi)|\Phi\rangle=\sum_{IK\sigma} g_{IK\sigma}\cos[(M-K)\psi]\,|IK\sigma\rangle. \tag{4}$$

Hence, the component of the wave function with the desired M can be picked up by means of Gauss-Chebishev integration over ψ [5]. Let us define

$$\widehat{P}_{J_z=M}=\frac{\pi}{L}\sum_{j=1}^{L}\widehat{Q}_M(\psi_j);\quad \psi_j=\frac{(2j-1)}{2L}\pi. \tag{5}$$

It is clear from the above that this operator acts on $|\Phi\rangle$ as a true projector as long as $L>(I_{\max}+|M|)/2$, where $I_{\max}$ is the maximal spin to which the N particles can be coupled in the given single particle basis:

$$\widehat{P}_{J_z=M}|\Phi\rangle=\sum_{I\sigma} g_{IM\sigma}|IM\sigma\rangle=:|\Phi_M\rangle. \tag{6}$$

The state $|\Phi_M\rangle$ is an eigenstate of $\widehat{J}_z$ with eigenvalue M, but in general is not an eigenstate of $\widehat{J}^2$.

We now proceed further to pick up the component of good $\widehat{J}^2$. Consider a rotation on angle β along the y-axis, sandwiched between two $\widehat{P}_{J_z=M}$. Clearly,

$$\widehat{P}_{J_z=M}\widehat{R}_y(\beta)\widehat{P}_{J_z=M}|\Phi\rangle=\sum_{I\sigma} g_{IM\sigma}d^I_{MM}(\beta)|IM\sigma\rangle. \tag{7}$$

Expressing the small d-function through the Jacobi polynomials [5]

$$d^I_{MM}(\beta)=\cos^{2M}(\beta/2)P^{(0,2M)}_{I-M}(\cos\beta) \tag{8}$$

one realizes that the desired J-value can be picked up by means of Gauss-Jacobi integration over $\cos\beta$. After some algebra one arrives to the final finite form of the projection operator

$$\widehat{P}_{JM}=\mathcal{N}\sum_{i=1}^{L}\sum_{j=1}^{L}\sum_{k=1}^{L'} e^{iM(\alpha_i+\gamma_j)}\cos^{-2M}(\beta_k/2)\,W_k\,\widehat{R}(\alpha_i\beta_k\gamma_j), \tag{9}$$

where N is irrelevant normalization factor, and

$$\alpha_i,\ \gamma_i=\pm\frac{(2i-1)}{2L}\pi,$$

$$\beta_k=\arccos(\eta_k),\ \text{where}\ P^{(0,2M)}_{L'+1}(\eta_k)=0,$$

$$W_k=\{P'^{(0,2M)}_{L}(\eta_k)\,P^{(0,2M)}_{L'+1}(\eta_k)\}^{-1}.$$

Whenever $L>(I_{\max}+|M|)/2$ and $L'>(I_{\max}-M)/2$, the finite representation (9) is exact. Thus, one needs $(I_{\max}-M+2).[(I_{\max}+|M|+2)]^2/2$ distinct orientations of $|\Phi\rangle$ in order to pick up the desired angular momentum eigenstate, and this number cannot be reduced further without imposing symmetry restrictions on $|\Phi\rangle$.

Now, let us turn to the application of the above formalism to a realistic case. The system under consideration is the nucleus ^{28}Si viewed as an inert ^{16}O core plus 12 nucleons in the $1s-0d$ oscillator shell, interacting with each other through a modified Wildenthal force [6]. The single particle energies are -4.15 MeV ($d_{5/2}$), -3.98 MeV ($s_{1/2}$) and 0.93 MeV ($d_{3/2}$). ^{28}Si is the most difficult nucleus in the $s-d$ shell, since the dimensions of the corresponding irreducible shell-model subspaces are very large, so the problem is far of being trivial and in fact is on the limit of the conventional shell-model configuration mixing (SCM) approach. We chose this nucleus for the sake of comparison with the exact SCM treatment using the same force.

Due to the symmetries of the force, it is possible to work in this case with identical proton and neutron Slater determinants. This means that 36 complex variables specify a ^{28}Si Slater determinant. The minimization of $\langle\Phi|\widehat{H}|\Phi\rangle$ with respect to the 72 variables yields a Hartree-Fock triaxial state $|\Phi_{\rm HF}\rangle$ with energy $E_{\rm HF}=-132.78$ MeV and dispersion $D_{\rm HF}=35.76$ MeV^2, while the minimization of $\widehat{\Phi}|H^2|\Phi\rangle-\langle\widehat{\Phi}|H|\Phi\rangle^2$ yields $|\Phi_{\rm DS}\rangle$ with $E_{\rm DS}=-132.51$ MeV and $D_{\rm DS}=32.79$ MeV^2. These numbers are rather close to each other, which seems to be a general feature [3, 4]. They further indicate, with respect to the large values of $D_{\rm HF}$ and $D_{\rm DS}$, that neither $|\Phi_{\rm HF}\rangle$ nor $|\Phi_{\rm DS}\rangle$ is a good approximation to the true ground state wave function. After these states have been obtained, a projection to good angular momentum is in order. Hovever, we first check the convergence properties of the finite representations (7) and (9). Figure 1 shows the behaviour of the quantity $\langle\Phi_{\rm HF}|\,\widehat{H}\widehat{P}_{J_z=M}|\Phi_{\rm HF}\rangle/\langle\Phi_{\rm HF}|\widehat{P}_{J_z=M}|\Phi_{\rm HF}\rangle$ for $M=0{,}2$, and 4 with changing L. For ^{28}Si in the $s-d$ shell $I_{\max}=14$ and one expects the curves to saturate at $L=8$, 9 and 10 respectively. Obviously, it happens earlier, which means that states with large J_z values do not mix in $|\Phi\rangle$ and hence the deviation from axial symmetry in $|\Phi\rangle$ is weak. On the other hand, the gain of energy upon projection on $M=0$ amounts to 1.9 MeV indicating the importance of the axial symmetry restoration. Figure 2 shows similar curves for the angular momentum-projected energy $\langle\Phi_{\rm HF}|\widehat{H}\widehat{P}_{JJ}|\Phi_{\rm HF}\rangle/\langle\Phi_{\rm HF}|\widehat{P}_{JJ}|\Phi_{\rm HF}\rangle$ for $J=0{,}2$ and 4 as a function of L'. Saturation is expected at $L'=8$, 7 and 6 respectively. Again, it takes place earlier, thus indicating relatively small contribution of high spin states to the HF ground state. The above results give us confidence in the reliability and stability of the projection technique. They also indicate that for an approximate angular momentum projection of HF ground states it is safer to decrease L than L'.

Finally, we compare the lowest three members of the ground state band of ^{28}Si, obtained by angular momentum projection of $|\Phi_{\rm HF}\rangle$ and $|\Phi_{\rm DS}\rangle$. They are shown in Fig. 3

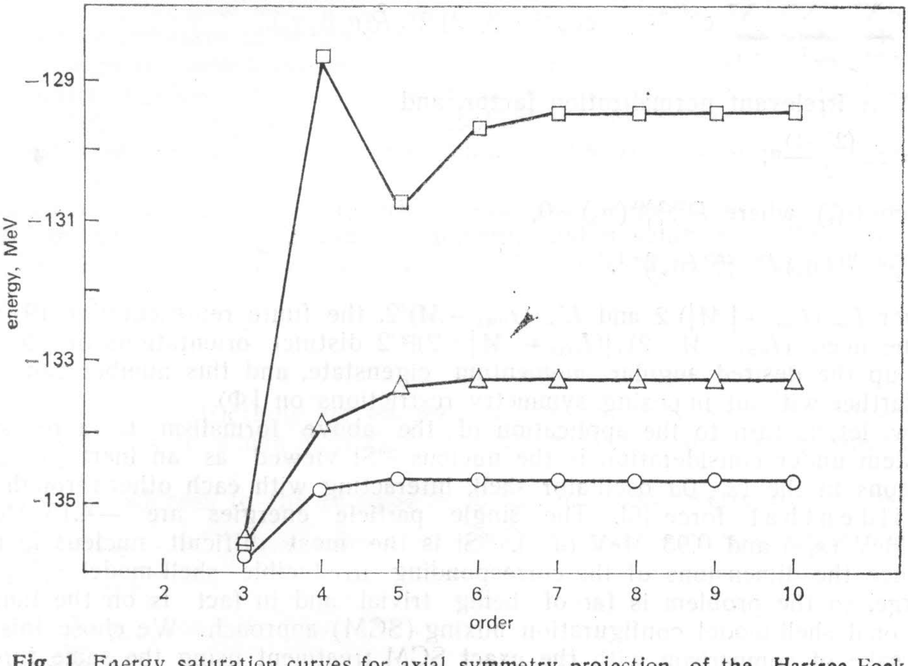

Fig. 1. Energy saturation curves for axial symmetry projection of the Hartree-Fock state on $M=0,2$ and 4. On the x-axis is the order of Gauss-Chebishev formula: ○ — $J_z=0$; △ — $J_z=2$; □ — $J_z=4$

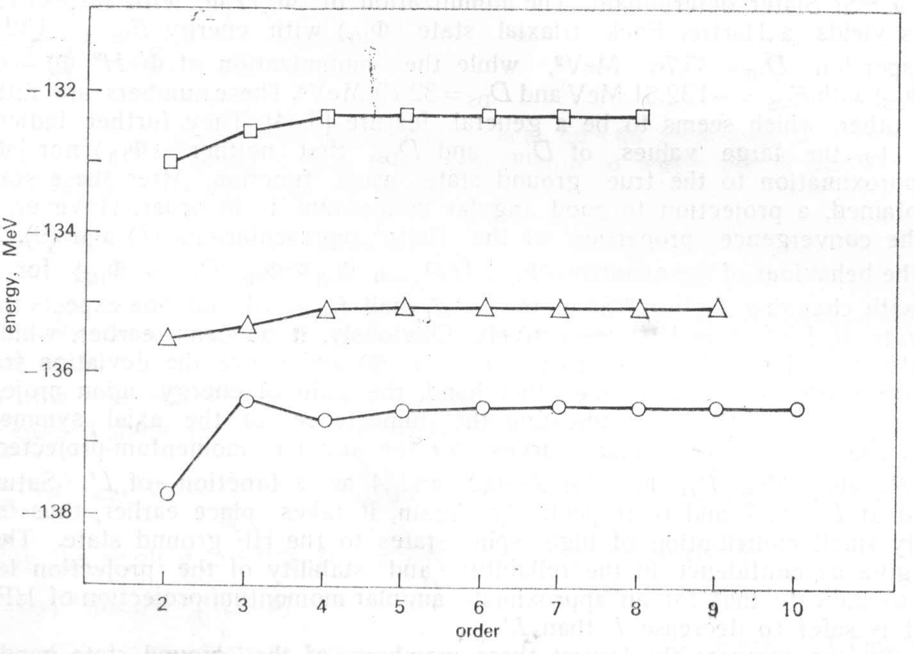

Fig. 2. Energy saturation curves for full angular momentum projection of the Hartree-Fock state on $J=J_z=0,2$ and 4. On the x-axis is the order of the Gauss-Jacobi formula: ○ — $J=0$; △ — $J=2$; □ — $J=4$

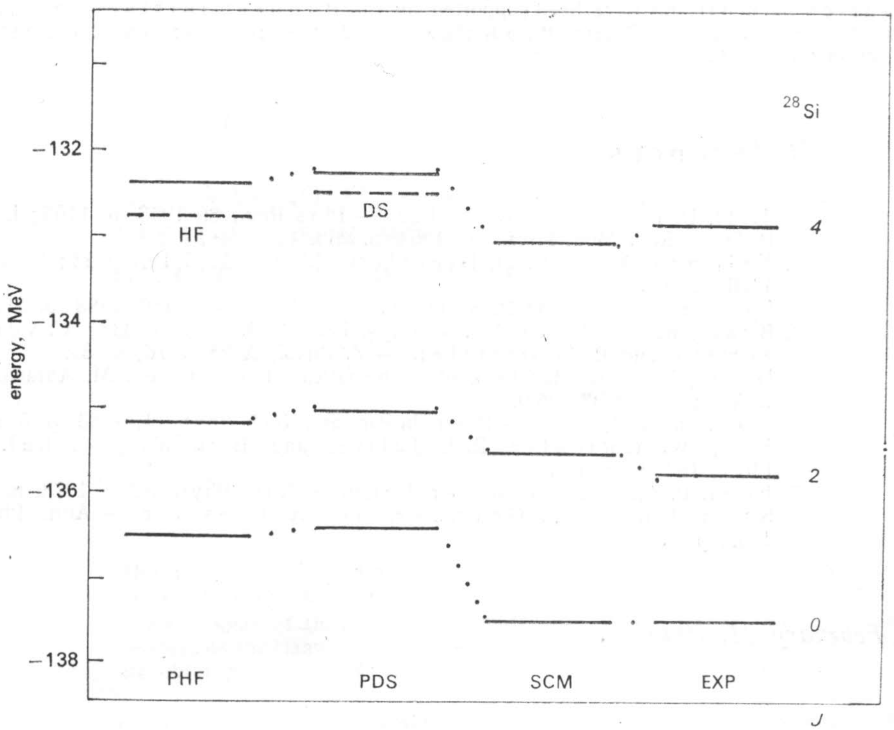

Fig. 3. The lowest three members of the ground-state band in ^{28}Si as given by projection of the Hartree-Fock state (HF), projection of the minimal dispersion state (DS), shell configuration mixing (SCM) and experiment (EXP). Indicated are also the energies of the corresponding intrinsic states

together with the exact SCM results and the experimental spectrum (taken from [7]). The last is included just to illustrate the adequacy of the used interaction to the chosen basis and is normalized to the SCM results. We should mention that prior angular momentum projection the orientation of the z-axis is adjusted in each case separately such that the axial symmetry projection on $J_z = J$ gives minimal energy. This is necessary because we do not use the more complicated procedure for angular momentum projection [8] which makes the results independent of the initial orientation of the deformed Slater determinant that is to be projected.

The spectra shown in Fig. 3 lead to the following conclusions:

a) $|\Phi_{HF}\rangle$ $|\Phi_{DS}\rangle$ give almost identical states upon angular momentum projection. Thus, no advantage of the state of minimal dispersion to the one of minimal energy is apparent. This is in contrast to the results of a schematic model [3]. The situation may be different for different two-body interaction, but no general rule seems to exist as to which state is better.

b) The release of the axial symmetry restriction to the mean field appears to be quite important. This work shows that calculations without axial symmetry restriction on the underlying states are both feasible and useful.

Acknowledgements. We are grateful to Prof. Dr. K. W. Schmid for the interest and fruitful discussions. Parts of this work have been performed during our stay at the Kernforschungsanlage Jülich GmbH and have been supported by the Bundesministerium für Forschung und Technologie (Intern. Büro-Karlsruhe) and the Bulgarian Committee of Science (contract no. 802).

References

1. Hill, D. L. and J. A. Wheeler. — Phys. Rev., 89 1953, p. 1106; Löwdin, P. O. — Rev. Mod. Phys., 36, 1964, p. 966.
2. Keleman, A., and R. M. Dreizler.—Z.Phys., A275, 1975 p. 23; Ibidem, A278, 1976, p. 269.
3. Dimitrov, V, I. and B. Slavov. — Nucl. Phys., A480, 1988, p. 312.
4. Bhatt, K. and J. Parikh. — Phys. Lett., 44B, 1973, p. 338; C. von Charzewski and R. M. Dreizler. — Z. Phys., A278, 1976, p. 35.
5. Davis, F. — In: Handbook of mathematical functions, ed. M. Abramovitz and I. A. Stegun (NBS-1964).
6. Wildenthal, B. H. — Progr. in Part. and Nucl. Phys., 11, 1983, p. 5; Brown, B. A, W. A. Richter, R. E. Julies, and B. H. Wildenthal. — Ann. Phys., 182, 1988, p. 191.
7. Endt, P. M. and C. van der Leun. — Nucl. Phys., A310, 1978, p. 1.
8. Schmid, K. W., F. Grümmer, and A. Faessler. — Ann. Phys., 180, 1987, p. 1.

Received February 21, 1990