Fast, efficient calculations of the two-body matrix elements of the transition operators for neutrinoless double-β decay

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We present a new, fast algorithm and computing code developed to efficiently calculate the two-body matrix elements (TBMEs) of the neutrinoless double-beta decay transition operator, which are necessary for the shell model calculation of the double-beta decay matrix elements in the closure approximation. The improvement consists of a rearrangement of the expression of the TBMEs that allows us to do the radial integrals analytically, and thus only the integration over the momentum remains to be performed numerically. This fast algorithm is an important step forward in investigating quenching effects of the transition operator by considering their evolution in increasingly larger shell model spaces.

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Neutrinoless double-beta ($0\nu\beta\beta$) decay is a beyond standard model (SM) process of major interest for understanding neutrino properties. Indeed, its discovery would decide if neutrinos are their own antiparticles [1], and would give a hint regarding the scale of their absolute masses. The present status of these investigations can be found in several more recent reviews [2–5], which also contain therein a comprehensive list of references in the domain. Of particular interest is the effective neutrino mass, a parameter entering the $0\nu\beta\beta$ decay half-lives, which depends on the neutrino masses, neutrino oscillating parameters, and Majorana phases. Thus, to extract information about neutrino properties one needs a precise computation of the nuclear matrix elements (NMEs) which also enter the half-lives formula. This problem still represents a challenge in the theoretical study of the $0\nu\beta\beta$ decay. Typical calculations of the NMEs are performed using a bare transition operator [5]. This is almost always the case even if one uses different approaches: proton-neutron quasiparticle random phase approximation (pnQRPA) [6–10], shell model (ShM) [11–14], interacting boson approximation (IBA) [15], projected Hartree-Fock Bogoliubov (PHFB) [16] and energy density functional (EDF) method [17], which are the most common methods of calculation of these matrix elements. This is equally true even if one uses an improved transition operator that considers higher order effects in the nucleon current (HOC) [18,19]. In principle the most reliable of these approaches to perform calculations for the NMEs (relevant for $0\nu\beta\beta$ decay) is the ShM, since it incorporates all types of correlations and uses effective nucleon-nucleon (NN) interactions which are checked with other spectroscopic calculations for nuclei from the same region. However, it has to face the problem of the large model spaces and the associated computational resources. Also, it is well known that in ShM calculations of the two-neutrino ($2\nu\beta\beta$) matrix elements the Gamow-Teller operator needs to be quenched, to better describe the experimental data for beta decays and charge-exchange reactions. Therefore, it is important to know if the $0\nu\beta\beta$ transition operator has to be effectively modified when used in relatively small model spaces. Work in this direction was recently reported in Ref. [20] where an effective operator was analyzed for the $0\nu\beta\beta$ decay of ^{82}Se in the $jj44$ model space consisting of the $f_{5/2}$, $p_{3/2}$, $p_{1/2}$, and $g_{9/2}$ orbitals. For these calculations up to eight major harmonic oscillator shells (MHOS) were used, which implies that one needs all two-body matrix elements of the $0\nu\beta\beta$ transition operator in these large spaces. In addition, there were recent proposals [21,22] to investigate the modifications of the transition operator in increasingly larger shell model spaces for a fictitious $0\nu\beta\beta$ decay of a p-shell nucleus. The calculations reported in Ref. [20] were performed using a bare operator without higher order contributions in the nucleon current. In these calculations the integral over momentum in the transition operator can be analytically done, which makes the calculation of its two-body matrix elements very fast. It is however known that the effect of the higher order contribution in the nucleon current is a reduction of the $0\nu\beta\beta$ matrix element by 20%–30%. This reduction could be further amplified by the equivalent effective operator. Therefore, it is important to investigate this effect, which would require knowledge of the two-body matrix elements of the bare transition operator in a large number of MHOS, e.g., 8 to 12. In our previous works [14,23], we started to develop an efficient nuclear ShM approach to accurately calculate the NMEs for both $2\nu\beta\beta$ and $0\nu\beta\beta$ decay modes. The approach used in Ref. [14] to calculate the TBMEs of the transition operator that includes higher order terms in the nucleon current needs to calculate two-dimensional integrals, on the relative momentum and the relative coordinate. This approach was sufficiently fast for calculating the two-body matrix elements in a single major

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shell, such as the pf shell. However, calculations of these two-body matrix elements in 8–12 major shells would be intractable with this approach.

In this paper we present a new, improved (fast, efficient) ShM code which reduces substantially the computing time of calculation of the TBMEs of the $0\nu\beta\beta$ decay transition operator, which are necessary to calculate the NMEs. To calculate the TBMEs, normally two-dimensional integrations need to be done, one in the coordinate space and one in momentum space. The main improvement in this code is a rearrangement of the expression of TBMEs that allows us to do the radial integrals (the integrals in coordinate space) analytically when harmonic oscillator (HO) single particle wave functions are used. Therefore, only the integration over the momentum remains to be performed numerically. We first compare our results for NMEs with other similar results from literature performed with both ShM and other methods. Then, we compare the CPU times of our code with the CPU times of our previous code [14], for the same calculations. We note that these times decrease significantly. We get an estimation of an average CPU time per TBME and note that the new code proves very promising for more elaborate calculations in many MHOS.

The $0\nu\beta\beta$ decay $(Z, A) \rightarrow (Z+2, A) + 2e^-$ requires that the neutrino and the antineutrino are identical and massive particles. Considering that this decay occurs only by exchange of light neutrinos between nucleons and in the presence of left-handed weak interactions, the lifetime can be expressed as

$$\left(T^{0\nu}_{1/2}\right)^{-1} = G^{0\nu}(E_0, Z) \mid M^{0\nu} \mid^2 \left(\frac{\langle m_\nu \rangle}{m_e}\right)^2. \tag{1}$$

$G^{0\nu}$ is the phase space factor depending on the energy decay E_0 and nuclear charge Z, and $\langle m_\nu \rangle$ is the effective neutrino mass parameter depending on the first row elements of the neutrino mixing matrix U_{ei}, Majorana phases $e^{i\alpha_i}$, and the absolute neutrino mass eigenstates m_i (see, e.g., Ref. [5]). The nuclear matrix elements are

$$M^{0\nu} = M^{0\nu}_{GT} - \left(\frac{g_V}{g_A}\right)^2 M^{0\nu}_F, \tag{2}$$

where $M^{0\nu}_{GT}$ and $M^{0\nu}_F$ are the Gamow-Teller (GT) and the Fermi (F) parts, respectively. Usually a tensor part appears as well, but the numerical calculations have shown that its contribution is small [14]; consequently, it will be neglected in the following. The matrix elements can be expressed as the sum of products of two-body transition densities (TBTD) and matrix elements for two-particle states (TBMEs),

$$M^{0\nu}_\alpha = \sum_{j_p j_{p'} j_n j_{n'} J_\pi} \mathrm{TBTD}(j_p j_{p'}, j_n j_{n'}; J_\pi) \times \langle j_p j_{p'}; J_\pi \| \tau_{-1}\tau_{-2} O^\alpha_{12} \| j_n j_{n'}; J_\pi \rangle, \tag{3}$$

The calculation of the matrix elements of the two-body transition operators O^α_{12} (α = GT, F) can be decomposed into products of reduced matrix elements within two subspaces spanned by the spin and relative wave functions of two-particle states [14]. The most difficult step in the computation of TBMEs is the radial part of these operators, which contains the neutrino potentials. Neutrino potentials depend weakly on the intermediate states, and are defined by integrals of momentum carried by the virtual neutrino exchanged between the two nucleons [19]:

$$H_\alpha(r) = \frac{2R}{\pi}\int_0^\infty j_0(qr)\frac{h_\alpha(q)}{\omega}\frac{1}{\omega + \langle E \rangle} q^2 dq \equiv \int_0^\infty j_0(qr) V_\alpha(q) q^2 dq, \tag{4}$$

where $R = 1.2A^{1/3}$ fm, $\omega = \sqrt{q^2 + m_\nu^2}$ is the neutrino energy, and $j_0(qr)$ is the spherical Bessel function. We use the closure approximation in our calculations, and $\langle E \rangle$ represents the average excitation energy of the states in the intermediate odd-odd nucleus that contribute to the decay. The expressions of h_α (α = F, GT) [19] are the same as in Eqs. (8) and (9) of Ref. [14], which include finite nucleon size (FNS) contributions and higher order terms in the nucleon currents (HOC).

To compute the radial matrix elements $\langle nl|H_\alpha|n'l'\rangle$ we use the (HO) wave functions $\psi_{nl}(r)$ (depending on the HO parameter ν) corrected by a factor $[1 + f(r)]$, which takes into account the short-range correlations (SRC) induced by the nuclear interaction,

$$f(r) = -ce^{-ar^2}(1 - br^2), \tag{5}$$

where a, b, and c are constants which have particular values in different parametrizations [19,24]. Including HOC and FNS effects, the radial matrix elements of the neutrino potentials become

$$\langle nl \mid H_\alpha(r) \mid n'l' \rangle = \int_0^\infty r^2 dr\, \psi_{nl}(r)\psi_{n'l'}(r)\,[1 + f(r)]^2 \times \int_0^\infty q^2 dq\, V_\alpha(q) j_0(qr)\,, \tag{6}$$

The calculation of the radial matrix elements (6) requires the numerical computation of two integrals, one over the coordinate space and the other over the momentum space:

$$\mathcal{I}_\alpha(\mu; m) = \int_0^\infty q^2 dq\, V_\alpha(q) \times \left(\frac{2}{\pi}\right)^{\frac{1}{2}} (2\nu)^{\frac{m+1}{2}} \int_0^\infty dr\, e^{-\mu r^2} r^m j_0(qr), \tag{7}$$

where $\mu = \nu$, $\nu + a$, $\nu + 2a$, and m is an integer. However, one can reduce the computation to only one integral by rearranging the expression of the radial integral in coordinate space as a sum of terms with the same power of r, and perform analytically this integral taking advantage of some mathematical recursion formulas:

$$\left(\frac{2}{\pi}\right)^{\frac{1}{2}} (2\nu)^{\frac{m+1}{2}} \int_0^\infty dr\, e^{-\mu r^2} r^m j_0(qr) = \left(\frac{2\nu}{2\mu}\right)^{\frac{m+1}{2}} (m-1)!! \sum_{k=0}^{\frac{m}{2}-1} (-1)^k \binom{\frac{m}{2}-1}{k} \times \frac{e^{-\frac{q^2}{4\mu}}}{(2k+1)!!(2\mu)^k} q^{2k}. \tag{8}$$

Similar approaches to calculate TBMEs were reported in Refs. [15,25,26].

Finally, the radial matrix element can be expressed as a sum of integrals over the momentum space:

$$\langle nl \mid H_\alpha(r) \mid n'l' \rangle = \sum_{s=0}^{n+n'} A_{l+l'+2s}(nl, n'l') \mathcal{K}_\alpha(m), \qquad (9)$$

where $A_{l+l'+2s}$ are coefficients independent of r:

$$A_{l+l'+2s}(nl, n'l') = \left[\frac{n!(2l+2n+1)!!}{2^n} \frac{n'!(2l'+2n'+1)!!}{2^{n'}} \right] \times (-1)^s \sum_k \frac{1}{k!(n-k)!(2l+2k+1)!!} \times \frac{1}{k'!(n'-k')!(2l'+2k'+1)!!}, \qquad (10)$$

with $\max(0, s-n') \leqslant k \leqslant \min(n, s), k+k' = s$. Here $\mathcal{K}_\alpha(m)$ is a sum of six $\mathcal{I}_\alpha(\mu; m)$ integrals over momentum,

$$\mathcal{K}_\alpha(m) = \frac{1}{\sqrt{2\nu}} \left[\mathcal{I}_\alpha(\nu; m) - 2c\mathcal{I}_\alpha(\nu+a; m) + 2c \left(\frac{b}{2\nu} \right) \mathcal{I}_\alpha(\nu+a; m+2) + c^2 \mathcal{I}_\alpha(\nu+2a; m) - 2c^2 \left(\frac{b}{2\nu} \right) \mathcal{I}_\alpha(\nu+2a; m+2) + c^2 \left(\frac{b}{2\nu} \right)^2 \mathcal{I}_\alpha(\nu+2a; m+4) \right], \qquad (11)$$

where a, b, and c are the parameters entering Eq. (5).

We developed a new code for computing the TBMEs necessary for the ShM calculations of the NME involved in $0\nu\beta\beta$ decays, based on the formalism described above. The new code has a flexible user interface, which allows the selection of various nuclear effects. In order to obtain the NMEs, the TBTD are calculated using the method described in Ref. [14]. For ^{48}Ca we used the GXPF1A [27] effective interaction in the full pf model space, and for ^{82}Se we used JUN-45 [28] effective interactions in the $jj44$ model space. Our code is also flexible for use with different SRC types such as Miller-Spencer [24] and the coupled cluster model (CCM) with Argonne V18 and CD-Bonn parametrizations [19]. A first step was to compare the results obtained with our code with results from the literature obtained with similar nuclear effects and parametrizations. As one can see from Table I, our results

TABLE I. Comparison between the results of the present work and other similar results from the references indicated. All calculations include FNS, HOC, and SRC of Jastrow type with Miller-Spencer parameters.

$M^{0\nu}$	^{48}Ca	^{82}Se
Present work	0.57	2.47
[14] (2010 ShM)	0.57	
[12] (2008 ISM)	0.59	2.11
[13] (2009 ISM)	0.61	2.18
[9] (2007 QRPA)		2.77

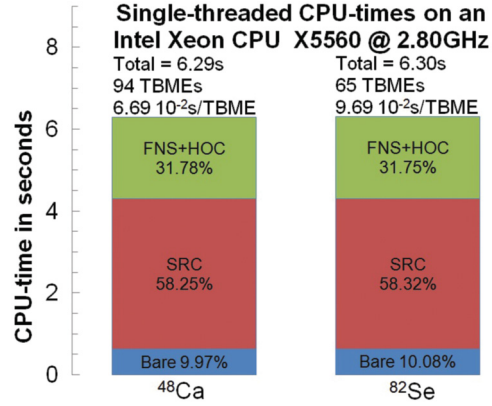

FIG. 1. (Color online) CPU times for the computation of the TBMEs.

are in good agreement with previous ones, provided that the same nuclear nuclear effects are included in the calculations.

We have also analyzed the performance of our code in getting improved computing speed. In Fig. 1 we show the single-core CPU times needed to compute the TBMEs.

In the case of ^{48}Ca, there are 94 TBMEs requiring a total of 6.29 s of CPU time on our test machine equipped with Intel Xeon X5560 CPUs. This translates into an average of 6.7×10^{-2} s for each individual TBME. When computing the product of wave functions, the dependence on the n and l quantum numbers of the nucleon orbits is reflected in the CPU times, as one can see in the difference between the average CPU time per TBME of ^{48}Ca and those of ^{82}Se. ^{82}Se has required a total of 6.30 s for the computation of its 65 TBMEs, thus needing an average time of 9.7×10^{-2} s for each TBME. Even then, we can still calculate TBMEs for ^{82}Se almost as fast as for the simpler case of the ^{48}Ca nucleus. Figure 1 also shows the contribution of the SRC and FNS + HOC effects to the total computation time for the TBMEs. "Bare" means that neither SRC nor FNS + HOC effects were considered. With our new method and code, we obtain an improvement in speed by a factor of about 30, as compared to the code used in Ref. [14], where more than 3 min were needed instead of 6.3 s. The performance of the new code makes us confident that it is now possible to rapidly, accurately, and efficiently compute TBMEs for many nuclear shells. This task is very challenging for the TBME code of Ref. [14]. For example, if one wants to investigate the effective transition operator in only eight MHOS [20], one needs to calculate about 434 000 TBMEs (GT plus F). The actual average time per TBME is about 1.7 s, but as remarked above, is increasing with the raise of the angular momenta of the single-particle orbits involved. Using a conservative estimate of about 10 s per TBME, one could conclude that one needs about 50 days of single-threaded processing power to calculate all necessary TBMEs. This time could be reduced by a factor of, say, 500 if the calculation of the TBMEs is distributed via a load-balancing algorithm [29], when using 1000 cores with 50% efficiency. However, this reduction might not be sufficient if nine or ten MHOS need to be used. The new algorithm presented here could be extremely useful in reducing the calculation time by another factor of about 30.

In summary, we developed a fast, efficient code for computing the TBMEs, which are part of the NMEs necessary for the analysis of the $0\nu\beta\beta$ decays. The improvement consists of a faster computation of the radial matrix elements using correlated HO wave functions. Their computation normally requires the numerical evaluation of two-dimensional integrals, one over the coordinate space and the other over the momentum space. By rearranging the expressions of the radial matrix elements, the radial integrals can be performed analytically over the coordinate space, thus the computation reduces to summing up a small number of integrals over momentum. We checked our code by comparing the values of the NMEs for ^{48}Ca and ^{82}Se calculated with our new code with similar results from literature, and we found a quite good agreement. Further, we estimated the CPU times for one single core needed to compute the TBMEs with our code and compare them with the similar CPU times obtained with our previous code requiring two-dimensional integrals. We find a significant reduction of the computational time, by a factor of about 30. We also estimated the average CPU time per single TBME in the cases ^{48}Ca and ^{82}Se and found very small values. This achievement makes us confident that it is now possible to rapidly, accurately, and efficiently compute TBMEs for many major harmonic oscillator shells, which were very time consuming in our earlier approach. The calculation of the TBMEs in eight MHOS could be done in about 1–2 days using the present single-threaded code. Extension to more than eight MHOS would require the parallelization of the code using a load-balancing algorithm. These TBMEs can be further used to investigate the effective transition operator needed for $0\nu\beta\beta$ decay analyses.

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