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Abstract

I discuss numerical many-body techniques based on the Lanczos algorithm and their applications to nuclear structure problems. Examples include shape coexistence, inclusive response functions, and weak interaction rates in ^{160}Ge ; weak-coupling descriptions of the 0^+ bands in isotopes of Ge and Se; and the evaluation of the nuclear Green's functions that arise in two-neutrino $\beta\beta$ decay and in nuclear anapole and electric dipole moment calculations.

As most of my nuclear structure studies have involved light nuclei and relatively low spin, my presence on the program of this high spin conference is a bit amusing. Despite the incongruity, some of the issues my collaborators and I have addressed are also central to this conference: shape coexistence, band mixing, and deformation. We have tried to describe such phenomena in light- and medium-mass nuclei from the starting point of a g -matrix derived directly from the NN interaction. Our tools are a set of powerful algorithms based on the work of Lanczos.¹ Some of the techniques we use might be equally effective for heavy nuclei and high spin, particularly when the spin is close to the limiting value in the chosen shell model space.

The basic tool, the Lanczos algorithm, allows one to find the extremum (lowest and highest) eigenvalues and associated eigenvectors of a very large matrix iteratively. With standard workstations, matrices of dimension $\sim 10^6$ by 10^6 can be treated in this way. In contrast, standard methods for fully diagonalizing matrices are usually limited to about $\sim 10^3$ by 10^3 . An even more powerful aspect of this algorithm, due to its connections with the method of moments, is that it can be used to generate inclusive response functions and Green's functions iteratively. Thus the Lanczos algorithm has proven useful in a wide variety of problems, including the nuclear shell model, atomic and molecular structure, spin-lattice problems in condensed matter physics, and Hamiltonian lattice gauge theory.

Consider a Hamiltonian H , defined over a finite Hilbert space of dimension N , and a starting normalized vector $|v_1\rangle$ in that space. We begin to construct a basis for representing H by

$$H|v_1\rangle = \alpha_1|v_1\rangle + \beta_1|v_2\rangle$$

where $|v_2\rangle$ is a normalized vector representing that part of $H|v_1\rangle$ orthogonal to $|v_1\rangle$. Proceeding

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$$\begin{aligned} H|v_2\rangle &= \beta_1|v_1\rangle + \alpha_2|v_2\rangle + \beta_3|v_3\rangle \\ H|v_1\rangle &= \beta_2|v_2\rangle + \alpha_3|v_3\rangle + \beta_4|v_4\rangle \end{aligned}$$

and so on. Note that the term $\beta_1|v_1\rangle$ must appear in the first line above because H is Hermitian. Also note that $|v_1\rangle$ does not appear in the second line above because everything that connects to $H|v_1\rangle$ other than $|v_1\rangle$ is defined as $|v_2\rangle$. Similarly, $H|v_4\rangle$ will contain nothing proportional to $|v_1\rangle$ or $|v_2\rangle$. Thus H has been cast in a tridiagonal form

$$H = \begin{pmatrix} \alpha_1 & \beta_1 & 0 & 0 \\ \beta_1 & \alpha_2 & \beta_2 & 0 \\ 0 & \beta_2 & \alpha_3 & \beta_3 \\ 0 & 0 & \beta_3 & \alpha_4 \\ \vdots & & & \ddots \end{pmatrix} \quad (1)$$

If this procedure is continued for N steps, the full H would then be in tridiagonal form. However the power of the algorithm derives from the information in the tridiagonal Lanczos matrix when the procedure is truncated after n iterations, $n \ll N$. If $\{\psi_{E_i}, i = 1, \dots, N\}$ are the exact eigenfunctions of H , then

$$\langle v_1 | H^N | v_1 \rangle = \sum_{i=1}^N |\langle v_1 | \psi_{E_i} \rangle|^2 E_i^N \equiv \sum_{i=1}^N f(E_i) E_i^N$$

The distribution $\{f(E_i), i = 1, N\}$ can be thought of a set of N weights f and measures E_i (the eigenvalues) characterizing the distribution of $|v_1\rangle$ in energy, i.e., the f 's determine a complete set of moments. The truncated Lanczos matrix, when diagonalized, provides the information needed to construct a distribution $\{g(\tilde{E}_i), i = 1, \dots, n\}$ which has the same $2n-1$ lowest moments in E as the exact distribution $\{f(E_i)\}$. That is, the Lanczos algorithm provides, at each iteration, a solution to the classical moments problem.² As Whitehead has emphasized^{2,3}, the speed and numerical stability of this moments algorithm is a very special property of Lanczos, and leads to marvelous procedures for evaluating total response functions and Green's functions in various many body applications.

If, as n increases, the Lanczos algorithm continues to accurately characterize the $(2n-1)$ lowest moments, clearly it must describe the extremum eigenvalues very faithfully: these are given enormous weight for large powers of H because they lie so far from the centroid of the distribution $\{f(E_i)\}$ in E . Thus a second important property of Lanczos is that some of the $\tilde{E}_i$ in the distribution $\{g(\tilde{E}_i)\}$ must quickly converge to the exact extremum eigenvalues of the matrix H . That is, we can use Lanczos as an efficient matrix diagonalization scheme provided we are interested in extremum eigenvalues.

Thus one concludes that the Lanczos algorithm is almost always adequate for physical applications. For instance, in nuclear physics we tend either to study familiar, low lying excitations (for which the Lanczos algorithm can provide the eigenvalues and eigenfunctions) or total nuclear responses (which Lanczos can characterize by its moments, even if all of the contributing discrete states cannot be determined). In either

case, it is straightforward to use the Lanczos algorithm on matrices of order $10^6 \times 10^6$, a scale that often arises in problems of physical interest.

The shell model code I use is about 10 generations removed from the original parent, the Glasgow code of Rex Whitehead and collaborators³ that was distributed in the mid-1970's. Although the early revisions John Dubach and I made to the Glasgow code were substantial, the present code remains almost identical to the original in its mathematical outline. Most of the revisions focused on improvements in speed, exportability, and adaptability. We also coupled Glasgow to new codes for generating density matrices for arbitrary one- and two-body operators.

The Glasgow code works in the m -scheme, rather than in subspaces of definite J , in order to exploit the natural connection between Fock-space fermion Slater determinants and computer words: each fermion single-particle state is associated with a bit in a computer word and can be occupied (bit = 1) or unoccupied (0). If the number of single-particle states exceeds the computer word size, more than one word can be used to represent the Slater determinant. Each of the vectors $|v_1\rangle, |v_2\rangle$, etc., forming the basis for Eq. (1) are stored as a list of amplitudes, corresponding to the list of all possible Slater determinants of the chosen total M that exist in the Hilbert space. If H contains only one- and two-body operators, the Lanczos algorithm requires us to evaluate

$$\sum_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \langle \alpha\beta | H | \gamma\delta \rangle_A |v_1\rangle$$

where $\langle \alpha\beta | H | \gamma\delta \rangle_A$ are the antisymmetrized two-body matrix elements that must be supplied by the user. One of the clever ideas of the Glasgow code was the realization that efficient bit-manipulation algorithms could be used to evaluate $a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$ acting on Slater determinants stored as computer words.

Since only M is fixed, the Lanczos algorithm will generate the extremum eigenvalues and eigenfunctions for all states $J \geq M$. In fact, since angular momentum is not explicitly imposed, the convergence to states of good J is a powerful numerical check. Within the m -scheme one can use time-reversal symmetry (if $A = N + Z$ is even) to select only even or only odd J states, and charge conjugation symmetry (if $N = Z$) to select even isospin states or odd isospin states.

Although most shell model practitioners tend to concentrate on light nuclei, the m -scheme might be interesting from the perspective of high spin. Heavy nuclei often require very large single-particle spaces, but our existing codes permit up to 120 distinct s.p. states. While the full Hilbert space is then enormous, one could choose M to be only slightly smaller than the maximum J that could be formed in this space, thereby eliminating all states with $J < M$ and making the dimensions of the Hilbert space reasonable.

The Glasgow group's review provides an excellent discussion of properties and possible applications of the Lanczos algorithm.³ A few of the relevant points are:

- 1) Although spherical single-particle bases are commonly used, there is no requirement to do so. For instance, a Nilsson basis could be adopted.

- 2) For moderately large shell model problems ($N \sim 10^5$), 200 iterations typically yield 10 fully converged states at the low energy end of the spectrum.
- 3) If the space is separable, spurious center of mass motion can be removed by adding a (large) multiple of the center of mass Hamiltonian H_{cm} to H .
- 4) Common UNIX workstations with adequate disk space (Gbyte) are suitable for calculations with $N \lesssim 10^6$. We have adapted our code for supercomputers, but have been disappointed with the results: it does not fully vectorize, and the disk space and memory demands are often troublesome in multi user environments.

Calvin Johnson and I recently completed a study of the structure of ^{16}O and of axial charge transitions that made heavy use of Lanczos techniques.⁴ The one-body axial-charge operator $\vec{\sigma}(t) \cdot \vec{p}(t)$ transforms under particle-hole conjugation like the more familiar E1 operator, and thus its matrix elements are suppressed by and very sensitive to 2p2h pairing correlations. One of the most thoroughly studied axial-charge transitions is the $0^+ \leftrightarrow 0^-$ β decay and μ capture transition in ^{16}O . This transition has been an important test of strong exchange-current corrections. (The two-body axial-charge operator determined from PCAC and current algebra is of the same order, $\frac{5}{2}$, as the one-body term and typically increases transition rates by a factor of two.) The μ -capture transition has been exploited as a test of $g\rho/g_A$ and its deviations in nuclei from the Goldberger-Treiman value. In addition, there is a strong connection between the axial-charge β -decay operator and hadronic weak interactions: the parity-nonconserving two-body interaction, when reduced to an effective one-body form, becomes the axial charge. Thus our ability to correctly describe the effects of correlations on the $A=16$ axial-charge transition is quite relevant to similar shell model studies in ^{14}N , ^{18}F , ^{19}F , and ^{21}Ne , where hadronic PNC measurements have been made.

The structure of ^{16}O also provides a classic example of shape coexistence. Brown and Green (BG) first pointed out that the $K^\pi = 1/2^+$ and $1/2^-$ Nilsson levels near $A = 16$ were nearly degenerate for large positive β , so that the spherical closed-core 0^+ state could strongly mix with a deformed 4p4h excitation and with a deformed 2p2h excitation of favored symmetry. An extreme weak coupling calculation, mixing these three states with a $\delta 2h\omega$ interaction $V_{\delta 2h\omega}$, yielded wave functions that successfully reproduced many of the observed properties.⁵ Johnson and I were interested in whether similar shape coexistence would emerge naturally from a complete microscopic calculation employing a realistic g -matrix.

Finally, the Gamow Teller distribution for $A = 16$ is an interesting quantity that can be studied by exploiting the moments properties of the Lanczos algorithm. The ^{16}O GT distribution is entirely a measure of ground-state correlations. Many theoretical calculations fail to reproduce the observed GT strength in the low energy tail of this distribution.

The Brown and Green work suggested that we focus on $V_{\delta 2h\omega}$, ignoring $V_{4h\omega}$ and more exotic terms. It is clear that first-order perturbation theory demands that any calculation that includes $V_{\delta 2h\omega}$ must contain the $4h\omega$ basis states: without these, the $2h\omega$ basis states are repelled by the ground state, with no compensating effect from the $4h\omega$ states. [Despite this, most " $2h\omega$ " calculations of ^{16}O and similar nuclei omit $4h\omega$ states, and compensate for this omission by an ill-advised readjustment of $V_{\delta 2h\omega}$ that

distorts the mixing of $0h\omega$ and $2h\omega$ states.] The resulting full $4h\omega$ single-particle basis is very large [1s, 1p, 2s1d, 2p1f, 3s2d1g, 3p2f1h], spanning four computer words on 32-bit machines. Since time-reversal and charge-conjugation symmetries can be applied, the basis for the four needed calculations (even and odd J and T) are moderate, $N \sim 90,000$.

In the spirit of BG, we allowed the N-N residual interaction to operate only in the 1p-2s1d shell, but projected spuriousity by allowing H_{cm} to operate everywhere. Kuo's Reid soft-core bare g -matrix⁶ was employed for $V_{2h\omega}$.

Fig. 1 A comparison of experiment and the $4h\omega$ ^{16}O shell-model spectrum of $T=0$ states. The spectrum resulting from diagonalizing the same Hamiltonian in a $2h\omega$ space is also shown.

In the second column of Fig. 1, 1 show the resulting spectrum of $T = 0$ states. The third column shows the effect of removing interactions with the $4h\omega$ states, which

are responsible for about an 8 MeV shift in the positions of states (dominantly) $2\hbar\omega$ in character.

The BG and shell model $0\hbar\omega$, $2\hbar\omega$, and $4\hbar\omega$ probabilities for the first 0^+ states are compared in Table I. They cannot be completely in accord: for instance, the BG spherical state is mixed only among three states, while in the realistic calculation it mixes with a complete set of $2\hbar\omega$ and $4\hbar\omega$ 0^+ states. Yet there is substantial agreement between the schematic and microscopic results. In Table II shell model $B(E2)$ values, calculated with bare charges and with radial wave functions from the Ginocchio potential⁷, are compared to experiment. The systematics are very well reproduced. Further technical details relevant to Fig. 1 and Tables I and II are given in Ref. [4].

Often one is interested in the inclusive response of some nucleus, initially in its ground state, to some perturbation. This can be accomplished by applying the Lanczos algorithm to the starting vector

$$|v_1\rangle = \hat{O}|g.s.\rangle$$

where $\hat{O}$ is the operator of interest. In our ^{16}O calculation we followed this procedure for

$$\hat{O} = \sum_{i=1}^A \vec{\sigma}(i) \tau_{\pm}(i)$$

thereby generating the distribution of $B(\text{GT})$ strength shown in Fig. 2. Relative to a $2\hbar\omega$ shell model calculation, the integrated strength increases by $\sim 50\%$, and the strength at low excitation energies is strongly enhanced, although not sufficiently to reproduce experiment.

Fig. 2 The $4\hbar\omega$ (solid line) and $2\hbar\omega$ (dotted line) $B(\text{GT})$ spectra in ^{16}O . In each case excitation energies are measured relative to the lowest 1^+1 level.

Table I. Comparison of the shell model (SM) and Brown Green (BG) $0p0h$, $2p2h$, and $4p4h$ probabilities for the first three 0^+ states in ^{16}O .

Probability	g.s.		$0_2^+(6.05 \text{ MeV})$		0_3^+	
	Bg	SM	BG	SM	BG	SM
$0p0h$	0.76	0.42	0.07	0.04	0.07	0.03
$2p2h$	0.22	0.45	0.05	0.05	0.73	0.68
$4p4h$	0.02	0.13	0.88	0.90	0.10	0.30

Table II. Experimental, shell-model, and schematic-model ^{16}O $B(E2)$ values. Ginocchio potential single particle wave functions were used in the shell model calculation.

Transition	Expt.	SM	BG ⁵
$2_1^+(6.92) \rightarrow 0_1^+(0.0)$	7.4 ± 0.2	4.3	5.3
$2_1^+(6.92) \rightarrow 0_2^+(6.05)$	65 ± 7	53	103
$2_2^+(9.84) \rightarrow 0_1^+(0.0)$	0.074 ± 0.007	0.054	
$2_2^+(9.84) \rightarrow 0_2^+(6.05)$	2.9 ± 0.7	0.68	
$2_3^+(11.52) \rightarrow 0_1^+(0.0)$	3.6 ± 1.2	2.2	3.3
$2_3^+(11.52) \rightarrow 0_2^+(6.05)$	7.4 ± 1.2	4.8	7.7
$4_1^+(10.36) \rightarrow 2_1^+(6.92)$	156 ± 14	63	152
$4_2^+(11.10) \rightarrow 2_1^+(6.92)$	2.4 ± 0.7	5.1	

Even though many 1^+ states exist in $^{16}\text{F}/^{16}\text{N}$, experiment cannot resolve all of these. The distribution shown in Fig. 2 corresponds to our Lanczos distribution $\{g(\tilde{E}_i), i = 1, \dots, n\}$ folded with a resolution function that approximates the resolution achievable in (p, n) mappings of GT strength. The distribution is fully converged ($n \approx 200$). The important point is that the Lanczos algorithm permits one to effectively extract, from a large matrix, all of the information that is relevant for comparisons to inclusive cross sections.

An interesting extension of the Lanczos shell-model techniques was undertaken

several years ago, motivated by the problem of double beta decay. Double beta decay is an exclusive process, usually involving only the transition to the daughter ground state, $J^\pi = 0^+$. Two transitions of experimental relevance are $^{76}\text{Ge} \rightarrow ^{76}\text{Se}$ and $^{82}\text{Se} \rightarrow ^{82}\text{Kr}$. The canonical spaces for these nuclei, $\{p_{1/2}, p_{3/2}, f_{5/2}, g_{7/2}, g_{9/2}\}$, lead to matrices that exceed 10^6 and are therefore beyond our capabilities to diagonalize directly.

The procedure we followed for these medium mass nuclei was p-n weak coupling. Writing $H = H_p + H_n + H_{pn}$, we treated H_{pn} as a perturbation. H_p and H_n were diagonalized separately, and a weak coupling basis was formed from the resulting wave functions

$$\{\psi_{ij}\} = \{|\psi_p^i(t) \otimes \psi_n^j(t)\rangle | J=0\}$$

We retained about 50 each of the lowest energy proton and neutron states, coupling them together to form a $J_0 = 0^+$ basis. H_{pn} was then diagonalized in this partial basis, one in which the most favored proton and neutron configurations should be well represented. [To carry this out in the m-scheme requires several clever tricks!]

Fig. 3 Excitation energies of the low-lying 0^+ states in the Ge isotopes as a function of neutron number. Ge and Se isotopes have both been studied as a function of neutron number and

Fig. 4 The solid lines give the weak-coupling predictions for the occupation numbers of the $2p_{3/2}$ and $1f_{5/2}$ subshells for the 0^+ ground states of the isotopes of Ge. The dashed lines are the corresponding results for the 0^+ states. The solid and empty circles give the experimental ($1f_{5/2}$) and ($2p_{3/2} + 2p_{1/2}$) occupation probabilities, respectively, of the ground states.

exhibit some dramatic physics. Fig. 3 shows that the 0^+ state plunges with increasing neutron number: perhaps a level crossing of the two lowest bands occurs at neutron number ≈ 40 . Fig. 4 shows that the proton occupation numbers correspondingly are undergoing rather sudden changes. (One expects that this may reflect the strong interaction between $1f_{5/2}$ (protons) and $1g_{9/2}$ (neutrons), shells with the same nodal structure. As neutrons are added to the $1g_{9/2}$ shell, the protons are polarized. The mixing of three 0^+ bands (spherical, $p_{3/2}^2 f_{5/2}^2$ (protons), $p_{1/2}^2 g_{9/2}^2$ (neutrons), and $p_{3/2}^2 f_{5/2}^2$ (protons) - $p_{1/2}^2 g_{9/2}^2$ (neutrons)) is an aspect of this polarization, and must change rapidly with neutron number.

Figs. 3 and 4 show that the weak coupling shell model with the Kuo (^{76}Ni) g matrix reproduces most of this complicated physics, and this gave us a great deal of confidence in our $\beta\beta$ decay predictions. The standard model 2ν rates we calculated were later measured and shown to agree to within about 50%.⁸ This in turn has boosted the confidence in the Majorana neutrino mass limits we extracted from calculations of $0\nu\beta\beta$ decay nuclear matrix elements.

The final, and perhaps most extraordinary, application of the Lanczos algorithm is in evaluating fully-interacting nuclear Green's functions. For instance, in $\beta\beta$ decay one needs the quantity

$$(0^+|\hat{0}_{GT}\frac{1}{E_0-H}\hat{0}_{GT}|0^+)$$

where $\hat{0}_{GT}$ is the GT operator. Defining $|v_1\rangle = \hat{0}_{GT}|0^+\rangle$, one can demonstrate

$$\frac{1}{E_0-H}|v_1\rangle = g_1(E_0)|v_1\rangle + g_2(E_0)|v_2\rangle + \dots$$

where the $|v_i\rangle$ are the Lanczos vectors and the $g_i(E_0)$ continued fractions formed from the entries in the tridiagonal Lanczos matrix. For example,

$$g_1(E_0) = \frac{1}{E_0 - \alpha_1 - \frac{\beta_1^2}{E_0 - \alpha_2 - \frac{\beta_2^2}{E_0 - \alpha_3 - \beta_3^2}}}$$

Roger Haydock has extensively explored Lanczos Green's functions methods in condensed matter physics.¹⁰ My experience in various nuclear physics applications has led me to conclude that this is a wonderfully stable and rapidly converging (often ~ 20 iterations) procedure to evaluate a quantity that is inherently very complex.

In $\beta\beta$ decay we have used this algorithm to complete a full fp-shell calculation of the transition $^{46}\text{Ca} \rightarrow ^{46}\text{Ti}$ ($g.s.$), thereby respecting all sum rules for the GT operator. Similar calculations for $^{76}\text{Ge} \rightarrow ^{76}\text{Se}$ and $^{82}\text{Se} \rightarrow ^{82}\text{Kr}$ are perhaps a workstation generation away. Other applications where nuclear polarizabilities must be evaluated include anapole moments, electric dipole moments, and $0^+ \rightarrow 0^+ 2\gamma$ transitions.

In conclusion, I hope the description of structure techniques we use in lighter nuclei might suggest some applications to high spin physics. The possibilities seem quite intriguing to me. It would be reassuring if tools could be developed to predict the properties of very high spin states from microscopic calculations based on realistic g matrices.

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