Neutrinoless double-$\beta$ decay of $^{124}$Sn, $^{130}$Te, and $^{136}$Xe in the Hamiltonian-based generator-coordinate method

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We present a generator-coordinate method for realistic shell-model Hamiltonians that closely approximates the full shell model calculations of the matrix elements for the neutrinoless double-beta decay of $^{124}$Sn, $^{130}$Te, and $^{136}$Xe. We treat axial quadrupole deformations and also triaxial quadrupole deformations, including the proton-neutron pairing amplitudes as generator coordinates. We validate this method by calculating and comparing spectroscopic quantities with the exact shell model results. A detailed analysis of the $0\nu\beta\beta$ decay nuclear matrix elements for $^{124}$Sn, $^{130}$Te, and $^{136}$Xe is presented. Our Hamiltonian-based generator-coordinate method produces $0\nu\beta\beta$ matrix elements much closer to the shell model ones, when compared to the existing energy density functional-based approaches. The remaining overestimation of $0\nu\beta\beta$ nuclear matrix element suggests that additional correlations may be needed to be taken into account for $^{124}$Sn, $^{130}$Te, and $^{136}$Xe when calculating with the Hamiltonian-based generator-coordinate method.

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I. INTRODUCTION

The possible detection of $0\nu\beta\beta$ decay is of great importance for unveiling the Majorana character of neutrinos, which would imply an extension to the standard model of electroweak interactions. Furthermore, if this transition is observed, the measurement of its decay rates can provide information about the absolute neutrino mass scale and mass hierarchy, but only if one can obtain accurate values of the underlying nuclear matrix elements (NMEs) governing the $0\nu\beta\beta$ decay [1]. At present, NMEs given by various nuclear models show significant uncertainties up to a factor of three [2, 3]. These large uncertainties preclude not only a definitive choice and amount of material that are required in expensive experiments, but also the inference of accurate values of absolute neutrino masses once a $0\nu\beta\beta$ decay rate is known [2]. Reducing the uncertainty in the matrix elements would be crucial for planning the expensive and complicated $\beta\beta$ experiments that draw near.

Several nuclear structure methods have been employed to calculate the $0\nu\beta\beta$ NMEs, including shell model (SM) [4, 5], interacting boson method (IBM) [9], quasi-particle random phase approximation (QRPA) [10, 11], and generator coordinate method (GCM) [13–16]. Both QRPA and GCM can incorporate energy density functional (EDF) theory [10, 14, 15]. The most obvious feature of EDF-based GCM calculations is that the $0\nu\beta\beta$ matrix elements are much larger than those of the SM. The overestimation could be the result of missing important high-seniority correlations in both the GCM ansatz and in the EDF itself [17]. Adding correlations in an EDF without having genuine operators to relate to, however, may lead to inconsistencies and unexpected results [18]. On the contrary, SM exactly diagonalizes an effective nuclear Hamiltonian ($H_{\text{eff}}$) in a valence space, which means that SM considers all possible correlations around the Fermi surface that can be induced by $H_{\text{eff}}$. However, this careful treatment of correlations restricts SM calculations to relatively small configuration spaces. Most SM calculations of $0\nu\beta\beta$ matrix elements are performed in a single harmonic oscillator shell, and hence may be unable to fully capture collective correlations [3].

One way to overcome some drawbacks of EDF-based GCM is to abandon the focus on functionals and return to Hamiltonians. Starting from an effective Hamiltonian allows us to include the important shell model correlations in a self-consistent way. In addition, an effective Hamiltonian is usually originated from a bare nucleon-nucleon interaction, and then adapted to a certain configuration space through many-body perturbation theory [19]. This means that the Hamiltonian-based GCM can be extended to larger valence space. The Hamiltonian-based GCM may thus be able to include both the important correlations of SM and large configuration spaces of EDF-based methods, without the drawbacks of either approaches.

An important question is which correlations are most relevant to $0\nu\beta\beta$ matrix elements, but are missing in the EDF-based GCM calculations. Both QRPA and SM calculations suggest that isoscalar pairing correlations quench the Gamow-Teller part of $0\nu\beta\beta$ matrix elements significantly [20, 22], while the implementation of isoscalar pairing for EDF has not yet been developed. Furthermore, although the axial deformation was taken as a generator coordinate in previous GCM works [13–15], the triaxial deformation that induces quadrupole correlations together with axial deformation is usually neglected in the study of NMEs. Recently, we developed a GCM code that works with realistic effective Hamiltonians, and we tested it onto the calculations of $0\nu\beta\beta$ NMEs for $^{48}$Ca and $^{76}$Ge within both a single shell and two major shells [24]. To fully address the effect of isoscalar $pn$ pairing and quadrupole correlations on $0\nu\beta\beta$ decay, we treat the isoscalar pairing amplitude, in addition to axial...
II. THE MODEL

In the closure approximation, we can write the $\nu\beta\beta$ decay matrix element in terms of the initial and final ground states, and a two-body transition operator. If the decay is produced by the exchange of a light-Majorana neutrino with the usual left-handed currents, the NME can be given by:

$$M^{0\nu} = M_{GT}^{0\nu} - \frac{g^2}{g_A^2} M_F^{0\nu} + M_T^{0\nu}$$

(1)

where $GT$, $F$, and $T$ refer to the Gamow-Teller, Fermi and tensor parts of the matrix elements. The vector and axial coupling constants are taken to be $g_V = 1$ and $g_A = 1.254$, respectively. We modify our wave functions at short distances with the “CD-Bonn” short-range correlation function [26]. A detailed definition of the form of the matrix element can be found in Ref. [27].

To compute the $0\nu\beta\beta$ matrix element in Eq. (1), one needs initial and final ground states $|I\rangle$ and $|F\rangle$, which can be provided by GCM. We use a shell model effective Hamiltonian ($H_{\text{eff}}$) in our approach. In a isospin scheme, its can be written as a sum of one- and two-body operators:

$$H_{\text{eff}} = \sum_a \epsilon_a \hat{n}_a + \sum_{a,b,c,d} \sum_{JT} V_{JT}(ab; cd) \hat{T}_{JT}(ab; cd),$$

(2)

where $\epsilon_a$ stands for single-particle energies, $V_{JT}(ab; cd)$ stands for two-body matrix elements (TBME’s), $\hat{n}_a$ is the number operator for the spherical orbit $a$ with quantum numbers $(n_a, l_a, j_a)$ and

$$\hat{T}_{JT}(ab; cd) = \sum_{MT_z} A_{JM_{TT_z}}^j(ab) A_{JM_{TT_z}}(cd)$$

(3)

is the scalar two-body density operator for nucleon pairs in orbits $a, b$ and $c, d$ coupled to the quantum numbers $J, M, T,$ and $T_z$.

The first step in the GCM procedure is to generate a set of reference states $|\Phi(q)\rangle$ that are quasiparticle vacua constrained to given expectation values $q_i = \langle O_i \rangle$ for a set of collective operators $O_i$. Here we take the operators $O_i$ to be:

$$O_1 = Q_{20}, \quad O_2 = Q_{22},$$

$$O_3 = \frac{1}{2} (P_0^t + P_0^t), \quad O_4 = \frac{1}{2} (S_0^t + S_0^t),$$

(4)

where

$$Q_{2M} = \sum_a r_a^{2} Y_{2M}^a,$$

$$P_0^t = \frac{1}{\sqrt{2}} \sum_l l^{|c_l^+ c_l^t|}_{000}^{L=0, J=1, T=0},$$

$$S_0^t = \frac{1}{\sqrt{2}} \sum_l l^{|c_l^+ c_l^t|}_{000}^{L=0, J=0, T=1},$$

(5)

with $M$ labeling the angular-momentum $z$-projection, $a$ labeling nucleons, and the brackets signifying the coupling of orbital angular momentum, spin, and isospin to various values, each of which has $z$-projection zero. In Eq. (5), the operator $c_l^+$ creates a particle in the single-particle level with an orbital angular momentum $l$, and $l \equiv 2l + 1$. The operator $P_0^t$ creates a correlated isovector pair and the operator $S_0^t$ a correlated isoscalar pair.

We include the effect of isoscalar pairing, we start from a Bogoliubov transformation that mixes neutrons and protons in the quasiparticle operators, i.e. (schematically),

$$\alpha^\dagger \sim u_p c_p^\dagger + v_p c_p + u_n c_n^\dagger + v_n c_n.$$

(6)

The actual equations in practical calculations sum over single-particle states in the valence space, so that each of the coefficients $u$’s and $v$’s in Eq. (6) would be replaced by matrices $U$ and $V$, as described in Ref. [28].

We further solve the constrained Hartree-Fock-Bogoliubov (HFB) equations for the Hamiltonian with linear constraints:

$$\langle H' \rangle = \langle H_{\text{eff}} \rangle - \lambda_Z (\langle N_Z \rangle - Z) - \lambda_N (\langle N_N \rangle - N) - \sum_i \lambda_i (\langle O_i \rangle - q_i),$$

(7)

where the $N_Z$ and $N_N$ are the proton and neutron number operators, and $\lambda_Z$ and $\lambda_N$ are corresponding Lagrange multipliers, the sum over $i$ includes up to three of the four $O_i$ in Eq. (1), and the other $\lambda_i$ are Lagrange multipliers that constrain the expectation values of those operators to $q_i$. We solve these equations many times, constraining each time to a different point on a mesh in the space of $q_i$.

Once we obtain a set of HFB vacua with various amounts of axial deformation, triaxial deformation, and
isoscalar pairing amplitude, the GCM state can be constructed by superposing the projected HFB vacua as:

$$|\Psi^J_{NZ\sigma}\rangle = \sum_{KK'} f^J_{q\sigma} |JK; NZ; q\rangle,$$

where $|JK; NZ; q\rangle \equiv \hat{P}^J_M \hat{P}^N \hat{P}^Z |\Phi(q)\rangle$. The $\hat{P}'s$ are projection operators that project HFB states onto well-defined angular momentum $J$ and its $z$-component $M$, neutron number $N$, and proton number $Z$. The weight functions $f^J_{q\sigma}$, where $\sigma$ is simply a enumeration index, can be obtained by solving the Hill-Wheeler equations \[29\].

$$\sum_{KK'} \left\{ \mathcal{H}^J_{KK'}(q;q') - E^J_{KK'} N^J_{KK'}(q;q') \right\} f^J_{q\sigma} = 0,$$

where the Hamiltonian kernel $\mathcal{H}^J_{KK'}(q;q')$ and the norm kernel $N^J_{KK'}(q;q')$ are given by:

$$\mathcal{H}^J_{KK'}(q;q') = \langle \Phi(q) | H_{\text{eff}} \hat{P}^J_M \hat{P}^N \hat{P}^Z | \Phi(q') \rangle,$$

$$N^J_{KK'}(q;q') = \langle \Phi(q) | \hat{P}^J_M \hat{P}^N \hat{P}^Z | \Phi(q') \rangle.$$

To solve Eq. (9), we diagonalize the norm kernel $N$ and use the nonzero eigenvalues and corresponding eigenvectors to construct a set of “natural states”. Then, the Hamiltonian is diagonalized in the space of these natural states to obtain the GCM states $|\Psi^J_{NZ\sigma}\rangle$ (see details in Refs. \[30\] \[31\]). With the lowest $J = 0$ GCM states as ground states of the initial and final nuclei, we can finally calculate the $0\nu\beta\beta$ decay matrix element $M^{0\nu}$ in Eq. (11).

III. CALCULATIONS AND DISCUSSIONS

We start by using our GCM employing an effective Hamiltonians in a model space that a SM calculation can be applied to. If the Hamiltonian-based GCM and the SM itself use the same Hamiltonian and the same valence space, the SM can thus be considered as the “exact” solution because it diagonalizes the Hamiltonian exactly. Therefore, comparing the results given by Hamiltonian-based GCM and SM indicates to what extent the GCM can capture the correlations relevant to $0\nu\beta\beta$ matrix elements.

For the calculations of the $0\nu\beta\beta$ decay NMEs of $^{124}\text{Sn}$, $^{124}\text{Te}$, $^{130}\text{Te}$, $^{130}\text{Xe}$, $^{136}\text{Xe}$, and $^{136}\text{Ba}$, we need a reliable effective Hamiltonian. Currently, the best option is using a fine-tuned effective Hamiltonian for the $jj55$-shell configuration space that compromises the $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, and $0h_{11/2}$ orbits. As a reference Hamiltonian, we use a recently proposed shell-model effective Hamiltonian called SVD Hamiltonian \[52\], which has been tested throughout the $jj55$ model space. This Hamiltonian accounts successfully for the spectroscopy, electromagnetic and Gamow-Teller transitions, and deformation of the initial and final nuclei that our calculations involve \[7\] \[8\]. Our complete calculations include both deformation parameters $q_1$ and $q_2$ (or equivalently deformation $\beta$ and $\gamma$) as generator coordinates, as well as one of the proton-neutron pairing parameters $q_3$ and $q_4$. The effect from triaxial shape fluctuations can be easily excluded by removing those triaxially deformed configurations from the set of reference states.
TABLE I: The g.s. energies (in MeV) obtained with SVD Hamiltonian by using GCM and SM for $^{124}$Sn, $^{124}$Te, $^{130}$Te, $^{130}$Xe, $^{136}$Xe, and $^{136}$Ba.

| Nuclei   | Axial GCM | Triaxial GCM | SM    |
|----------|-----------|--------------|-------|
| $^{124}$Sn | −15.659   | −15.686      | −16.052 |
| $^{124}$Te | −23.056   | −23.187      | −24.446 |
| $^{130}$Te | −25.646   | −25.711      | −26.039 |
| $^{130}$Xe | −32.510   | −32.619      | −33.313 |
| $^{136}$Xe | −34.896   | −34.921      | −34.971 |
| $^{136}$Ba | −40.282   | −40.362      | −40.745 |

A. Ground-State Energies and Spectra

The first study we perform with the Hamiltonian-based GCM is the comparison of the calculated ground-state (g.s.) energies and the low-lying spectra of $^{124}$Sn, $^{124}$Te, $^{130}$Te, $^{130}$Xe, $^{136}$Xe, and $^{136}$Ba with the SM calculations $^{[7]}$. Table I presents the g.s. energies obtained using the SVD Hamiltonian for both GCM approaches employed, with or without triaxially deformed configurations. These results are very close to the exact solutions given by SM, implying that our Hamiltonian-based GCM has captured a major part of important correlations in the ground states of these nuclei. Including triaxial deformation slightly improves the description of the g.s. energies, but the differences between results given by triaxial GCM and axial GCM are within 0.14 MeV. This is because these nuclei do not show evidence of triaxial deformation, neither theoretically nor experimentally, suggesting that the effect from including triaxially deformed configurations would not be remarkable.

Figure 1 shows the low-lying level spectra of these nuclei, compared to the SM calculations. Generally, the Hamiltonian-based GCM calculations are in reasonable agreement with the SM results, though our calculations tend to overestimate the energy levels given by SM. As a comparison, the EDF-based GCM gives much higher $2^+$ states for $^{124}$Sn, $^{124}$Te, $^{130}$Te, $^{130}$Xe, $^{136}$Xe, and $^{136}$Ba $^{[15]}$. The overestimation could be due to our GCM calculations, which exclude the multi-quasiparticle (or called broken-pair) excitation that breaks the time-reversal symmetry. The multi-quasiparticle excitations would lower the excited states significantly in these nearly spherical nuclei. The inclusion of non-collective configurations like multi-quasiparticle configurations would be important for a better description of the low-lying spectra of spherical and weakly-deformed nuclei. However, it is outside of scope of this work.

B. Occupation probabilities

It is known that the $0\nu\beta\beta$ NMEs are sensitive to the occupancies of valence neutron and proton orbits $^{[22]}$. To further verify how suitable the Hamiltonian-based GCM is in describing the nuclear structure and $0\nu\beta\beta$ decay aspects of the nuclei involved, we also calculate the neutron vacancies for $^{124}$Sn, $^{124}$Te, and $^{136}$Ba, as well as the proton occupancies for $^{124}$Te and $^{136}$Ba. Our results presented in Fig. 2 are compared to the SM calculations reported in Figs. 2-4 of Ref. $^{[7]}$ and Fig. 2 of Ref. $^{[8]}$. The occupation probabilities of the $1d_{5/2}$ and $1d_{3/2}$ orbitals are summed up and presented as $1d$, which is similar to the references used for comparison. The occupancies obtained with our GCM calculations are close to the values calculated by SM. The calculated occupancies, combined with the g.s. energies and level spectra mentioned above, leads us to consider that Hamiltonian-based GCM is suitable for the description of the relevant nuclear structure aspects for these initial and final nuclei involved in the $0\nu\beta\beta$ decay.

C. Analysis of the nuclear matrix elements for $^{124}$Sn, $^{130}$Te, and $^{136}$Xe

We calculate the matrix elements of $^{124}$Sn, $^{130}$Te, and $^{136}$Xe using our GCM approach. Recent interest in these
nuclei for $0\nu\beta\beta$-decay experiments [24, 25] presents a pressing need for accurate calculations of the $0\nu\beta\beta$ NMEs to guide the experimental effort.

Figure 3 illustrates the our calculated NMEs, compared to the values given by the SM and the EDF-based GCM employing non-relativistic Gogny D1S force and relativistic PC-PK1 force. It can be seen that previous GCM calculations produce NMEs which are about two times larger than the SM ones. In contrast, with our Hamiltonian-based GCM calculations we obtain the NMEs that are about only 40% larger than the SM results, significantly reducing the long-debated discrepancy between previous GCM and SM predictions.

To further understand this 40% overestimation given by our GCM calculations, the values for the $0\nu\beta\beta$ decay NMEs of $^{124}$Sn, $^{130}$Te, and $^{136}$Xe are listed in Table II, where we show the Gamow-Teller, the Fermi, and the tensor contributions. Generally, the Fermi and tensor parts of NMEs present good agreement between our GCM calculations and SM calculations, while the Gamow-Teller part of NMEs are noticeably larger in our GCM results, resulting in the 40% overestimation in the total $0\nu\beta\beta$ NMEs.

The analysis of the $0\nu\beta\beta$ NME is extended by looking...
at the decomposition of the NMEs over the angular momentum $I$ of the proton (or neutron) pairs (see Eq. (B4) in Ref. [34]), called $I$-pair decomposition. In this case, the NME can be written as $M_{\alpha} = \sum_I M_{\alpha}(I)$, where $M_{\alpha}(I)$ represent the contributions from each pair-spin $I$ to the $\alpha$ part of the NME. To analyse the deviation between the $M_{\alpha}^{\text{GT}}$, given by GCM and SM, Fig. 4 presents the $I$-pair decomposition for the Gamow-Teller part of our calculated $0\nu\beta\beta$ NMEs, compared to the one calculated by SM [2]. The bars in Figs. 4 can be added directly to get the Gamow-Teller part of NMEs. As we can see, the dramatic cancellation between the $I = 0$ and $I = 2$ contributions shown by the SM calculations is reproduced well by our GCM approach. However, SM calculations give more negative contributions with $I \geq 4$, which further reduce the Gamow-Teller NMEs. On the contrary, our GCM approach can barely produce any contributions with $I \geq 4$.

Figure 5 visualizes the differences in Gamow-Teller NMEs between our GCM and SM calculations against the pair-spin $I$, which can help us to identify where the differences mainly come from. If we only include the $I \leq 2$ contributions, the Gamow-Teller NMEs obtained by our GCM approach are close to the ones given by SM in all three nuclei involved. However, if the $I \leq 4$ contribution are taken into account, the differences are noticeably increased to about 0.5 for $^{124}\text{Sn}$ and $^{136}\text{Xe}$, and about 0.75 for $^{130}\text{Te}$. The inclusion of all possible pair-spin $I$ contributions would increase these differences even further. Apparently, the overestimation of Gamow-Teller NMEs is associated with those large-$I$-pair contributions, which may correspond to collective or non-collective correlations that are excluded from current GCM calculation.

Therefore, the deviation between our current Hamiltonian-based GCM and SM results may be related to the lack of some correlations which become important in $^{124}\text{Sn}$, $^{124}\text{Te}$, $^{130}\text{Te}$, $^{130}\text{Xe}$, $^{136}\text{Xe}$, and $^{136}\text{Ba}$. Since these nuclei are all near spherical or weakly deformed, one can expect the non-collective correlations, for example, quasiparticle excitations, may overcome the collective correlations. Currently, the reference states that the GCM method employs are HFB states imposed by the time-reversal symmetry, which exclude any multi-quasiparticle configurations. It would be of great interest if we could treat the quasi-particle excitation as an additional generator coordinate in the future. It could improve the description of $0\nu\beta\beta$ decay NME for these nuclei.

**IV. SUMMARY**

In this paper, we present a GCM calculation based on effective shell model Hamiltonians for the $0\nu\beta\beta$ decay NMEs of $^{124}\text{Sn}$, $^{130}\text{Te}$, and $^{136}\text{Xe}$ in the $jj55$ model space that compromises the $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, and $0h_{11/2}$ orbits. We use the SVD effective Hamiltonian that is fine-tuned with experimental data. To ensure the reliability of the results, we perform the Hamiltonian-based GCM calculations of the ground-state energies, low-lying level spectra, and occupancies of valence neutron and proton orbits. These are compared to the SM results obtained by exactly diagonalizing the same effective Hamiltonian. Our results are in reasonable agreement with the values obtained with the shell model. We also provide a detailed analysis of $0\nu\beta\beta$ decay NMEs for $^{124}\text{Sn}$, $^{130}\text{Te}$, and $^{136}\text{Xe}$. Our Hamiltonian-based GCM produces $0\nu\beta\beta$ decay NMEs that are about 40% larger than the ones obtained by SM, significantly reducing the large deviation between previous GCM and SM predictions. By checking the decomposition of the NMEs over the angular momentum $I$ of the proton or neutron pairs, we find that the remaining 40% overestimation of $0\nu\beta\beta$ decay NMEs may be associated with the exclusion of some non-collective correlations.

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