Nuclear Matrix Elements for Neutrinoless Double-Beta Decay

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Recent progress in nuclear-structure theory has been dramatic and a DOE-sponsored topical collaboration has formed in the US to apply new methods to the matrix elements that govern neutrinoless double-beta decay. I describe the *ab initio* nuclear-structure methods that are being applied, and discuss when and why traditional nuclear models are still useful. I also briefly discuss the old and vexing problem of the renormalization of the weak nuclear axial-vector coupling constant "in medium" and plans to resolve it.

1 Introduction

Neutrinoless double-beta ($0\nu\beta\beta$) decay occurs if neutrinos are Majorana particles, at a rate that depends on a weighted average of neutrino masses (see References [1,2] for reviews). New experiments to search for $0\nu\beta\beta$ decay are under development, and one or more tonne scale experiments may be funded. Extracting a mass from the results, however, or setting a reliable upper limit — even planning the experiments efficiently — will require accurate values of the nuclear matrix elements governing the decay. These cannot be measured and so must be calculated.

The matrix elements have been computed in traditional nuclear models, but vary by factors of two or three. Nuclear-structure theory is now at the point, however, where we can do so-called *ab initio* calculations in systems with up to 50 or 60 nucleons, and should soon be able treat heavier nuclei as well. *Ab initio* means, as far as we're concerned, "from first principles." One starts with an interaction among nucleons, usually obtained from chiral effective field theory, and solves the many-nucleon Schrödinger equation in a controlled approximation scheme with quantifiable errors. The development of this kind of theory and the urgency of calculating double-beta-decay matrix elements has led to the funding of a five-year "topical" collaboration of theorists to apply the new methods to double-beta decay.

In this paper, I review some of the more promising *ab initio* schemes for computing the double-beta matrix elements. I also discuss how more traditional phenomenological methods can be improved, and then examine the currently unsettling "renormalization" of the nuclear weak axial coupling constant g_A, and argue that the cause will be identified soon through an investigation of many-body currents and the effective enlargement of model spaces. Although the presence of difficult theoretical issues such as this one mean that we don't yet know how accurately we will be able to compute the matrix elements, we will certainly be significantly better positioned in five years than we are now.

2 Neutrinoless Double-Beta Decay

The lifetime for neutrinoless double-beta decay, if the exchange of the familiar light neutrinos is responsible, is given by the product of a phase space factor, an effective mass $m_\nu = \sum_i U_{ei}^2 m_i$,

where m_i is the mass of the $i^{\rm th}$ eigenstate and U_{ei} weights each mass by the mixing angle of the associated eigenstate with the electron neutrino, and $M^{0\nu}$ is the nuclear matrix element. The matrix element is complicated but can be simplified without significantly altering its value through the "closure approximation." In this approximation, and neglecting two-body currents (which I take up briefly later), one can write the matrix element as

$$M^{0\nu} = \frac{2R}{\pi g_A^2}\int_0^\infty q\,dq \qquad (1)$$
$$\times \langle f|\sum_{a,b}\frac{j_0(qr_{ab})\,[h_F(q)+h_{GT}(q)\vec{\sigma}_a\cdot\vec{\sigma}_b]+3j_2(qr_{ab})h_T(q)\vec{\sigma}_a\cdot\vec{r}_{ab}\vec{\sigma}_b\cdot\vec{r}_{ab}}{q+\overline{E}-(E_i+E_f)/2}\tau_a^+\tau_b^+\,|i\rangle\ ,$$

where $r_{ab}\equiv|\vec{r}_a-\vec{r}_b|$ is the distance between nucleons a and b, j_0 and j_2 are the usual spherical Bessel functions, $\bar{E}$ is an average excitation energy to which the matrix element is insensitive, and the nuclear radius $R\equiv 1.2A^{1/3}$ fm is inserted with a compensating factor in the phase-space function to make the matrix element dimensionless. The "form factors" h_F, h_{GT}, and h_T are[3]

$$h_F(q) \equiv -g_V^2(q^2)$$
$$h_{GT}(q) \equiv g_A^2(q^2) - \frac{g_A(q^2)g_P(q^2)q^2}{3m_p} + \frac{g_P^2(q^2)q^4}{12m_p^2} + \frac{g_V^2(q^2)(\mu_p-\mu_n)^2q^2}{6m_p^2} \qquad (2)$$
$$h_T(q) = \frac{g_A(q^2)g_P(q^2)q^2}{3m_p} - \frac{g_P^2(q^2)q^4}{12m_p^2} + \frac{g_V^2(q^2)(\mu_p-\mu_n)^2q^2}{12m_p^2}\,,$$

with

$$g_V(q^2) = \frac{1}{\left(1+q^2/(0.71\ {\rm GeV}^2)\right)^2} \qquad (3)$$
$$g_A(q^2) = \frac{1.27}{\left(1+q^2/(1.09\ {\rm GeV}^2)\right)^2}$$
$$g_P(q^2) = \frac{2m_pg_A(q^2)}{q^2+m_\pi^2} \qquad g_M(q^2) = 3.70g_V(q^2)\,.$$

Here m_p and m_π are the proton and pion masses, and $\mu_p-\mu_n=3.706$.

In this development I have assumed that the weak nuclear currents are given adequately by the impulse approximation, i.e. as the sum of the currents associated with individual free nucleons. This approximation can be avoided (or lessened) by including two-body currents that are due to pion exchange. These occur at higher order in chiral effective field theory.

3 Chiral Effective Field Theory

Some *ab initio* calculations begin with an explicit model for the interaction between two nucleons and among three nucleons, but these days it is more common to use the framework of chiral effective field theory to determine these interactions. The theory [4] is supposed to work at kinetic/potential energies of up to a few hundred MeV, so the only degrees of freedom are nucleons and pions. The chiral framework, which provides a counting scheme in powers of momentum or pion mass divided by a QCD scale Λ_{QCD} of about 500 MeV, allows one to write down all possible interactions that are consistent with the underlying spontaneously broken chiral symmetry at any order of p/Λ_{QCD} or m_π/Λ_{QCD}. Two-nucleon interactions begin with one Feynman digram at leading order, three-nucleon interactions with two diagrams at next-to-next-to leading order. The coefficients of the interactions up to any order are fit to data. As long as one truncates the theory at some order n, one has a Hamiltonian[a] that should reproduce any low-energy data up to $\mathcal{O}([p/\Lambda_{QCD}]^{n+1})$. These Hamiltonians, typically up to next-to-next-to-next-to leading order (N^{3}LO) are what is used increasingly frequently in *ab initio* work.

[a] There is not universal agreement the theory is sufficiently rigorous to be completely trustworthy.

4 *Ab Initio* Shell Model

I turn now to the many-body methods used in conjunction with the Hamiltonians described in the last section. Some nuclei are easier to apply such methods to than others. The easiest are those that can be represented in first approximation by a single spherical Slater determinant. Such nuclei have "closed shells," i.e. a specific number of protons or neutrons so that the nucleus is much more bound than the nucleus with one additional proton or neutron. Many-body methods handle these nuclei by systematically correcting the Slater determinant. "Open-shell" nuclei are more difficult because they require a more sophisticated starting point.

Such nuclei have been described for a long time by what is called the nuclear shell model. The model focuses on the nucleons outside the last closed shell(s), with the others taken to form an inert core. The last (valence) nucleons are allowed to correlate arbitrarily, though only within a few valence single-particle orbitals. For that reason the Hamiltonian described in the previous section must be replaced by a phenomenological Hamiltonian. Once that Hamiltonian has been determined (generally through fits to nuclear data in isotopes close to those one cares about), the model works quite well. In our context, however, it has a problem. We are computing the matrix element of a complicated two-body nuclear operator. The "bare operator" of Eq. (1) may not sufficient in a limited space, for the same reason the bare Hamiltonian is not. Thus, even if the model describes spectra well, it may err considerably in its predictions of double-beta matrix elements.

Researchers are now, however, beginning to map *ab inito* calculations into shell-model calculations. Among the *ab initio* approaches in which this can be done are coupled clusters theory [5] and the in-medium similarity renormalization group (IMSRG) [6,7]. The idea behind both approaches is to construct a unitary transformation that transforms the full many-body Hamiltonian into block diagonal form, with a piece $H_{\rm eff}$ in the shell-model space that reproduces the lowest-lying energies exactly. Figure 1 presents the idea graphically, in terms of projection operators typically labeled $\hat{P}$ and $\hat{Q}$.

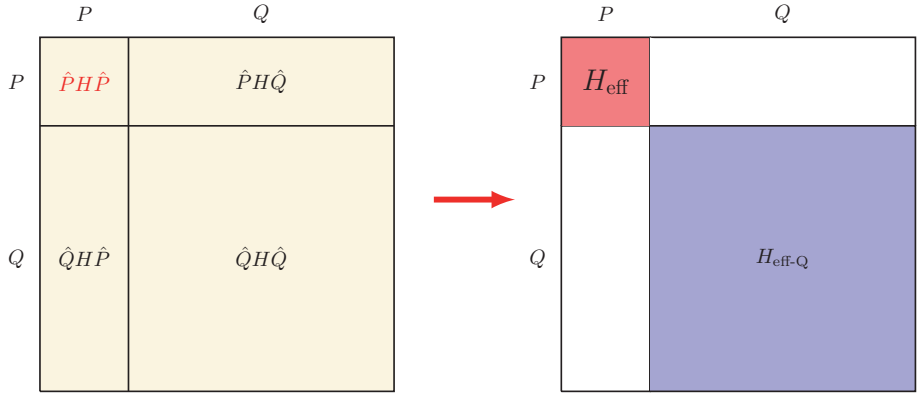

Figure 1 – Representation of unitary transformation for construction of effective shell-model Hamiltonian $H_{\rm eff}$. The operator $\hat{P}$ projects onto the shell-model (valence) space with an inert core, and the operator $\hat{Q}$ projects onto onto the rest of the many-body Hilbert space. After the transformation, the two spaces are decoupled.

Coupled cluster theory is based on replacing a single Slater determinant with the completely

general correlated state vector:

$$|\text{corr}\rangle = e^T |SD\rangle \tag{4}$$
$$T = \sum_{mi} t_{mi} a_m^\dagger a_i + \sum_{mnij} t_{mn,ij} a_m^\dagger a_n^\dagger a_i a_j + \dots .$$

Here $|SD\rangle$ is a Slater determinant and i, j label occupied orbitals in that determinant while m, n label empty orbitals. Thus the operator T creates one-particle one-hole configurations, two-particle two-hole configurations, etc. The presence of these operators in the exponent means the correlations are iterated and many-particle many-hole excitations are present, even when the series is truncated at the point indicated in Eq. (4).

Coupled clusters theory has reached the point at which the correlated closed-shell state above can be generalized to states containing two or three valence particles outside closed shells. The procedure for obtaining a shell-model interaction, e.g. in a valence space appropriate for ^{76}Ge (a prime double-beta decay candidate) goes something like this:

1. Begin with a two- and three-nucleon Hamiltonian from chiral effective field theory [8].

2. Do *ab initio* coupled-clusters calculations of the ground state of the closed shell nucleus ^{56}Ni, of the low-lying eigenstates states of the closed-shell-plus-one nuclei ^{57}Ni and ^{57}Cu, and of the low-lying states of the closed-shell-plus-two nuclei ^{58}Ni, ^{58}Cu, and ^{58}Zn. Eventually, when it becomes possible, do the same in closed-shell+three nuclei as well.

3. Perform a "Lee-Suzuki" mapping [9] of the low-lying states in these nuclei onto states in the valence shell containing one and two (and eventually, three) nucleons. The mapping is designed to maximize the overlap of the full ab initio eigenstates with their shell-model images, while preserving orthogonality of the images [10].

4. Use the mapping of states to construct the shell-model interaction H_{eff} that gives the image states the same energies as their parents. Construct an effective double-beta operator that gives the same matrix elements between image states as the bare operator does between the associated parents. The formalism that allows this step has long been worked out.

5. Put 4 protons and 16 neutrons (for ^{76}Ge) and 6 protons and 14 neutrons (for ^{76}Se) in the valence shell and use the effective interaction and decay operator derived in the previous step to calculate the ground-state-to-ground-state decay matrix element.

The last step, of course, is where things get tricky, because in principle, many-body effective interactions will be needed once more nucleons are in the valence shell. There are arguments that the effects of these fall off with the number of nucleons involved in the interaction. There is no power-counting scheme that tells us how fast, but one expects three body interactions and operators to be sufficient. The expectation can be checked by including four-body operator approximately. Such checks are how error is estimated in *ab initio* work.

The program has just begun to be carried out, starting in lighter nuclei. Reference [11] uses coupled cluster calculations in ^{16,17,18}O to predict the spectra of oxygen isotopes with more neutrons. Figure 2 shows the results. The left column for each isotope contains predictions, the middle column the experimental data, and the right column the "predictions" of the USD shell-model interaction [12] that was fit long ago to lots of data *in neighboring nuclei*. The coupled-clusters-generated interaction, which uses only data in two- and three-nucleon systems to obtain the N^{3}LO chiral interaction, produces results which are at least as good. Though researchers have yet to investigate matrix elements of the double-beta operator, the initial results for energy levels are extremely promising. Including an effective three-nucleon interaction, from still extremely difficult *ab initio* calculations in ^{19}O and ^{17}C (ensuring that predictions exactly match the *ab initio* results in those isotopes) should improve the spectra further.

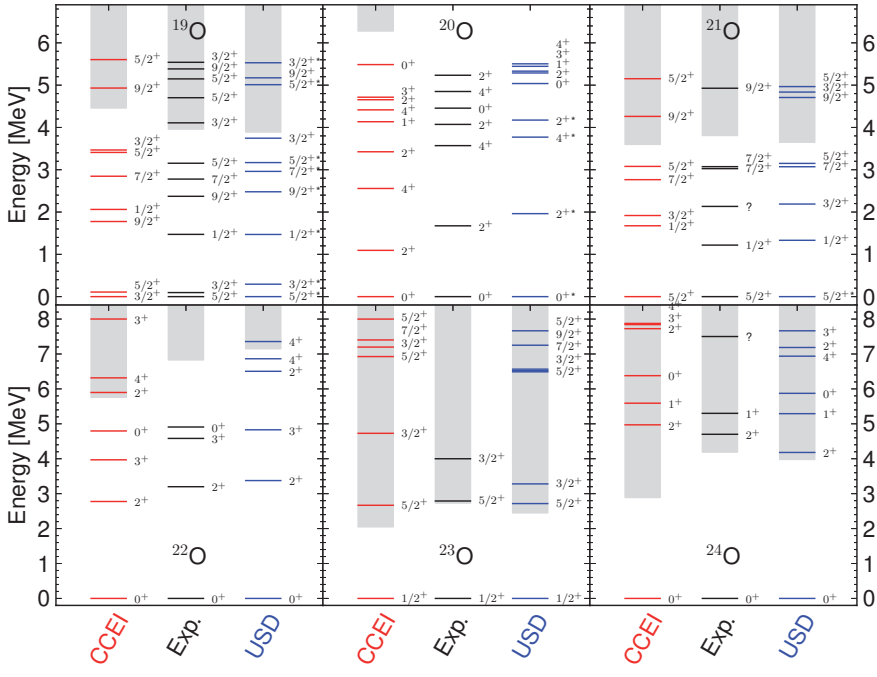

Figure 2 – Spectra of neutron-rich oxygen isotopes. The left column contains the results of *sd*-shell-model calculations with an effective Hamiltonian derived form ab initio chiral two- and three-body forces [8] and coupled-cluster calculations in ^{16,17,18}O. The middle column contains experimental data and the right column contains the predictions with the phenomenological USD interaction [12] that was fit to data in the same shell.

A similar program is being undertaken in the IMSRG; it has actually been taken a bit further. [7] The idea of that method is to write down flow equations for the unitary transformation that decouples the shell-model space from everything else, that is, to decouple the spaces incrementally. The flow equations are subject to truncation, like the operator in Eq. (4), but they are truncated at each step in the flow. The method takes advantage of normal ordering with respect to the decoupled space to minimize the effects of truncation.

Figure 3 compares the predictions of this approach, again with the chiral N^{3}LO interaction, for spectra of neon and magnesium isotopes with experimental data and with the predictions of a traditional phenomenological shell-model calculation. The leftmost column is the result of an incomplete IMSRG calculation that ignores chiral three-body interactions. The next column shows results with those interactions included; one can see that they are essential for a good description of the spectrum. Again, we see that with everything included the spectra are as good as that produced by our best phenomenology, here in nuclei with both valence protons and neutrons, including isotopes that exhibit collective rotation. (The two in the bottom panel have a characteristic $J(J+1)$ spectrum.)

5 Heavier Nuclei

For heavier complicated nuclei such as ^{130}Te or ^{150}Nd, fully ab initio calculations in the region are still a ways off. The main problem is the chiral-effective-theory Hamiltonian, which, for reasons that are not fully understood, tends to over-bind in nuclei with more than 100 nucleons.

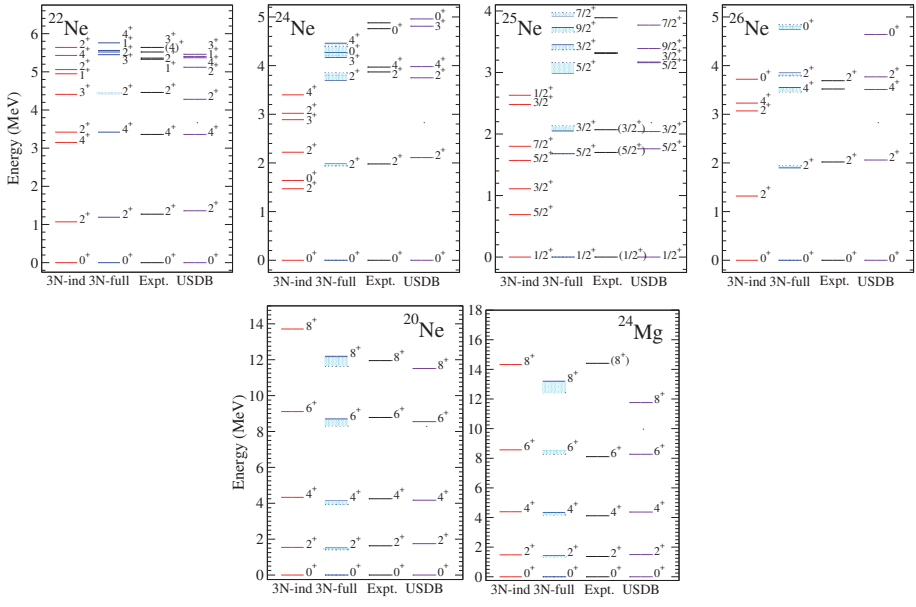

Figure 3 – Figure taken from Reference [7]. The top part shows spectra of neutron-rich neon isotopes. The leftmost column contains the results of *sd*-shell-model calculations with an effective Hamiltonian derived form ab initio chiral two-body forces [8] and IMSRG flow-equations. The next column to the left includes the chiral three-body interactions. The third column from the left contains contains experimental data and the rightmost column contains the predictions with the phenomenological USDB interaction [12] that was fit to data in the same shell. The bottom part shows the same for isotopes of Ne and Mg with collective spectra (containing a rotational band).

Thus the shell model and other phenomenological methods will still be important. Some of these models — the interacting boson model [13], the quasiparticle random phase approximation (see, e.g., Reference [14]), and the generator coordinate method [15,16] — emphasize collective degrees of freedom. To use these methods one must be convinced that collective degrees of freedom are the most important for double-beta decay. Is that really the case? Recent work [17] suggests that it is.

Figure 4 from that work shows the results of several calculations for the Gamow-Teller part of the double-beta matrix element in isotopes of titanium and chromium. ($N_{\rm parent}$ is the number of neutrons in the decaying nucleus.) Double-beta decay in these isotopes will never be observed, but one can calculate the matrix elements nonetheless. The figure shows the results of three calculations in a shell model space (the fp shell). The solid line connects results with the venerable KB3G shell-model effective interaction. The red dashed curve connects results generated by an approximate Hamiltonian $H_{\rm coll.}$ that includes only collective terms in the interaction. Here "collective" refers to a piece that generates deformation, one that generates superfluid correlations among like particles, and one that generates superfluid correlations between neutrons and protons. The rest of the shell-model Hamiltonian is discarded. The red and black line are nearly on top of one another, showing that in these isotopes, anyway, collective degrees of freedom are sufficient. The dashed blue curve connects results for which neutron-proton superfluid correlations have been omitted. One sees that such correlations are essential for a correct result. This fact often surprises nuclear-structure theorists because pairing between neutrons and protons typically manifests itself only delicately. When it comes to double-beta decay, however, that pairing is crucial.

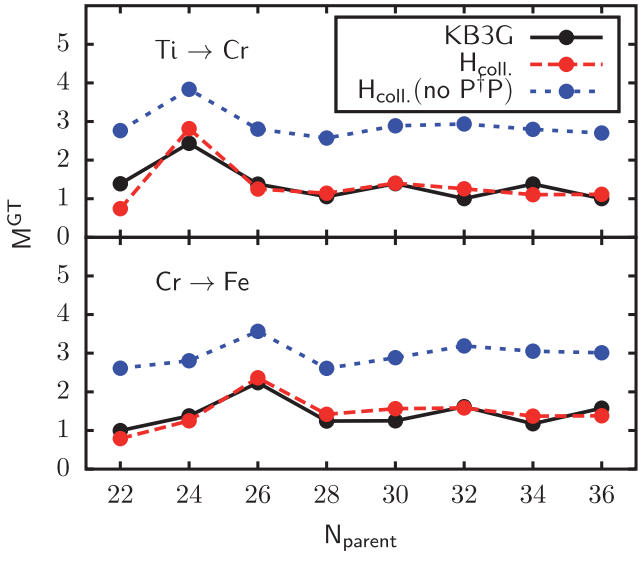

Figure 4 – Gamow-Teller part of the neutrinoless double-beta-decay matrix elements, M^{GT}, for the decay of Ti isotopes into Cr (top panel), and Cr isotopes into Fe (bottom), as a function of the neutron number $N_{\rm parent}$ of the initial nucleus. Results are shown for the KB3G interaction (black, solid line), the collective interaction $H_{\rm coll}$ (red, dashed line), and $H_{\rm coll}$ without the isoscalar (neutron-proton) pairing term (blue, short-dashed line).

The results of this work suggest that nuclear models that include only collective degrees of freedom can correctly predict double-beta decay rates. Such models have a long history in nuclear theory and are well understood. Typically they do not treat neutron-proton pairing explicitly, but they are capable of including it and work to make them do so is underway.[16]

I turn finally to the renormalization of the axial-vector coupling g_A. It has been know for some time (see, e.g., Reference [12]) that matrix elements for β and two-neutrino double-beta decay are smaller in reality than in our calculations. If neutrinoless matrix elements are as small compared to our calculations as two-neutrino matrix elements, experiments are in trouble. Fortunately, the issue can now be investigated systematically. There can only be two sources of the quenching: many-body weak currents, which would alter the predictions of calculations with the one-body Gamow-Teller operator, and model space truncation, i.e. the omission of important configurations. Work is now beginning to examine both these sources. The effects of many-body currents have traditionally been thought to be small[18], but the construction of those currents in chiral effective field theory — currents that should go along with the interactions used by ab initio calculations — may lead to larger effects [19,20]. Crucially, however, those effects should be smaller for neutrinoless decay than for two-neutrino decay. The issue should be cleared up by careful EFT parameter fits in the near future. The other source of quenching, model-space truncation, can be investigated in the ab initio shell-model calculations described earlier. Those implicitly include many configurations from outside shell-model spaces in the effective interactions and operators. We should soon be able to see whether neutrinoless decay is quenched, and if so, by how much.

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