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Toward *ab initio* calculations of astrophysical reaction rates

Kenneth M. Nollett[*†]
Physics Division, Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
USA
E-mail: nollett@anl.gov

There has been tremendous progress in recent years in the description of nuclei as collections of interacting nucleons: the low-lying energy spectra of many light nuclei have been successfully computed from the vacuum nucleon-nucleon interaction and an additional three-nucleon interaction. These *ab initio* calculations have mostly focused on static properties of nuclei, particularly the energies of their bound and narrow states. However, much more can be done, and there is an important opportunity to compute cross sections for low-energy nuclear reactions that are important for astrophysics. Such calculations will provide new constraints on cross sections because they will be *completely independent of experimental data on the reactions in question*. I discuss in particular calculations of scattering and capture cross sections from realistic interactions using the quantum Monte Carlo computational methods, which have been very successful at computing energies of nuclei up to $A = 12$. We have made a first pass at radiative capture in $A = 6$ and $A = 7$ systems as well as the first-ever calculation of scattering in a five-nucleon system using realistic nucleon-nucleon interactions.

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[*]Speaker.

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1. Nuclei as collections of nucleons

Ab initio nuclear theory is the search for the most fundamental description of the nucleus possible. In practice, this means describing nuclei as collections of nucleons interacting with each other. We seek to characterize the nucleon-nucleon interaction, understand how nuclear properties arise from that interaction, and predict nuclear properties.

Many important pieces of the *ab initio* puzzle have fallen into place in the last 15 years. There are now a half-dozen "realistic" nucleon-nucleon potentials that describe the large body of available nucleon-nucleon scattering data accurately [1]. The same time period has seen great advances in both computational methods and available computing power.

The work that I describe here is based on the Argonne v_{18} (or AV18) nucleon-nucleon interaction [2]. It derives its name from its 18 operator terms (with, *e.g.*, spin-orbit, tensor, and scalar character). AV18 is a local interaction with a strong repulsive core, a strong tensor interaction, and one-pion-exchange character at long range.

Computation of $A > 2$ systems is complicated by a three-nucleon interaction (TNI) that is important for both binding energies and spin-orbit splittings of nuclei and is not reducible to iterated nucleon-nucleon interactions. The work described here is based on two types of TNI: the Urbana models [3] and the more recent Illinois models [4]. The Illinois models, and in particular the Illinois-2 (hereafter IL2) model, contain four terms with operator and spatial structures fixed by models of their origin in two- and three-pion exchange processes. Only the strengths of these terms were fitted to data, by matching computed nuclear energies of 17 bound and narrow states with $A \leq 8$ to their experimental energies.

2. Quantum Monte Carlo methods

I discuss only work by my collaborators and me at Argonne, Los Alamos, Illinois, Jefferson Lab, and Pisa using the quantum Monte Carlo methods. We solve the many-body Schrödinger equation,

$$H\Psi(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_A) = E\Psi(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_A)\,, \tag{2.1}$$

where H is the Hamiltonian, $\mathbf{r}_i$ are particle coordinates, and E is an energy eigenvalue. The wave function Ψ is a vector in spin/isospin space, so Eq. (2.1) constitutes a large set of coupled equations; in the largest nucleus we compute, ^{12}C, it amounts to some 270,000 coupled partial differential equations in 36 variables. We first apply the variational Monte Carlo (VMC) method to obtain an approximate Ψ, and then use the Green's function Monte Carlo (GFMC) method to project the true wave function out of this result. These methods involve operations on random samples of Ψ at discrete points in the $3A$-dimensional configuration space rather than the basis of spatial orbitals used in most numerical methods.

The calculation of nuclear wave functions by the VMC method utilizes a sophisticated variational wave function, specified by hand but based on long experience with light nuclei [5]. The variational trial function takes the form

$$\begin{aligned}\Psi_T \;=\; &[\text{3-body operator functions}] \times [\text{2-body operator functions}] \\ &\times [\text{scalar functions}] \times [\text{shell-model-like orbital/spin/isospin structure}]\,,\end{aligned}$$

with each factor in brackets containing a product of functions of the particle separations. The "shell-model-like" part establishes antisymmetry and specifies the spin, parity, and isospin of the desired state. All parts of Ψ_T contain variational parameters, which are adjusted by hand to minimize

$$E_V \equiv \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0 \tag{2.2}$$

so that E_V approximates the true ground-state energy E_0 for the specified quantum numbers. The calculation of E_V is achieved by Monte Carlo integration.

VMC wave functions provide good approximations to the true wave functions for many applications, particularly for $A = 3$ and 4. In larger nuclei, they are 1 MeV or more above the true binding energy per *p*-shell particle. We use the GFMC method to obtain the true ground state from Ψ_T, by the transformation

$$\Psi = \lim_{\tau \to \infty} \exp\left[-\left(H - E_0\right)\tau\right] \Psi_T \,. \tag{2.3}$$

We write the operator in Eq. (2.3) as integrals over a series of short-time-step Green's functions and evaluate the integrals by a Monte Carlo method for gradually increasing values of τ [5]. Rapid convergence requires that Ψ_T contain only the ground state and small "contaminations" of high excitation, so a good Ψ_T from VMC is crucial.

GFMC calculations of properties of light nuclei based on the AV18+IL2 interaction have been quite successful. Some 60 observed states have now been computed using AV18+IL2, with a root-mean-squared deviation of 700 keV from the measured *absolute* energies of those states [5]. We also have extensive results for other static properties like charge radii and electromagnetic moments. For reasons arising from the fact that GFMC only produces discrete samples of $\Psi(\tau)$, we largely neglected "off-diagonal" quantities like electroweak decay rates until recently. These are now being computed with good success; several instances are presented in Ref. [6].

Our calculations of bound and narrow states are all based on Ψ_T with the form of a bound state; its amplitude decreases rapidly at large radius, and the GFMC propagation retains this property as long as the state is narrow enough. Broad states cannot be computed in this way because the GFMC propagation evolves them toward zero-energy scattering states of separated clusters. Calculating broad states will require learning to treat unbound states explicitly as scattering states.

When we learn to solve scattering problems, we will also be able to compute electroweak-capture cross sections, and this presents an opportunity for nuclear astrophysics. Astrophysical cross section experiments are typically difficult, and there is often disagreement among the small number of measurements that have been made for a given cross section. Completely *ab initio* calculations can provide completely independent information about reactions. When experiments have not been done or cannot be done, *ab initio* calculations should be able to provide reliable predictions because they take advantage of precise knowledge of the underlying interaction. A review of reaction calculations using realistic potentials may be found in Ref. [7].

3. A first pass at radiative capture

To produce radiative-capture cross sections, one must compute both bound and scattering states and then matrix elements connecting them. As a first pass at computing radiative-capture cross sections, we addressed three astrophysically interesting alpha-capture cross sections – $\mathrm{D}(\alpha,\gamma)^6\mathrm{Li}$

[8], ^{3}H$(\alpha,\gamma)^7$Li, and ^{3}He$(\alpha,\gamma)^7$Be [9] – that can all be computed as direct captures at energies below a few MeV. We avoided the off-diagonal GFMC problem by using VMC wave functions for all bound states. Instead of solving scattering problems, we wrote each initial-state wave functions as the product of two bound clusters and a phenomenological correlation describing their relative motion. This correlation was computed from a one-body Schrödinger equation with a potential fitted to reproduce elastic-scattering data.

These calculations were successful overall, considering their limitations. The results for ^{3}H$(\alpha,\gamma)^7$Li are quite close to the experimental data. Our results for ^{3}He$(\alpha,\gamma)^7$Be are about 20% too low, though they do pass through some of the lower data and they have the correct energy dependence (a result of attention paid to the long-range tails of the VMC wave functions). We regard these results as a successful proof of concept, keeping in mind that the wave functions used are not exact solutions.

Our results for D$(\alpha,\gamma)^6$Li are within 15% of the measured cross sections at energies below the deuteron-breakup threshold, and we also regard this as reasonable agreement. The $E1$ amplitude for this reaction is suppressed by an isospin selection rule, so that $E2$ capture dominates at $0.5 < E < 3$ MeV. We computed the $E1$ amplitude including several usually-small (spin-dependent, retardation, and pion-charge) terms, and found by far the largest contribution to be the inclusion of the mass-energy of the nucleon-nucleon interaction in the definition of the center-of-mass frame. The $E1$ amplitude has been observed in angular distributions at 2 MeV [10], but the forward-backward asymmetry in the differential cross section has the opposite sign from that predicted.

4. The first calculation of $A = 5$ scattering

The major remaining barrier to accurate cross-section calculations is the need for *ab initio* computations of scattering states. We recently completed the first-ever calculation of scattering in a five-nucleon system with realistic potentials using the GFMC method [11], producing cross sections for neutron-alpha elastic scattering up to a few MeV. This system is relatively simple because the alpha particle is very compact and has no excitations within 20 MeV of its ground state.

Calculations of scattering states require both a variational description of scattering for Ψ_T and a method to impose scattering boundary conditions on the GFMC calculation. We formulate scattering as a particle-in-a-box problem with the boundary condition $\hat{\mathbf{r}}\cdot\nabla_{\mathbf{r}}\psi = \gamma\psi$ at the surface of the (spherical) box, where $\mathbf{r}$ is the separation of the two clusters and γ is a number. By varying the value of γ, we obtain solutions at different energies and match them across the boundary onto phase-shifted scattering wave functions. Enforcing the boundary condition in the GFMC calculation required developing a method of images that had not been used for extensive calculations before.

For n-^{4}He scattering, the main difficulty was obtaining the high precision (~ 100 keV out of ~ 30 MeV) needed for accurate cross sections near threshold. This required a larger box than expected (9 fm) and careful attention to problems of obtaining accurate GFMC solutions for such a diffuse wave function. The results provide a nice illustration of the role of the TNI in producing spin-orbit splitting between the $J^\pi = 3/2^-$ and $J^\pi = 1/2^-$ p-wave resonances. The AV18+IL2 interaction matches the data quite well, in contrast to the cases of AV18 alone or with the Urbana IX TNI.

5. Prospects for the future

Our next task is to compute proton-^{4}He scattering as a learning case with Coulomb interaction between the scattering clusters. We will then compute $n+{}^3$H and $p+{}^3$He for comparison against existing results from other methods [12], and eventually move on to cluster-cluster problems beginning with $\alpha+\alpha$ scattering. When the scattering methods have been well tested, we will use them as initial states for electroweak capture calculations. Nucleon-transfer reactions should also be accessible in the very long term, but they will be significantly more difficult.

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