Current Status of Very-Large-Basis Hamiltonian Diagonalizations for Nuclear Physics

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Today there are a plethora of many-body techniques for calculating nuclear wave functions and matrix elements. I review the status of that reliable workhorse, the interacting shell model, a.k.a. configuration-interaction methods, a.k.a. Hamiltonian diagonalization, and survey its advantages and disadvantages. With modern supercomputers one can tackle dimensions up to about 20 billion! I discuss how we got there and where we might go in the near future.

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1 Introduction and relevance of nuclear structure

Some of my colleagues think nuclear structure theory, in particular the nuclear shell model, is as old-fashioned as the horse-and-buggy. But really it’s is the exact opposite. Nuclear structure theory has lots of exciting developments. These developments push the shell model from phenomenology to rigorous first-principle calculations, driven partly by new ideas but above all by the explosion in computing capabilities. While in the early days solving a $25 \times 25$ matrix was the height of computation [Halbert and French, 1957], today we find extremal eigenvalues of matrices exceeding dimensions of $2 \times 10^{10}$ [Forssén et al., 2018].

Aside from the intrinsic physics interest of nuclei, careful microscopic calculations are needed for many applications. Detection of known and unknown particles, from neutrinos [Suzuki et al., 2006] to dark matter [Anand et al., 2014], as well as experiments testing fundamental symmetries, such as neutrinoless double-$\beta$ decay [Horoi and Brown, 2013] and nonconservation of parity and time-reversal symmetries [Haxton and Wieman, 2001], often require knowledge of matrix elements in complex nuclei. For such calculations to be reliable and both precise and accurate, they need to be founded on solid microscopic calculations. Fortunately, in many cases modern nuclear structure theory is rising to the challenge.

2 Key ideas in large-basis diagonalization

This paper deals solely with diagonalization of the many-body Hamiltonian in a basis built from shell-model single-particle states, also called the configuration-interaction method or the interacting shell model [Brussard and Glaudemans, 1977, Brown and Wildenthal, 1988, Caurier et al., 2005]. The idea is straightforward: expand a state $|\Psi\rangle$ in a basis \{|$\alpha\rangle$\} (assumed to be orthonormal, $\langle \alpha | \beta \rangle = \delta_{\alpha,\beta}$),

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha} |\alpha\rangle;$$  

(1)

minimizing $\langle \Psi | \hat{H} | \Psi \rangle / \langle \Psi | \Psi \rangle$ leads to the eigenvalue equation

$$\sum_{\beta} H_{\alpha,\beta} c_{\beta} = E c_{\alpha},$$  

(2)

where $H_{\alpha,\beta} = \langle \alpha | \hat{H} | \beta \rangle$ is the matrix element of the many-body Hamiltonian $\hat{H}$ in this basis. I deal with the question of the choice of basis in section 3.

We can broadly classify configuration-interaction (CI) calculations into two categories, phenomenological and $ab$ initio. Phenomenological calculations are older, and usually assume a fixed cored and a relatively narrow valence space, such as the $1s_{1/2} - 0d_{3/2} - 0d_{5/2}$ space with a fixed $^{16}$O core, or the $1p-0f$ space with a fixed $^{40}$Ca...
The interactions actually start from some *ab initio* underlying interaction, and then adjusted to many-body spectra in the target space [Brown and Richter, 2006]. Because of this, it is fair to call them *semi*-phenomenological. By *ab initio* I mean a potential fitted to few-body data, such as nucleon-nucleon scattering and the binding energies of the $A = 2, 3$ and other light systems. These interactions are most commonly built from chiral effective field theory [Entem and Machleidt, 2003], but not always [Wiringa et al., 1995, Shirokov et al., 2016]. Despite having essentially the same few-body input, different choices such as cut-off regulators [Dyhdalo et al., 2016] can strongly influence the final many-body energies.

Purely *ab initio* CI calculations are often called *no-core shell model* (NCSM) calculations [Navrátil et al., 2009, Barrett et al., 2013], precisely because there is no core: all particles, in principle, are active, and the standard methodology increases the model space until convergence: see section 4 below.

In between these two are attempts to derive *ab initio* effective interactions, with no adjustable parameters, for phenomenological-like valence spaces for medium and heavy nuclei, via a double projection (Okubo-Lee-Suzuki) method [Dikmen et al., 2015], via coupled clusters [Jansen et al., 2014], and via the in-medium similarity renormalization group [Stroberg et al., 2017].

Because we cast the many-body Schrödinger equation as a matrix equation, the main computational task becomes solving a matrix eigenvalue problem. While some bases are larger than others, as discussed below, almost all CI calculations involve large enough dimensions that it would be foolish to try to find all eigenpairs. Instead, one solves for extremal eigenvalues using Arnoldi-type algorithms, almost always the Lanczos algorithm [Whitehead et al., 1977], although there have been attempts to use other methods [Shao et al., 2018].

### 3 Basis states for configuration interaction

How to construct the basis set $\{|\alpha\rangle\}$? One choice is to use many simple states. The most common building block are Slater determinants (antisymmetrized products of single-particle states) or more generally the occupation-space representations of Slater determinants using creation and annihilation operators. Furthermore, one often uses an is *M*-scheme basis, where each Slater determinant has the same fixed total $M$ or $J_z$, that is, the $z$-component of angular momentum. This is easy because $J_z$ is an additive quantum number. Many CI shell model codes use an *M*-scheme basis, most notably **ANTOINE** [Caurier and Nowacki, 1999], **MFDn** [Sternberg et al., 2008], **BIGSTICK** [Johnson et al., 2013, 2018], and **KSHLL** [Shimizu, 2013]. *M*-scheme bases are simple, amenable to a bit occupation representation ideal for digital computers [Whitehead et al., 1977], and one can compute matrix elements in the basis efficiently.
The drawback is one needs a large number of $M$-scheme basis states to build up nuclear correlations.

There are more sophisticated bases. $J$-scheme basis states have fixed total angular momentum $J$. The most widely used $J$-scheme codes are OXBASH [Brown et al., 1985] and its successor NuShellX [Brown and Rae, 2014]. As such, the $J$-scheme basis has smaller dimensions than the $M$-scheme. One can go even further, to so-called symmetry-adapted bases, based upon groups such as SU(3) [Dytrych et al., 2013] or Sp(3,R) [McCoy et al., 2018]. When judiciously truncated in the choice of irreps (subspaces defined by the Casimir operators of the group), such calculations can be even smaller in dimension.

Dimensions alone do not measure the computational burden. From Eq. (2) the real computational burden is in the nonzero matrix elements of the Hamiltonian. $M$-scheme bases are very sparse, as small as $\sim 10^{-6}$, while $J$-scheme bases, smaller in dimensions, can have more nonzero matrix elements, and symmetry-adapted bases yet more [Dytrych et al., 2016]. Furthermore, $J$-scheme basis states are generally represented as a linear combination of $M$-scheme states, and symmetry-adapted states are either a linear combination of $M$-scheme states or require non-trivial recursion algorithms, making calculation of the nonzero matrix elements a significant burden; by contrast, in the $M$-scheme matrix elements are so simple they can be recomputed efficiently on-the-fly, dramatically reducing the memory load, albeit at a price of a more complicated algorithm [Caurier and Nowacki, 1999, Johnson et al., 2018]. There is no ‘best’ basis, only the recognition of trade-offs.

In addition to the choice of many-body basis states, there is the question of the underlying single-particle basis. Phenomenological calculations either assume a harmonic oscillator basis or a Woods-Saxon like basis, but in general as matrix elements are primarily tuned to spectra, the single-particle basis is ambiguous. More rigorous ab initio calculations such as the no-core shell model (NCSM) do have definite single-particle bases, almost always harmonic oscillator which aids in removing spurious center-of-mass motion. Yet harmonic oscillator wave functions have a steep, unphysical fall off. Hence there have been many efforts to introduce better wave functions [Caprio et al., 2012], a question which has proved challenging. The most promising seem to be natural orbitals [Constantinou et al., 2017], orbitals that diagonalize the ground state one-body density matrix.

4 Convergence and extrapolation

Phenomenological calculations take place in a fixed set of valence orbits (unfortunately common usage often conflates orbits and shells), with interactions tuned to that valence space, such as the $1s$-$0d$ or $sd$-space [Brown and Richter, 2006]. Ab initio calculations, conversely, imply a result in a unrestricted or infinite space. Because any
actual calculation must be done in a finite space, one must investigate the convergence as the space is increased, and in many cases, extrapolate to the infinite limit.

In default NCSM calculations [Barrett et al., 2013], one defines the model space by two parameters: the harmonic oscillator frequency $\Omega$, or, more often, $\hbar \Omega$, for the single-particle basis states, and $N_{\text{max}}$, the maximum number of oscillator quanta allowed above the lowest configuration; historically this has also been called $N\hbar \Omega$. Typically one wants to extrapolate to infinite $N_{\text{max}}$ and $\hbar \Omega$.

One strategy is to use an exponential extrapolation, e.g. fitting energies to a form $a + b \exp(-cN_{\text{max}})$ [Heng et al., 2017]. This is inspired by similar exponential extrapolations in phenomenological shell model calculations where even the finite model space is so large one must truncate and extrapolate [Horoi et al., 1999]. For the NCSM, however, the results are not very robust. Instead, recent work has found more robust extrapolation by combining $N_{\text{max}}$ and $\hbar \Omega$ into infrared and ultraviolet parameters, and following the convergence in those parameters [Coon et al., 2012, More et al., 2013, Wendt et al., 2015]. This can also be linked to interpreting $N_{\text{max}}$ as a finite ‘wall’ [Furnstahl et al., 2012].

In a way, these extrapolations are brute force, and limited by the capability of modern computers. The basis dimension grows exponentially with the number of orbits / $N_{\text{max}}$ and particles, which is why size-extensive methods such as coupled clusters [Hagen et al., 2010] are attractive, but which have their own set of limitations. These limitations inspire alternatives to the standard NCSM prescription: rather than brute force computation in a larger basis, build in smarter bases, such as use of better single orbitals such as natural orbitals [Constantinou et al., 2017], and selected irreducible representations in symmetry-adapted bases which efficiently exploit deformation degrees of freedom [Dytrych et al., 2013, McCoy et al., 2018]. These lose, however, the powerful machinery of extrapolation applied to standard NCSM calculations.

Finally, rather than being ‘smarter’ in our physics, one can ride a current trend and hand over insights to the computer, with novel extrapolations using machine learning [Negoita et al., 2018]. The initial results are impressive, and it remains to see how widespread such techniques can be applied.

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