Evaluation of the theoretical nuclear matrix elements for $\beta\beta$ decay of $^{76}$Ge

B. A. Brown,1 D. L. Fang,2 and M. Horoi3

1Department of Physics and Astronomy, National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan 48824-1321, USA
2College of Physics, Jilin University, Changchun 130012, China
3Department of Physics, Central Michigan University, Mount Pleasant, Michigan 48859, USA

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The nuclear matrix elements for two-neutrino double-β and zero-neutrino double-β decay of $^{76}$Ge are evaluated in terms of the configuration-interaction (CI), quasiparticle random-phase approximation (QRPA), and interacting boson methods. We point out deficiencies in all of these models and suggest ways that some of them can be corrected. The final results are obtained from the CI method corrected for configuration admixtures involving orbitals outside of the CI configuration space by using results from QRPA, many-body-perturbation theory, and the connections to related observables. The CI two-neutrino matrix element is reduced due to the inclusion of spin-orbit partners and to many-body correlations connected with Gamow-Teller $\beta$ decay. The CI zero-neutrino matrix element for the heavy neutrino is enhanced due to particle-particle correlations that are connected with the odd-even oscillations in the nuclear masses. The CI zero-neutrino matrix element for the light neutrino contains both types of correlations that approximately cancel each other. The uncertainty from short-range correlations is also considered.

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Many properties of the active neutrinos are measured, but it is not yet established whether they are Dirac- or Majorana-type particles and their absolute masses are not known. Left-right symmetric extensions to the standard model provide an explanation for the nonzero masses of the left-handed light neutrinos and predict the existence of right-handed heavy neutrinos [1]. Neutrinoless double-$\beta$ ($0\nu\beta\beta$) decay of nuclei provides unique information and constraints on these neutrino properties [2–6]. The $\beta\beta$-decay process and the associated nuclear matrix elements (NMEs) have been investigated by using several approaches including the quasiparticle random-phase approximation (QRPA) [4,7–29], the configuration-interaction (CI) model [30–38], the interfering boson model (IBM) [39–41], the generator coordinate method [42], and the projected Hartree-Fock-Bogoliubov model [43].

Assuming contributions from the light left-handed ($\nu$) neutrino-exchange mechanism and the heavy right-handed ($N$) neutrino-exchange mechanism, the decay rate of a neutrinoless double-$\beta$ decay process can be written as [4,36]

$$[T_{1/2}^{0\nu}]^{-1} = G^{0\nu}(|M^{0\nu}|^2|\eta|^2 + |M^{0\nu}|^2|\eta_N|^2),$$

(1)

where $G^{0\nu}$ is the phase-space factor [44,45], $M$ are the NMEs, and $\eta$ are combinations of the neutrino masses [4,36].

Since the experimental decay rate is proportional to the square of the calculated nuclear matrix elements, it is important to calculate these matrix elements with good accuracy to be able to determine the absolute scale of the neutrino masses. However, the theoretical methods used give results that differ from one another by factors of up to 2 to 3. It is important to understand the nuclear structure aspects of these matrix elements and why the models give differing results. This Rapid Communication is part of a larger theoretical effort to address the theory recommendations of the Report to the Nuclear Science Advisory Committee on neutrinoless double-$\beta$ decay [46].

From an experimental point of view $^{76}$Ge is one of the most investigated $\beta\beta$-decay candidates. The two modes of $\beta\beta$ decay are shown in Fig. 1. The experimental half-life for the standard $2\nu$ decay is $T_{1/2}^{2\nu} = 1.50(10) \times 10^{21}$ yr with a resulting NME of $M^{2\nu} = 0.140(5)$ MeV$^{-1}$ [47]. $^{76}$Ge is the only isotope for which an observational claim for neutrinoless double-$\beta$ decay has been made with $T_{1/2}^{0\nu} = 1.2 \times 10^{25}$ yr [48,49]. The Germanium Detector Array-II (GERDA-II) [50] and the Majorana demonstrator [51], the second generation of the germanium-based experiments, are in progress. The most sensitive limits on $0\nu\beta\beta$ decay half-lives obtained from germanium-based experiments are those of the Heidelberg-Moscow experiment [52], the international germanium experiment [53], and the GERDA-I experiment [54]. The combination with the results from these experiments yields $T_{1/2}^{0\nu} > 3 \times 10^{25}$ yr (90% confidence limit) [54].

In this Rapid Communication we discuss the NME for the $\beta\beta$ decay of $^{76}$Ge obtained with the CI, QRPA, and IBM-2 methods. We will show that all of these methods have deficiencies. Some of the deficiencies can be addressed with many-body perturbation theory (MBPT) approaches and connections to other observables.

The nuclear matrix elements can be presented as a sum of Gamow-Teller (GT) ($M_{GT}$), Fermi ($M_F$), and tensor ($M_T$) matrix elements (see, for example, Refs. [35,55],

$$M = M_{GT} - \left( \frac{g_V}{g_A} \right)^2 M_F + M_T,$$

(2)

where $g_V$ and $g_A$ are the vector and axial constants, correspondingly. We use $g_V = 1$ and $g_A = 1.27$. The $M_n$ are matrix elements of scalar two-body potentials. The Gamow-Teller has the form $V_{GT}(r, A, \mu) \sigma_z \gamma_1 \gamma_2$, and the Fermi has the form $V_F(r, A, \mu) \gamma_1 \gamma_2$, where $\gamma$ are the isospin lowering operators. The neutrino potentials depend on the relative distance among...
the two decaying nucleons $r$, the mass number $A$, and the closure energy $\mu$ [37]. The radial forms are given explicitly in Ref. [35]. For the heavy-neutrino exchange, the potential does not depend on $\mu$. For the light-neutrino matrix element the closure approximation is good to within 10% [38].

The operators for $M_{GT}$ are given to a good approximation by $f(r)\sigma_1\sigma_2\tau_1\tau_2$, where $f(r)^{2\nu} = 1$ (in closure), $f(r)^{0\nu} = a/r$, and $f(r)^{0N} = b/r$ where the constants $a$ and $b$ depend on $A$, $\mu$, and the short-range correlation (SRC). The results discussed below follow from the expansions of the many-body matrix elements for these three operators in terms of the particle-hole ($ph$) in $^{76}$As or particle-particle ($pp$) intermediate states in $^{74}$Ge [56].

The $2\nu$ tensor NME is zero, and the Fermi NME is zero since isospin is conserved. For $0\nu$ and $0N$ the Fermi and tensor parts are both relatively small, and we define a correction factor for these given by $R_{GT} = M/M_{GT}$, where $M$ contains all three terms of Eq. (2). The CI calculations give $R_{GT}^{0\nu} = 1.10(3)$. Larger values of 1.23 for QRPA [16] and 1.33 for IBM-2 [39] were obtained with the older calculations. But more recently, it was found that the $2\nu$ Fermi matrix element was not zero because isospin was being treated incorrectly in QRPA [25] and IBM-2 [41]. After this was corrected the new $M_{GT}^{2\nu}$ values are now zero in all methods. The new results for $R_{GT}^{2\nu}$ are 1.10 [25] and 1.19 [29] for QRPA and 1.04 [41] for IBM-2. Taking these results into account we adopt a correction factor from the tensor plus Fermi contributions of $R_{GT}^{0\nu} = 1.12(7)$. The ratio for the heavy neutrino is 1.20 for CI, 1.26 for QRPA [29], and 1.00 for IBM-2 [41]. The adopted correction factor is $R_{GT}^{0N} = 1.13(13)$.

In the following we first focus on results for $M_{GT}$. At the end, the total matrix element $M$ will be obtained from $M_{GT}$ via a product of correction factors $R$ given by $M = [M_{GT}](CI)[R_{1}][R_{3}][R_{GT}]$. $R_{GT}$ is defined above. We start with the use of SRCs [55] based on the charge dependent (CD)-Bonn potential [57]. At the end we will give a value and error for the correction to this $R_{1}$, based on a range of assumptions about the SRCs. $R_{1}$ represents the correction coming from a “vertical” expansion of the CI model space that includes the effect of orbitals below and above those in $jj44$. $R_{3}$ is the main focus of this paper.

The model space for CI and IBM-2 is $jj44$ that consists of the four valence orbitals $0f_{5/2}$, $1p_{3/2}$, $1p_{1/2}$, and $0g_{9/2}$ for protons and neutrons. The model spaces for QRPA are the 21 orbitals with oscillator quanta $N \leq 5$ where $N = 2n + \ell$ for protons and neutrons. The QRPA results are also given when the evaluations of the NME are restricted to $jj44$ and to $fpg$ ($jj44$ plus $0f_{7/2}$ and $0g_{9/2}$). In addition to our own CI calculations with the JUN45 [58] and jj4bpn [59] Hamiltonians, we will show results from the gcn28:50 Hamiltonian [60] for $2\nu$ [61], $0\nu$ [33], and $0N$ [62].

The method and parameters used for the QRPA calculations1 are similar to those used in Ref. [25]. For the particle-particle channel in order to restore the isospin symmetry, we follow the formalism introduced in Refs. [23,25] by separately fitting the $T = 0$ and $T = 1$ parts of the interaction. For the $T = 1$ part, $g_{pp}^{T=1} = 0.985$ is taken to give $M_{GT}^{pp} = 0$. For the $T = 0$ particle-particle channel, two parameter sets were used: (a) $g_{pp}^{T=0} = 0.673$ reproduces the experimental value for $M_{GT}^{2\nu}$, and (b) $g_{pp}^{T=0} = 0.643$ gives a value for $M_{GT}^{2\nu}$ that is a factor of $(1/0.75)^2$ larger than experiment, anticipating that there may be MBPT corrections beyond QRPA that could reduce the strength to low-lying states.

Results for the $2\nu\beta\beta$ NME are shown in Fig. 2. This NME is completely determined by $J^{pp}_N = 1^{+}$ intermediate states in $^{76}$As. In CI the summation over the intermediate including the energy denominator (Eq. (2) in Ref. [61]) is obtained with the strength-function method [63]. The IBM-2 result is not shown because it uses an approximation for the NME based on the closure result for the operator $\sigma_1\sigma_2\tau_1\tau_2$ together with average closure energies from other methods (Eq. (16) in Ref. [41]). Experiment is reduced by a factor of about 0.45 compared to CI. $R_{GT}^{2\nu} = M^{2\nu}/M^{2\nu}$(CI) denotes the correction beyond the $jj44$ model space due to a vertical expansion that includes correlations from orbitals below and above the $jj44$ model space. The QRPA results for $jj44$ and

1The single-particle energies are taken from a Woods-Saxon potential with Coulomb corrections. All of the residual interactions for QRPA are obtained from solutions of the Bruckner $G$ matrix based on the CD-Bonn one-boson exchange nucleon-nucleon potential. We solve the BCS equations with the CD-Bonn pairing interactions adjusted to give the experimental five-point mass pairing gap. The renormalization factors are $g_{ph}^{pp} = 0.858$ and $g_{ph}^{pp} = 0.978$ for $^{76}$Ge and $g_{ph}^{pp} = 0.894$ and $g_{ph}^{pp} = 1.008$ for $^{76}$Se. For the renormalization of the QRPA residual interactions, we use $g_{ph} = 1.0$ for the particle-hole channel.
intermediate states. To summarize, relative to CI in the NME due to the energy denominator in the summation over space together with 2p-2h admixtures are required for the 2 model space, reductions due to a spin-orbit complete model high excitation energy [72] that gets removed from the 2B(GT) strength is associated with a spreading of strength to order to conserve the Ikeda sum rule, the reduction in low-lying compared to the empirical interaction vertex have shown that the influence of mesonic-exchange currents is small [69,70]. These results are that the reduction in GT strength was due to the model-space wave functions. Earlier calculations claimed this reduction using MBPT in terms of 2p-2h admixtures into factor relative to QRPA [67] and the 3(\Delta 1) Ikeda sum rule [68]. Arima et al. [69] and Towner [70] have explained this reduction using MBPT in terms of 2p-2h admixtures into the model-space wave functions. Earlier calculations claimed that the reduction in GT strength was due to \Delta excitations [71] in the nucleus. However, calculations with a realistic \(N \Delta \pi\) interaction vertex have shown that the influence of \(\Delta\) (and other mesonic-exchange currents) is small [69,70]. These results are compared to the empirical sd results in Fig. 13 of Ref. [65]. In order to conserve the Ikeda sum rule, the reduction in low-lying B(GT) strength is associated with a spreading of strength to high excitation energy [72] that gets removed from the 2v NME due to the energy denominator in the summation over intermediate states. To summarize, relative to CI in the jj44 model space, reductions due to a spin-orbit complete model space together with 2p-2h admixtures are required for the 2v\(\beta\beta\) NME. The observed factor of \(R_V = 0.45\) is consistent with expectations.

The results for 0N (heavy neutrino) are shown in Fig. 3. In addition to our own QRPA results, we show the QRPA result from Ref. [29]. The \(J_{pp}\) intermediate states are dominated by the 0\(^+\) ground state of \(^{76}\)Ge (see Ref. [56] for details on the analysis). In QRPA the NME increases by a factor of \(R_V^{0N} = 1.9\) as the number of orbitals included in the sums increases from jj44 to full (21 orbitals). This is due to the strong pairing (particle-particle) part of the Hamiltonians and the resulting increase in the number of coherent pairs contributing to the 0N NME. The pairing also gives rise to the odd-even staggering of the nuclear binding energies quantified by the pairing energies \(D\) [73,74]. For the germanium isotopes the experimental pairing energies are a factor of 1.45 larger than that obtained with the first-order expectation value of the CD-Bonn Hamiltonian. Based on the average of this result and the increase observed in QRPA, we will use \(R_V^{0N} = 1.65(25)\).

The results for 0v\(\beta\beta\) (light neutrino) are shown in Fig. 4. The largest term in the 0v NME is from the \(J_{pp} = 0^+\) ground state of \(^{74}\)Ge [56]. In QRPA the NME is nearly constant as the number of orbitals included in the sums increase. Qualitatively this is due to a competition between the reduction from the particle-hole channel observed for 2v and the enhancement due to the particle-particle channel observed for 0v. The connection of the 0v matrix elements with pairing has been previously discussed [31]. The new point of our analysis is that the increase expected from pairing coming from MBPT beyond the jj44 model space is canceled by the reduction from the ph-type correlations.

Contributions from states with \(J_{pp} > 0\) cancel part of the NME from \(J_{pp} = 0^+\). Within jj44 the reduction is dominated by the \(J_{pp} = 2^+\) states [56]. For the 0v NME within jj44,

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FIG. 2. (Color online) Nuclear matrix elements for 2\(\nu\)\(\beta\beta\) decay of \(^{76}\)Ge. The top point in green is the experimental value [47]. The QRPA results are shown for \(g_{pp}^{R_{0^0}} = 0.673\) (red dots) and \(g_{pp}^{R_{0^0}} = 0.643\) (red crosses). The CI results are shown for the JUN45 (dot), jj44bpn (cross), and gcn28.50 (triangle) Hamiltonians.

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FIG. 3. (Color online) The 0N NME for heavy-neutrino decay of \(^{76}\)Ge. See caption for Fig. 2. The QRPA point with the triangle is from Ref. [29].

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FIG. 4. (Color online) The 0v NME for light-neutrino decay of \(^{76}\)Ge. See captions for Figs. 2 and 3.
one finds $R_{pp}^{0\nu} = (M_{GT}^{0\nu}/[M_{GT}^{0\nu}(J_{pp} = 0^+)]) = 0.53$ for CI [56], 0.90 for IBM-2 [39], and 0.72 for QRPA. The reason for these differences may be due to the truncation within $jj$ made by IBM-2 and QRPA. For the $0N$ NME this ratio is $R_{pp}^{0\nu}$ = 0.89 in CI [56]; the cancellation from higher $J_{pp}$ is much less, the result is dominated by the $J_{pp} = 0^+$ contribution, and its connection to pairing is discussed above. In the $jj$ model space the agreement between the $0N$ NME (Fig. 3) for CI, QRPA, and IBM-2 is much better than that for $0\nu$ (Fig. 4) since the cancellation from higher $J_{pp}$ terms is small.

Holt and Engel [75] considered the effect of 2p-2h admixtures beyond the $jj$ model space by treating the effective transition operator in MBPT. They found a 20% increase in the $0\nu$ NME this ratio (Fig. 4) for CI, QRPA, and IBM-2 is much better than that for $0\nu$ (Fig. 4) since the cancellation from higher $J_{pp}$ terms is small.

The results shown above are based on the CD-Bonn SRC. This is the weakest of several SRCS that have been used [55]. The strongest is the AV18 SRC, and the UCOM [76] SRC is about half way between. For our final result we use the average of CD-Bonn and AV18 with an error that encompasses both. The result is that the $0N$ NMEs are multiplied by $R_{S}^{0\nu} = 0.80(20)$ and the $0\nu$ NMEs are multiplied by $R_{S}^{0\nu} = 0.97(3)$, where $R_{S}$ is the SRC correction relative to the CD-Bonn starting point.

Finally, we combine all of the factors discussed above in the form $M = [M_{GT}(CI)[R_{V}][R_{S}][R_{GT}]]$. Based on the experimental value for $2\nu$ the NME is

$$M_{2\nu} = 0.140(5) = [0.31(3)][0.45][1][1].$$

The second term is the empirical correction for $R_{V}$ due to mixing beyond the $jj$ model space. The error in the CI NME reflects the spread obtained with the three different Hamiltonians used (Fig. 2). For $0N$, $M_{0N}^{0\nu} = [155(10)][1.65(25)][0.80(20)][1.13(13)] = 232(80),$$

where the CI value is from Fig. 3. The error for $0N$ is dominated by the SRC correction. Finally for $0\nu$,

$$M_{0\nu}^{0\nu} = [3.0(3)][1.2(2)][0.97(3)][1.12(7)] = 3.9(8),$$

where the CI value is from Fig. 4. The error for $0\nu$ is dominated by an estimated uncertainty of 20% in the correction beyond $jj$. Comparison to previous values must take into account the isospin correction for QRPA and IBM discussed above and the choice of SRC (in our $R_{S}$ factor). The range is from 2.8 for CI [33] to 4.7 for IBM-2 [41] and 5.3 for QRPA [29].

Our result is in between these, but it is not an average since we have made comments on the deficiencies of all of these models. Using Eq. (1) with the experimental limit of the half-life ($T_{1/2}^{0\nu} > 3 \times 10^{25}$ yr [54]) and the phase-space factor from Ref. [44], we obtain $|\eta_{\nu|M_{\nu}e^2 < 0.3$ eV.

Sometimes the $2\nu$ correction factor (0.45 in this case) is expressed in terms of an effective $g_{A}$ value ($g_{A}^{\nu} = 0.85$ in this case). Since the factor ($g_{A}^{\nu}$4 appears inside the phase-space factor of Eq. (1), one might think that the decay rate for $0\nu$ and $0N$ could be reduced by a factor of $|g_{A}^{\nu}|2^{1/2} = 0.20$ [41,77]. However, this $g_{A}^{\nu}$ is only for a specific operator associated with a specific observable ($2\nu\beta\beta$ decay) relative to a specific model (CI in $jj$). The operators involved in $0\nu$ and $0N$ decay are different (short ranged), and corrections beyond CI cannot be expressed in terms of an overall change in $g_{A}$. It is better to express the renormalizations in terms of factors, such as $R_{V}$, that are operator and model-space dependent.

The model-space truncation contributions to $R_{pp}$ should be understood. The error for the $R_{GT}$ correction could be reduced if reasons for the variations within the models is understood. The error for the $R_{V}$ correction could be reduced if the MBPT results, such as those in Ref. [75], should be expanded to include the renormalization of the separate effects in the ph and pp channels in order to compare to the results found previously relative to the $jj$ model space. This includes the reduction in Gamow-Teller $\beta$-decay strength [69,70] and the enhancements of the pairing strength seen in the $D$ values. The basic division between CI and its MBPT corrections from all other orbitals can be checked by no-core and $ab\ ini\ito$ CI in lighter nuclei where they are tractable. Other methods, such as in-medium similarity renormalization group [78] and coupled cluster [79], can be used in place of MBPT, and at this level the division between short-range renormalization $R_{S}$ and long-range renormalization $R_{T}$ might be merged. The CI results for the $A = 76$ region can be further checked against spectroscopic observables (occupation numbers are in good agreement with CI [33]) including two-nucleon transfer. Future results should be presented in terms of changes relative to the various contributions we have discussed, and evaluations for other cases of interest [46] should be performed.

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