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LETTER TO THE EDITOR

A novel projection technique in nuclear structure calculations

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Abstract. We present an exact projection technique based on the Lanczos algorithm for calculating eigenstates of an operator. The method is directly applicable to any intrinsic state expressible in terms of a sum of Slater determinants, does not depend on intrinsic symmetries, and can be used to project eigenstates of any one- or two-body operator.

The projection of eigenstates of a physically important operator from an intrinsic state which is not itself an eigenstate of the operator is a familiar problem in nuclear physics. In the case of angular momentum projection from a deformed intrinsic state the favourite method is the integral technique of Hill and Wheeler (1953). This method requires complex numerical integration and is normally used only when the assumption of axial symmetry in the intrinsic state reduces the problem to integration over one variable. Even this simplification has some difficulties as care must be taken in the numerical integration procedure, especially for high spin states. An exact non-integral method exists and has been used with some success in the nuclear 2s–1d shell (Watt 1972). This method can be used with symmetry restrictions less severe than axial symmetry but requires considerable programming effort if a range of nuclei is to be investigated.

We have developed a new projection technique (Morrison 1973) which has the advantage that it does not require any symmetries in the intrinsic state and is suitable for application to a range of nuclei without modification. The method is based on the Lanczos algorithm used in the Glasgow shell model program (Whitehead 1972). A full discussion is given in this reference and only the salient points will be mentioned here. The method is to diagonalize the operator whose eigenstates are required in a special basis prepared by the Lanczos method. This approach has also been used analytically by Warke (1974) to derive qualitative results, but for axial intrinsic states only.

Let A be a real symmetric $n \times n$ matrix, and let $\boldsymbol{v}_1$ be an arbitrary $n \times 1$ vector normalized to 1. New vectors $\boldsymbol{v}_2, \boldsymbol{v}_3, \ldots$ are formed by iteration thus:

$$\begin{aligned} A\boldsymbol{v}_1 &= \alpha_1\boldsymbol{v}_1 + \beta_1\boldsymbol{v}_2 \\ A\boldsymbol{v}_2 &= \beta_1\boldsymbol{v}_1 + \alpha_2\boldsymbol{v}_2 + \beta_2\boldsymbol{v}_3 \\ A\boldsymbol{v}_3 &= \beta_2\boldsymbol{v}_2 + \alpha_3\boldsymbol{v}_3 + \beta_3\boldsymbol{v}_4 \\ &\vdots \\ A\boldsymbol{v}_n &= \beta_{n-1}\boldsymbol{v}_{n-1} + \alpha_n\boldsymbol{v}_n \end{aligned} \tag{1}$$

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At the ith step $\boldsymbol{v}_{i+1}$ is the normalized remainder after orthogonalizing with respect to $\boldsymbol{v}_i$ and $\boldsymbol{v}_{i-1}$. The vectors $\boldsymbol{v}_i$ form an orthonormal basis in which the matrix A takes on tri-diagonal form, which is important because it is easy to find the eigenvalues and eigenvectors of a tri-diagonal matrix.

If it happens that a vector $\boldsymbol{v}_i$, $i<n$, is zero, then the process is continued by introducing a new arbitrary vector and iterating until the space is spanned. This leads to a factorization of the full n-dimensional space S^n into partitions of dimension m_1, $m_2, \ldots, m_K$:

$$S^n = S^{m_1} + S^{m_2} + \ldots + S^{m_K} \tag{2}$$

with

$$n = m_1 + m_2 + \ldots + m_K. \tag{3}$$

If V is the matrix whose columns are the vectors $\boldsymbol{v}_i$, then the matrix

$$C = V^{-1}AV \tag{4}$$

now takes on block diagonal form, the submatrices arising from the spaces S^{m_1}, $S^{m_2}, \ldots, S^{m_K}$. This transformation of A preserves the eigenvalues, and if $\boldsymbol{b}_i$, λ_i are the ith eigenvector and eigenvalue of the matrix C, then $V\boldsymbol{b}_i$ is the eigenvector of A corresponding to eigenvalue λ_i.

However A need not be a matrix. It can be an abstract operator and the vectors can be kets expressed as a sum of Slater determinants. To form $A|v_i\rangle$ we use the rules for operating with A on the ket $|v_i\rangle$ instead of ordinary matrix multiplication. This process is no better than conventional methods if the full n operations are needed to find the eigenstates of A. In the shell model context where A is the hamiltonian, this is avoided because the numerically largest eigenvalues converge rapidly and 100 iterations are usually more than adequate.

In the context of projection, the situation is even better. It is not necessary to iterate until convergence has occurred because the full space always factorizes into very small subspaces. Each subspace contains at most one eigenvector corresponding to each of the different eigenvalues of the operator. For example the eigenstates of $\boldsymbol{J}^2$ and $\boldsymbol{T}^2$ are highly degenerate leading to a reduction of the full space into partitions as in equation (2). The dimension of the first partition S^{m_1} is equal to the number of eigenstates of $\boldsymbol{J}^2$ or $\boldsymbol{T}^2$ in the intrinsic state $|v_1\rangle$ and is very small, typically of order 10. In principle, the eigenvalues and eigenvectors are produced exactly after $m_1 - 1$ iterations as the space S^{m_1} is linearly independent of all the remaining subspaces. The method therefore produces projected eigenstates rather than simply matrix elements as in most projection methods, and energies, transition rates etc can then be calculated in a straightforward manner using standard shell model techniques.

To illustrate this point further, consider an axial Hartree–Fock solution $|v_1\rangle$ obtained in the 2s–1d shell. We may write

$$|\boldsymbol{v}_1\rangle = \sum_J a_J |J, \alpha_J\rangle$$

where the state $|J, \alpha_J\rangle$ is the single state of angular momentum J contained in $|v_i\rangle$, and is one out of perhaps several thousand states of angular momentum J needed to span the complete space S^n in the 2s–1d shell. But these states $|J, \alpha_J\rangle$, one for each J, span the subspace S^{m_1}. Operating on the vector $|v_1\rangle$ with $\boldsymbol{J}^2$ gives a different linear combination of the same basis states $|J, \alpha_J\rangle$, and so $\boldsymbol{J}^2|v_1\rangle$ is another vector

in S^{m_1}. Thus the first $m_1 - 1$ iterations only produce vectors in the subspace S^{m_1} of S^n. By halting the Lanczos process when the basis S^{m_1} is exhausted, we obtain all the eigenstates contained in the intrinsic state and no others.

The terminating vector is never exactly zero as rounding errors in the calculation remove the exact independence of the space S^{m_1}. These small inaccuracies, if ignored, would generate components of the other subspaces and finally span the whole space. The projection process would then generate all possible eigenstates out of these round-off errors. For this reason the projection procedure is terminated if a state of very low normalization is produced. Fortunately these errors do not seriously affect the results due to the few iterations normally required. Indeed the high degree of numerical stability of the Lanczos process means that eigenstates of J^2 present as very small proportions of the intrinsic state can be projected successfully.

The method has been used for angular momentum and isospin projection from Hartree–Fock–Bogoliubov intrinsic states in a number of 2s–1d shell nuclei (MacDonald *et al* 1973). Here we illustrate the power of the method by presenting some results of calculations for the nucleus ^{22}Ne. The intrinsic state is not restricted to have the symmetries normally imposed on such states, and all bands with $K = 0, 1, 2, \ldots, 10$ are represented. Further details of this solution are given by Morrison (1973). In

Table 1. Projection data for the nucleus ^{22}Ne. The energies E are given for states of angular momentum J projected from the $K = 0$, 1 and 2 bands. All states have $T = 1$ and the percentage of each state in its K band is given in the row marked %.

	J	0	1	2	3	4	5
$K = 0$	E	−34·18	−29·34	−33·20	−28·62	−31·32	−26·88
	%	41·0	0·06	38·0	0·05	16·0	0·02
$K = 1$	E		−29·29	−31·29	−30·40	−29·10	−27·64
	%		0·5	48·0	32·0	5·0	11·3
$K = 2$	E			−33·27	−30·39	−31·38	−27·55
	%			70·0	2·5	22·0	0·46

	J	6	7	8	9	10
$K = 0$	E	−28·32	−23·17	−23·53	−19·18	−18·35
	%	4·0	10^{-3}	0·5	10^{-3}	0·02
$K = 1$	E	−26·71	−24·08	−23·09	−19·52	−18·58
	%	0·8	2·0	0·11	0·14	0·006
$K = 2$	E	−28·32	−24·00			
	%	5·1	0·05			

practice, all other projection methods rely heavily on symmetries in the intrinsic state. This method requires no symmetries. The HFB state is expressed as a sum of Slater determinants and all those with the same K are selected. Angular momentum and isospin projection are then performed to give the desired state and the energies calculated.

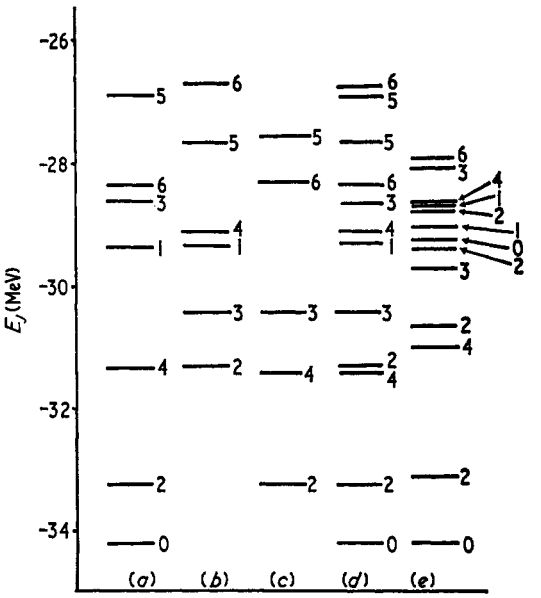

Figure 1. Projected HFB spectra for the nucleus ^{22}Ne. Spectra (*a*), (*b*) and (*c*) arise from the $K = 0$, 1 and 2 bands of the intrinsic state while (*d*) is the superposition of these and (*e*) is the shell model spectrum.

The results are tabulated in table 1 and the excitation energies of the low-lying states are compared in figure 1 with the exact shell model results of Halbert *et al* (1971). Of particular interest is the accurate determinations of the energy of the $J = 1$ state not obtainable from self-consistent calculations using any symmetries in the intrinsic state. Also from the percentage overlap figures we see that the process is accurate even for states present as very low proportions of the intrinsic wavefunction.

Projection using the Lanczos method is therefore accurate and easily applicable to situations where the intrinsic state has no special symmetries. The restriction in applicability of the method is to those nuclei where the Slater determinant basis is not too large to handle which at present limits calculations to one or two major shells in the harmonic oscillator basis.

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