

## Problems Associated with the Fitting of Low-Energy Spectra in a Truncated Vector Space\*

N. Ullah† and L. E. H. Trainor

*Department of Physics, University of Toronto, Toronto, Ontario, Canada*

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We show that it is possible to fit the low-energy spectrum in a truncated space using any one of a variety of pseudo-Hamiltonians together with a suitable choice of a set of orthonormal wave functions. Numerical examples are used for illustration.

### I. INTRODUCTION

The concept of effective interactions has been used for a long time in the fitting of low-energy nuclear spectra. In its simplest and most direct form the concept arises when a shell-model space is truncated and an effective Hamiltonian introduced to obtain a fit with the low-lying states of given angular momentum and parity.<sup>1</sup> It is usually assumed, at least implicitly, that the eigenfunctions of the effective Hamiltonian are sufficiently close to the true nuclear wave functions to make them useful in calculating nuclear properties other than energy spectra. That this procedure has severe limitations is now well known, e.g., through the use of effective charges radically different from their nominal values.

Before discussing what the purpose of the present paper is, let us discuss what it is not, in order to avoid possible confusion. Our purpose is not to formulate an alternative method to those already employed in the problem of fitting low-energy nuclear spectra; nor is it to formulate a new theory of effective operators.<sup>2</sup> Rather our purpose is to make explicit in a particular and perhaps dramatic way what is already well known, namely, that any method relying on the truncation of vector spaces and the diagonalization of the corresponding finite matrices for the system energy, is subject to large errors when these wave functions are used in calculating other nuclear properties, such as transition probabilities.

In practice, one is usually concerned with a finite subset of the total problem, e.g., one might be trying to fit the first 10 or 20 energy levels in the spectrum of a particular nucleus. Taking the experimental values for these energy levels to define the "exact problem," one attempts to find a Hamiltonian whose eigenvalues in a truncated vector space match those of the "exact problem." We point out in the present paper in a very explicit way that there are infinitely many ways of choosing a Hamiltonian and an associated set of wave functions such that the matrix of the Hamiltonian

with respect to the set simulates the finite matrix of the "exact problem." We shall refer to such a Hamiltonian and its associated set of wave functions as "simulated."

It is important in understanding our work to realize that we are not dealing with a standard eigenvalue problem in which one has some approximate or effective Hamiltonian with a known or presumed spectrum. For our simulation, the wave functions of the set associated with the simulated Hamiltonian are chosen in such a way that they reproduce the matrix elements of the "exact problem," i.e., in the finite subspace, the matrix is diagonal with values equal to those of the exact problem. However, as we have remarked earlier, these wave functions are not the eigenfunctions of the simulated Hamiltonian.

The importance of our work is that it deals directly with the problem as it appears in practice, namely, it deals directly with the lack of uniqueness of operators and wave functions in truncated vector spaces. Our contribution is not so much that we discover the problem – this has been done before – but that we organize it in a way that we believe is illuminating and possibly even useful.

The importance of the present study can be seen, for example, in the kind of problem which arises when the nuclear moment of inertia for a rotational band is calculated using the Skyrme formula:

$$\lambda = \frac{\hbar^2}{2g} = \frac{\langle \psi | H J^2 | \psi \rangle - \langle \psi | H | \psi \rangle \langle \psi | J^2 | \psi \rangle}{\langle \psi | J^4 | \psi \rangle - \langle \psi | J^2 | \psi \rangle^2}.$$

As shown by Wong, Tienhaara, and Trainor,<sup>3</sup> this formula is exact provided that the spectrum is known to be  $J(J+1)$  and  $|\psi\rangle$  represents an arbitrary linear combination (intrinsic state) of exact eigenfunctions in the band. In practice, one uses some approximation to  $|\psi\rangle$ , e.g., the deformed Hartree-Fock state. The present study makes it clear that once an approximate expression is used for  $|\psi\rangle$ , it is no longer true that the exact Hamiltonian is the best choice for calculating the matrices in the numerator of the Skyrme formula; our present formulation, however, does not tell us what is in fact

the best choice of effective Hamiltonians – this is the problem of constructing effective operators, and goes beyond the scope of the present work.

We present the formulation of our problem in Sec. II and give several simple examples in Sec. III to illustrate the principles involved. In Sec. IV we discuss briefly how effective operators other than the Hamiltonian come into the picture. Concluding remarks and discussions are summarized in Sec. V.

## II. FORMULATION OF THE PROBLEM

Let  $\psi_\alpha$ ,  $E_\alpha$  be the eigenfunctions and eigenvalues, respectively, of some exact Hamiltonian  $H$ . In matrix notation, we have

$$\langle \psi_\alpha | H | \psi_\beta \rangle = E_\alpha \delta_{\alpha\beta} \quad (1a)$$

and

$$\langle \psi_\alpha | \psi_\beta \rangle = \delta_{\alpha\beta}. \quad (1b)$$

The  $\psi_\alpha$  form a complete, orthonormal basis.

Consider now an  $N$ -dimensional subspace of functions  $\psi_\alpha$ ,  $\alpha = 1, 2, \dots, N$ , and let  $\kappa$  be a relatively arbitrary (arbitrary in the sense to be specified below) Hermitian operator (pseudo-Hamiltonian) defined in the subspace. We raise the question whether it is possible to find a set of wave functions  $\phi_\alpha$  such that the matrix elements of  $\kappa$  with respect to them correspond with the matrix elements of  $H$  with respect to the  $\psi_\alpha$ ,

$$\langle \phi_\alpha | \kappa | \phi_\beta \rangle = \langle \psi_\alpha | H | \psi_\beta \rangle = E_\alpha \delta_{\alpha\beta}, \quad (2a)$$

i.e., whether we can find a set of functions  $\phi_\alpha$  associated with  $\kappa$  such that the matrix elements of  $\kappa$  produce the diagonalized Hamiltonian in the truncated  $N$ -dimensional subspace. If we *do not* impose any orthonormality conditions of the type

$$\langle \phi_\alpha | \phi_\beta \rangle = \delta_{\alpha\beta}, \quad (2b)$$

it is straightforward to show that conditions (2a) can be satisfied by an infinity of different choices of the set  $\phi_\alpha$ . [We return below to the question of also imposing conditions of type (2b).]

We proceed as follows: Let us look for solutions to (2a) which can be expressed in the form of an expansion in the  $N$ -dimensional subspace of eigenfunctions  $\psi_\beta$ :

$$\phi_\alpha = \sum_{\beta=1}^N C_{\beta\alpha} \psi_\beta, \quad (3a)$$

or in a matrix notation

$$\Phi = \Psi C. \quad (3b)$$

Substituting (3a) in (2a), we obtain the matrix equation

$$C^\dagger \kappa C = E, \quad (4)$$

where  $\kappa$  is the matrix with elements

$$\kappa_{\alpha\beta} = \langle \psi_\alpha | \kappa | \psi_\beta \rangle.$$

Since  $\kappa$  is Hermitian, it can be diagonalized by some unitary matrix  $V$ ; hence,

$$V \kappa V^\dagger = d, \quad (5)$$

where  $d$  is the diagonal form of  $\kappa$ .

Letting  $d^{-1/2}$  be the diagonal matrix whose elements are the inverse square roots of the (diagonal) elements of  $d$ , and similarly  $E^{1/2}$  be the diagonal matrix whose elements are the square roots of the (diagonal) elements of  $E$ , then a solution (3a) to the problem is given by the choice

$$C = V^\dagger d^{-1/2} u E^{1/2}, \quad (6)$$

where  $u$  is an *arbitrary* unitary matrix. This follows at once by substituting (6) into (4), using (5).

Thus we have found an infinity of solutions to our problem (namely, those corresponding to the arbitrariness in the choice of the elements of the unitary matrix  $u$ ), but most of them are not very useful since they fail to satisfy orthogonality and normalization conditions. In fact, we now impose such conditions in order to select out the most useful set of solutions.

First let us discuss the case where  $\kappa$  is a real symmetric matrix and the coefficients of  $C$  are chosen to be real. (Later we generalize to Hermitian  $\kappa$  and complex coefficients.) The solution can now be written

$$C = \tilde{T} d^{-1/2} O E^{1/2}, \quad (7)$$

where  $T$  is the orthogonal matrix which diagonalizes  $\kappa$  and  $O$  is an arbitrary orthogonal matrix which we would like to fix by imposing orthonormality conditions of the type (2b). Now an  $N \times N$  orthogonal matrix has  $\frac{1}{2}N(N-1)$  independent parameters. This gives us exactly enough freedom to *satisfy orthonormality conditions of the type (2b) on exactly  $(N-1)$  of the  $N$  vectors  $\phi_\alpha$* , with a proviso to be explained below.

In other words, given a Hermitian matrix  $H$  with diagonal form  $E$ , and a real symmetric matrix  $\kappa$ , we are able to find a set of solutions  $\phi_\alpha$  satisfying

$$\langle \phi_\alpha | \kappa | \phi_\beta \rangle = E_\alpha \delta_{\alpha\beta} \quad (2a)$$

for  $\alpha, \beta = 1, 2, \dots, N$ , and

$$\langle \phi_\alpha | \phi_\beta \rangle = \delta_{\alpha\beta}$$

for  $\alpha, \beta = 1, 2, \dots, N-1$ . The  $N$ th vector  $\phi_N$  is not normalized nor is it orthogonal to the other  $N-1$ . By judicious choice of the orthogonal matrix  $O$ , one can easily arrange that the unnormalized vector corresponds to the highest eigenvalue of  $H$  in the set  $E_1, E_2, \dots, E_N$ .

If we write the normalization and orthogonality

conditions out explicitly, we have from (7) and (2a)

$$\sum_{\lambda=1}^N \frac{(E_\alpha E_\beta)^{1/2}}{d_\lambda} O_{\lambda\alpha} O_{\lambda\beta} = \delta_{\alpha\beta}, \quad \alpha, \beta = 1, 2, \dots, N-1. \quad (8)$$

For  $\alpha = \beta$ , we obtain the conditions

$$\sum_{\lambda=1}^N \frac{1}{d_\lambda} O_{\lambda\alpha}^2 = \frac{1}{E_\alpha}, \quad \alpha = 1, 2, \dots, N-1. \quad (9)$$

Clearly, if we choose an energy scale which makes all eigenvalues positive, we have

$$\frac{1}{E_\alpha} = \sum_{\lambda=1}^N \frac{1}{d_\lambda} O_{\lambda\alpha}^2 \leq \frac{1}{d_1} \sum_{\lambda=1}^N O_{\lambda\alpha}^2 = \frac{1}{d_1}, \quad (10)$$

where  $d_1$  is the lowest eigenvalue of the diagonalized  $\kappa$  matrix. Hence, for a given level  $\alpha$ , one requires that  $d_1 \leq E_\alpha$ . If for a given matrix  $\kappa$  this turns out not to be the case, the method fails; but it evidently works for a modified matrix  $\kappa$  obtained by subtracting a constant value from  $\kappa$ . This is the proviso referred to above.

If we take  $\kappa$  to be Hermitian so that  $u$  is a unitary matrix and the  $C_{\alpha\beta}$  are complex expansion coefficients, we have the following situation. An  $N$ -dimensional unitary matrix has  $N^2$  independent real parameters. On the other hand,  $N$  orthogonal vectors require  $N(N-1)$  orthogonality conditions and  $(N-1)$  vectors require  $(N-1)$  normalization conditions for a total of  $N^2 - 1$ . Hence, if we limit our unitary matrix to the class with  $\det u = 1$ , we have exactly the right number of free parameters to satisfy these conditions. Again the orthonormalization conditions require

$$\sum_{i=1}^N \frac{(E_\alpha E_\beta)^{1/2}}{d_\lambda} u_{\lambda\alpha}^* u_{\lambda\beta} = \delta_{\alpha\beta}, \quad (11)$$

for  $\alpha, \beta = 1, 2, \dots, N-1$ , and by the same argument as that following (9), we require  $\kappa$  to be such that  $d_1$  lies lower than the lowest eigenvalue  $E_1$  of the exact Hamiltonian  $H$ . With this restriction we have again simulated the spectrum of  $H$  in the truncated  $N$ -dimensional space using the matrix  $\kappa$  and a set of  $N$  vectors  $\phi_\alpha$ ,  $(N-1)$  of which are normalized, but all  $N$  are orthogonal.

One might ask, why not remove the restriction  $\det u = 1$  and extend the normalization to the  $N$ th

vector  $\phi_\alpha$ . If we do this, (11) becomes

$$\sum_{\lambda=1}^N \frac{E_\alpha}{d_\lambda} u_{\lambda\alpha}^* u_{\lambda\alpha} = 1;$$

if we now divide out by  $E_\alpha$  and then sum on  $\alpha$ , we obtain

$$\sum_{\lambda=1}^N \frac{1}{d_\lambda} = \sum_{\alpha=1}^N \frac{1}{E_\alpha}. \quad (12)$$

Hence, if we attempt to extend the normalization to all  $N$  vectors  $\phi_\alpha$ , we end up with the requirement that the harmonic mean of the eigenvalues of  $\kappa$  must equal the harmonic mean of the eigenvalues of  $H$ . Since this restriction is not likely to be satisfied for an arbitrary choice of  $\kappa$ , we chose to relax the condition on normality of  $\phi_N$  and to impose the condition  $\det u = 1$  instead.

### III. NUMERICAL EXAMPLES

In order to illustrate what happens in a practical example, let us consider four nucleons moving in  $p_{1/2}$  and  $d_{5/2}$  orbits outside a  $^{12}\text{C}$  core with the choice  $\epsilon_{p_{1/2}} = -4.95$  and  $\epsilon_{d_{5/2}} = -1.1$  MeV for single-particle energies. These single-particle energies are taken from  $^{13}\text{C}$  spectrum and have been used in the Hartree-Fock calculations on light nuclei.<sup>4</sup> For the exact Hamiltonian we choose a 50-MeV Rosenfeld interaction and consider the subspace of dimension  $N=3$  corresponding to the  $J^\pi = 0^+$ ,  $T=0$  wave functions arising from the configurations  $(p_{1/2})^4$  and  $(p_{1/2})^2(d_{5/2})^2$ . Exact diagonalization yields the three eigenvalues  $E_\alpha$  shown in Table I. Also shown in Table I are the exact eigenfunctions  $\psi_\alpha$  corresponding to the  $E_\alpha$  as expressed in terms of the component configurations.

Regarding  $\kappa$  as an approximate Hamiltonian, we take it again to be a Rosenfeld interaction, this time with a 60-MeV strength but with the same single-particle energies. Constructing  $\kappa$  in the basis of exact eigenfunctions, we obtain the matrix elements in Table II. Table III gives the eigenvalues  $d_i$  of  $\kappa$ , together with the elements of the matrix  $T$  which diagonalizes it. The matrix elements of the orthogonal matrix  $O$  are uniquely determined by requiring that the first two functions  $\phi_1$

TABLE I. Exact eigenvalues  $E_\alpha$  and the eigenfunctions  $\psi_\alpha$  expressed as a linear combination of the three  $J^\pi = 0^+$ ,  $T=0$  wave functions obtained from the configurations  $(p_{1/2})^4$ ,  $(p_{1/2})^2(d_{5/2})^2$ .

Exact eigenvalues $E_\alpha$	Exact eigenfunctions $\psi_\alpha$		
	$(p_{1/2})^4_{0^+,0}$	$(p_{1/2})^2(d_{5/2})^2_{a0^+,0}$	$(p_{1/2})^2(d_{5/2})^2_{b0^+,0}$
-35.40042	0.87717	-0.15315	0.45510
-24.19305	0.41361	0.72243	-0.55409
-16.30320	-0.24392	0.67427	0.69704

TABLE II. Matrix of the approximate Hamiltonian  $\kappa$  in the basis of  $\psi_\alpha$ .

$\alpha \backslash \beta$	1	2	3
1	-38.87552	0.55871	-0.32949
2	0.55871	-26.34818	-0.15537
3	-0.32949	-0.15537	-17.05219

and  $\phi_2$  are orthonormal. These matrix elements are given in Table IV, and the components  $C_{\alpha\beta}$  of the expansion (3a) for  $\phi_\alpha$  are given in Table V. [These coefficients are easily calculated from the matrix (7).] From Tables II and V, one can easily verify that

$$\langle \phi_\alpha | \kappa | \phi_\beta \rangle = E_\alpha \delta_{\alpha\beta}$$

and that  $\phi_1$  and  $\phi_2$  are orthonormal.

We have repeated the calculation assuming complex coefficients for the  $C_{\alpha\beta}$  instead of real coefficients and using a unitary matrix with  $\det u = 1$  in place of  $O$ . The solution for  $u$  is given in Table VI, and the corresponding solutions for the  $\phi_\alpha$  are given in Table VII in terms of the complex coefficients  $C_{\alpha\beta}$ . In this case one can arrange all of the vectors to be orthogonal, and all but the last one to be normalized.

As a second example, we used the same Hamiltonian for the exact problem (with eigenvalues and eigenfunctions as given in Table I) but for the "approximate" Hamiltonian  $\kappa$  we chose

$$\kappa = \frac{1}{2} (\sum_i \epsilon_i + \sum_i h_i), \quad (8')$$

where  $\epsilon_{p_{1/2}} = -6.20$  MeV,  $\epsilon_{d_{5/2}} = 0.65$  MeV, and the  $h_i$  are the single-particle Hartree-Fock Hamiltonians for the 50-MeV Rosenfeld interaction. The calculation proceeds in the same way as in the first example (assuming real coefficients  $C_{\alpha\beta}$ ) and the results are expressed in Tables VIII–XI in parallel to Tables II–V, for example I.

#### IV. EFFECTIVE OPERATORS

Formally it is easy to construct effective operators which give the same matrix elements with respect to the  $\phi_\alpha$  as do the exact operators with respect to the correct eigenfunctions  $\psi_\alpha$ . This construction is, however, of limited practical in-

TABLE III. The orthogonal matrix  $T$  which diagonalizes the matrix  $\kappa$ .

$d_i$	Diagonalizing matrix $T$		
	$T_{i1}$	$T_{i2}$	$T_{i3}$
-38.90512	0.99891	-0.04426	0.01475
-26.32639	0.04399	0.998865	0.01830
-17.04422	-0.01554	-0.01763	0.99972

TABLE IV. Orthogonal matrix  $O$  determined from the orthonormalization of  $\phi_1$  and  $\phi_2$ .

$i \backslash j$	1	2	3
1	0.92928	0.17623	0.32464
2	-0.28754	0.89681	0.33623
3	-0.023188	-0.40580	0.88406

terest, since it requires the knowledge of  $\psi_\alpha$ .

Consider the operator

$$\Omega_{\text{eff}} = \sum_{\alpha, \beta=1}^N (C\Omega\bar{C})_{\alpha\beta} |\psi_\alpha\rangle \langle \psi_\beta|, \quad (9'a)$$

where

$$(C\Omega\bar{C})_{\alpha\beta} = \sum_{\lambda, \nu=1}^{N-1} C_{\alpha\lambda} \langle \psi_\lambda | \Omega | \psi_\nu \rangle C_{\beta\nu}. \quad (9'b)$$

From the definition of  $\Omega_{\text{eff}}$  in (9'a) and (9'b) and from the expansion for  $\phi$  in (3a), we can write, for  $\sigma, \omega = 1, 2, \dots, N-1$ ,

$$\begin{aligned} \langle \phi_\sigma | \Omega_{\text{eff}} | \phi_\omega \rangle &= \sum_{\alpha, \beta=1}^N C_{\alpha\sigma} C_{\beta\omega} (C\Omega\bar{C})_{\alpha\beta} \\ &= \sum_{\alpha, \beta=1}^N \sum_{\lambda, \nu=1}^N C_{\alpha\sigma} C_{\beta\omega} C_{\alpha\lambda} C_{\beta\nu} \langle \psi_\lambda | \Omega | \psi_\nu \rangle \\ &= \langle \psi_\sigma | \Omega | \psi_\omega \rangle, \end{aligned} \quad (10')$$

where we have used the orthogonality relations for the first  $N-1$  vectors  $\phi_\sigma$ . In other words, the transition operator between exact eigenstates  $\psi_\sigma$  can be replaced by an effective transition operator between the states  $\phi_\alpha$ , if we exclude the  $N$ th state.

#### V. REMARKS AND DISCUSSION

We have shown in Sec. II that for any choice of Hermitian operator  $\kappa$  (which we may regard as a simulated Hamiltonian), it is possible to find an associated set of wave functions  $\phi_\alpha$  such that

$$\langle \phi_\alpha | \kappa | \phi_\beta \rangle = E_\alpha \delta_{\alpha\beta}, \quad (2a)$$

where the  $E_\alpha$  are the eigenvalues of the Hamiltonian of the system in the  $N$ -dimensional truncated space defining the "exact problem" referred to in the Introduction. Further, we have shown that (2a) can be accomplished with sufficient freedom left over to require  $(N-1)$  of the  $\phi_\alpha$  to be orthonormal. We can formally convert (2a) into a re-

TABLE V. Wave functions  $\phi_\alpha$  in terms of the exact set  $\psi_\alpha$ .

$\phi_\alpha$	$C_{1\alpha}$	$C_{2\alpha}$	$C_{3\alpha}$
1	0.87599	-0.36639	-0.32712
2	0.18415	0.86110	-0.46555
3	0.20813	0.23975	0.87233

TABLE VI. Unitary matrix  $u$  with  $\det u = 1$  determined from the orthogonality of  $\phi_1$ ,  $\phi_2$ ,  $\phi_3$ , and normalization of  $\phi_1$  and  $\phi_2$ .

$i \backslash j$	1		2		3	
	Real	Imag.	Real	Imag.	Real	Imag.
1	0.49135	0.87096	0.0	0.0	0.0	0.0
2	0.0	0.0	0.51974	0.63803	-0.03687	-0.56695
3	0.0	0.0	0.47568	0.31068	0.30033	0.76617

TABLE VII. Wave functions  $\phi_\alpha$  with complex expansion coefficients.

$\phi_\alpha$	$C_{1\alpha}$		$C_{2\alpha}$		$C_{3\alpha}$	
	Real	Imag.	Real	Imag.	Real	Imag.
1	0.46818	0.82990	-0.02075	-0.03677	0.00691	0.01225
2	0.01311	0.02115	0.48768	0.60441	0.57568	0.38123
3	-0.00584	-0.03127	-0.03416	-0.45885	0.29312	0.74096

stricted eigenvalue problem by multiplying on the left by  $|\phi_\alpha\rangle$  and summing over  $\alpha$ . This yields

$$\sum_{\alpha} |\phi_\alpha\rangle \langle \phi_\alpha | \kappa | \phi_\beta \rangle = \kappa' |\phi_\beta\rangle = E_\alpha |\phi_\beta\rangle. \quad (11')$$

This eigenvalue problem is restricted in the sense that it holds only in the space of  $N$  dimensions. Moreover, if we restrict  $\alpha, \beta$  to the  $(N-1)$  dimensions where orthogonality holds, we see that  $\kappa$  and  $\kappa'$  have identical elements in this  $(N-1)$ -dimensional subspace.

We now ask what would happen if we chose for  $\kappa$  the proper effective Hamiltonian for the  $N$ -dimensional truncated space, say in the sense of Harvey and Khanna.<sup>2</sup> In this case  $\kappa$  is again diagonal, but this time the  $\phi_\alpha$  form a set of  $N$ -orthonormal functions rather than a set of only  $(N-1)$ -orthonormal functions, as obtained in the general case. In other words, the true "effective Hamiltonian" is selected out by the additional requirement that all  $N$  vectors form an orthonormal set.

In Sec. II we have expanded the functions  $\phi_\alpha$  in terms of the exact eigenfunctions  $\psi_i$ . So far as the fitting of energy spectra is concerned, we can easily show that it is not necessary to choose this particular set but any other convenient orthonormal set of functions  $\chi_i$  can be chosen for this purpose.

TABLE VIII. Matrix of the approximate Hamiltonian  $\kappa$  defined in terms of single-particle energies and Hartree-Fock single-particle Hamiltonians.

$\alpha \backslash \beta$	1	2	3
1	-33.68611	-5.76026	3.39704
2	-5.76026	-24.18611	1.60180
3	3.39704	1.60180	-22.41463

We would now like to discuss some of the possible applications of the formulation of Sec. II. The constrained solution of Sec. II tells us that for each choice of the pseudo-Hamiltonian  $\kappa$  we can find a set of wave functions  $\phi_\alpha$  such that the energy spectra can be fitted with them. We now ask whether there is some way of telling which of the mixed configuration set of wave functions  $\phi_\alpha$  is better for calculating other nuclear properties. This question can be answered to some extent by choosing some operator  $\Omega$  and calculating its matrix in  $\phi_\alpha$  representation. The representation which gives the values of the matrix elements  $\Omega_{\alpha\beta}$  closest to the experimental values of  $\Omega_{\alpha\beta}$  then provides us with the best mixed configuration wave functions. As an example we have taken  $\Omega$  to be the octupole-octupole operator<sup>5</sup>

$$\Omega = \chi r_1^2 r_2^2 \sum_q Y_{3q} Y_{3-q},$$

the matrix of which in the representation of Table I is given by

$$\begin{matrix} & (p_{1/2})^4_{0^+,0} & (p_{1/2})^2(d_{5/2})^2_a & (p_{1/2})^2(d_{5/2})^2_b \\ (p_{1/2})^4_{0^+,0} & \begin{bmatrix} 0 & -0.289 & 0.508 \\ -0.289 & -0.191 & -0.279 \\ 0.508 & -0.279 & 0.141 \end{bmatrix} \end{matrix}$$

Using the expansion coefficients of Table I we find

TABLE IX. Orthogonal matrix  $T$  which diagonalizes  $\kappa$  of Table VIII.

$d_i$	$T_{i1}$	$T_{i2}$	$T_{i3}$
-37.34688	0.87717	0.41361	-0.24392
-21.46998	-0.42649	0.90449	0.0
-21.46998	0.22063	0.10403	0.96979

TABLE X. Orthogonal matrix  $O$  for the second example of approximate Hamiltonian  $\kappa$ . It is determined from the orthonormalization of  $\phi_1$  and  $\phi_2$ .

$i \setminus j$	1	2	3
1	1.0	0.0	0.0
2	0.0	0.28	0.96
3	0.0	-0.96	0.28

that the "exact" value of  $\langle \psi_1 | \Omega | \psi_1 \rangle = 0.547$ . We now use the two different operators  $\kappa$  of the previous example (Sec. III) and the associated sets of wave functions  $\phi_\alpha$  given in Tables V and XI. Calculating the matrix element  $\langle \phi_1 | \Omega | \phi_1 \rangle$  for each of these two sets, we find that  $\langle \phi_1 | \Omega | \phi_1 \rangle = 0.589$  using Table V, while it has a vanishing value using Table XI. Clearly, in a choice between these two sets of wave functions, both of which fit the energy spectrum, the mixed configuration wave functions of Table V give much better agreement with the "exact" case.

TABLE XI. Wave functions  $\phi_\alpha$  in terms of the exact set  $\psi_\alpha$  for the second example.

$\phi_\alpha$	$C_{1\alpha}$	$C_{2\alpha}$	$C_{3\alpha}$
1	0.85401	0.40269	-0.23748
2	-0.35160	0.16282	-0.98828
3	-0.30295	0.78203	0.23662

Finally, we remark again that in problems where only a finite number of matrix elements enter the calculation, like the application of the Skyrme formula referred to in the Introduction, one can simulate the final result with endless pseudo-Hamiltonians and associated sets of wave functions. By this same fact, once an approximation has been entered into for the approximate wave functions in the problem, it is no longer clear what the best choice of operators is without solving the whole problem of effective operators.

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## Effects of the Giant Resonance on the Energy Spectra of Neutrons Emitted Following Muon Capture in $^{12}\text{C}$ and $^{16}\text{O}$

Michael E. Plett\* and Stanley E. Sobottka

*Department of Physics, University of Virginia, Charlottesville, Virginia* † 22903

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The spectra of neutrons emitted following muon capture in carbon and oxygen are presented with a resolution of 6.5% at 5 MeV and a precision of 5%. The carbon spectrum is dominated by a broad peak at 4.2 MeV, while the oxygen spectrum is dominated by a narrower peak at 5.1 MeV. Partial transition rates for these two peaks are given. This structure supports theoretical predictions of the excitation of the giant resonance in the capture process.

### 1. INTRODUCTION

Early attempts to calculate the total muon capture rate in complex nuclei in the context of either a Fermi-gas model or an independent-particle shell model<sup>1</sup> led to values about 1.5 times as high as the experimental rate. In order to explain this,

Barlow *et al.*<sup>2</sup> and Balashov *et al.*<sup>3</sup> independently postulated that the capture process proceeds through isobaric analogs of the photonuclear giant-resonance states. This raised the theoretical estimate of the average nuclear excitation from about 13 to about 22 MeV. The resultant reduction in neutrino momentum was sufficient to re-