Neutrinoless double beta decay of calcium isotopes

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Abstract: In this work, we compare neutrinoless double beta decay ($0\nu\beta\beta$) nuclear matrix elements (NMEs) in calcium isotopes obtained with two different methods, the nuclear shell model (NSM) and the generator coordinate method (GCM). We describe the steps needed to proceed with the calculations, and give indications on how to select reliable results. Additionally, we estimate the error in the GCM results. The ^{56}Ca isotope shows the biggest NME discrepancy, when comparing GCM to NSM, with 34%. For ^{44}Ca and ^{52}Ca, there is only a 7% and 5% discrepancy, and a slightly larger one of 24% for ^{48}Ca.

I. INTRODUCTION

New generations of experiments are emerging in search of unobserved phenomena that could help us reformulate and extend established theories. An example is the effort in the observation of the neutrinoless double beta decay ($0\nu\beta\beta$), where the violation of leptonic number could give us a hint in the matter-antimatter imbalance, and the need for a reformulation of the standard model of particle physics. Additionally, the absence of neutrinos in the decay would establish the Majorana nature of neutrinos, being both its particle and anti-particle [1, 2].

The nuclear shell model (NSM) is one of the most successful models in nuclear physics. It is an exact method, because all the nucleus possible states are taken into account, with the nuclear wave function being a superposition of all these states. However, in the NSM, the number of states scales exponentially with the number of particles, and is computationally unfeasible for heavy nuclei [1]. This motivates the need for approximate many-body methods that do not require using all these different states and therefore require less computational power. Results differ significantly between these methods and this is a relevant problem in current research, making it difficult to study the $0\nu\beta\beta$ decay.

In this work, we compare the NSM and the generator coordinate method (GCM), which uses the Hartree-Fock-Bogoliubov (HFB) approximation in the calculation of the nuclear wave functions. The HFB is a generalization from the Hartree-Fock method that allows us to obtain similar wave functions to those constructed by the NSM, but only using one initial Slater determinant [3, 4].

In this work, we compute the $0\nu\beta\beta$ nuclear matrix elements (NMEs) of the calcium isotopic chain for both approaches. Additionally, we estimate the error in the GCM calculations for the NME, and give some suggestions for the improvement of our results based on our findings and the ones obtained in [5].

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II. THEORY AND METHODOLOGY

A. The neutrinoless double beta decay ($0\nu\beta\beta$)

When a nucleus decays, it goes from the initial state to a lower energy state. In our case, we study the $0\nu\beta\beta$. The nuclear half-life is

$$(T^{0\nu}_{1/2})^{-1} = G_{0\nu} \cdot |M_{0\nu}|^2 \cdot m_{\beta\beta}, \tag{1}$$

where $G_{0\nu}$ is the phase-space factor, $m_{\beta\beta}$ is the effective neutrino mass, and $M_{0\nu}$ is the NME [2]. While $G_{0\nu}$ is known, $m_{\beta\beta}$ is not, as it represents physics beyond the standard model of particle physics [1].

We calculate the NME between the ground-states of the initial and final nuclei. The NME is formed of three parts according to their spin structure: the Fermi (F), Gamow-Teller (GT) and Tensor (T) matrix elements,

$$M_{0\nu} = M^{GT}_{0\nu} - M^{F}_{0\nu} + M^{T}_{0\nu}. \tag{2}$$

B. Nuclear shell model

The NSM is based on the empirical nuclear mean field approximation that reproduces magic numbers, using the

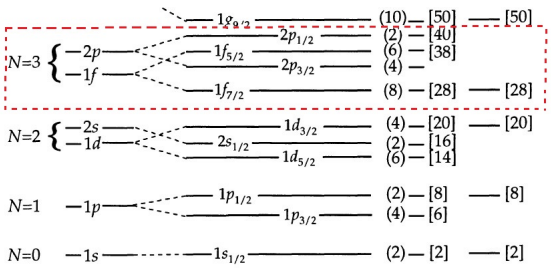

FIG. 1: **NSM single-particle orbitals [6]**. On the left side, levels given by the harmonic oscillator potential. On the right side, orbital-splitting due to the spin-orbit coupling, which leads to the magic numbers (numbers in parenthesis on right extreme).

surface corrected harmonic oscillator with spin-orbit coupling [6]:

$$U(r) = \frac{1}{2}m\omega^2 r^2 + D\mathbf{l}^2 - C\mathbf{ls}, \tag{3}$$

where m is the mass, $\mathbf{r}$ the position, $\mathbf{l}$ the angular momentum, $\mathbf{s}$ the spin, $\boldsymbol{\omega}$ the harmonic oscillator frequency and C and D are constant coefficients [6].

In the NSM, only a few nucleons, in a restricted number of states, are able to determine the properties of the nucleus. For example, in Fig.1, the orbitals inside the box define the calcium and titanium valence space, which is the pf shell for both neutrons and protons, and is composed of the $1f_{7/2}, 1f_{5/2}, 2p_{3/2}$, and $2p_{1/2}$ orbitals. As a result, the NSM Hilbert space is divided in three parts: the inert core (fully occupied orbits), the valence space (available orbits that can be occupied by the nucleons), and the external space (remaining empty orbits) [7].

Once the relevant levels for the valence space are selected, the NSM wave function is computed using an effective Hamiltonian,

$$H_{eff} = \sum_{ij} t_{ij} a_i^\dagger a_j + \frac{1}{2}\sum_{ijkl} v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k. \tag{4}$$

The Hamiltonian is diagonalized in the basis of many-body Slater determinants that can be built from the available single-particle states in the valence space. The nuclear wave function $|\Phi\rangle_{NSM}$ is a superposition of Slater determinants,

$$|\Phi\rangle_{NSM} = \sum_\alpha c_\alpha |\phi_\alpha\rangle, \quad |\phi_\alpha\rangle = \prod_i^N a_i^\dagger |0\rangle, \tag{5}$$

where $|\phi\rangle_\alpha$ are the Slater determinants, $|0\rangle$ is the particle vacuum, and $a_i^\dagger$ is the single-particle creation operator in the i state [7]. The number of Slater determinants needed in the calculation depends on the valence space and the nucleus.

The NME is then computed using the $0\nu\beta\beta$ operator $O^{0\nu}$ and the nuclear wave functions of the initial $|\Phi_i\rangle$ and final $|\Phi_f\rangle$ states,

$$M^{0\nu}_{NSM} = \langle\Phi_f| O^{0\nu} |\Phi_i\rangle_{NSM}. \tag{6}$$

We use the Nathan code for the NSM calculations [7]. Nathan has a computational limit of 10^{10} Slater determinants in the construction of the wave function. In cases like ^{124}Xe, this value is 10^{12}, and approximated many-body methods such as GCM are needed.

C. Generator coordinate method

For our GCM calculations, the starting point are the HFB states, which are a generalization of the Hartree-Fock states. Hartree-Fock is a mean-field method, where all the individual interactions between nucleons are reduced to an effective mean-field interaction. The variational principle is used to minimize the wave function energy and to determine the Hartree-Fock equations, which give us the system's ground-state.

1. Hartree-Fock-Bogoliubov

In order to generalize the Hartree-Fock scheme, we introduce the Bogoliubov transformation, which goes from the single-particle basis to the quasi-particle basis. The transformation is defined by the operators,

$$b_k^\dagger = \sum_i \left(U_{ik} a_i^\dagger + V_{ik} a_i\right), \quad b_k = \left(b_k^\dagger\right)^\dagger \tag{7}$$

where U_{ij} and V_{ij} are the mixing matrices that give us the quasi-particle states [8]. This transformation breaks the number of particles in the quasi-particle states, as a result of the particle-hole mixing, and, additionally, any other symmetries that we mix [6]. In our case, we do angular momentum mixing.

We find the HFB quasi-particle states with the variational principle applied to U_{ij} and V_{ij} matrices, using a trial wave function and a Hamiltonian with certain constraints,

$$H = H_{eff} - \lambda_Z Z - \lambda_N N - \sum_k \lambda_k Q_k, \tag{8}$$

where λ are Lagrange multipliers, Z the number of protons operator, N the number of neutrons operator and Q_k the coordinate operators.

2. The GCM state

The GCM wave function of our nucleus is a superposition of a set of HFB states $|\phi(\boldsymbol{\theta})\rangle$ projected to good quantum numbers,

$$|\Phi^{NZJ}\rangle_{GCM} = \sum_{\boldsymbol{\theta}} c^{NZJ}_{\boldsymbol{\theta}} P^N P^Z P^J |\phi(\boldsymbol{\theta})\rangle_{HFB}, \tag{9}$$

where J is the angular momentum, P are the projection operators, and c^{NZJ} are the coefficients that weight the projected HFB states.

$\boldsymbol{\theta}$ are the coordinates of the method, which give a fixed value to the coordinate operators Q_k. In our case, we use the deformation parameters β and γ as our generator coordinates, which are related to the quadrupole operators. The quadrupole describes the nucleus deformation, for it is a measure of the charge distribution and its deviation from the spherical form [6].

Projection is needed to restore the broken symmetries in the construction of the HFB states, resulting in the quantum numbers of the GCM state being well-defined. In order to find the c^{NZJ} coefficients, we need to solve

the Hill-Wheeler-Griffin equation (HWG),

$$\sum_{\boldsymbol{\theta}'} \left(\mathcal{H}^{NZJ}_{\boldsymbol{\theta}\boldsymbol{\theta}'} - E^{NZJ}\mathcal{N}^{NZJ}_{\boldsymbol{\theta}\boldsymbol{\theta}'}\right) c^{NZJ}_{\boldsymbol{\theta}'} = 0, \tag{10}$$

where $\mathcal{H}$ and $\mathcal{N}$ are the Hamiltonian and overlap kernels respectively,

$$\mathcal{H}^{NZJ}_{\boldsymbol{\theta}\boldsymbol{\theta}'} = \langle NZJ, \boldsymbol{\theta}| \, H_{eff} \, |NZJ, \boldsymbol{\theta}'\rangle \,, \tag{11}$$

$$\mathcal{N}^{NZJ}_{\boldsymbol{\theta}\boldsymbol{\theta}'} = \langle NZJ, \boldsymbol{\theta}|NZJ, \boldsymbol{\theta}'\rangle \,, \tag{12}$$

that we obtain with the HFB states for each (β,γ) deformation, and E^{NZJ} is the energy of the nucleus. To solve the equation, we diagonalize the overlap matrix, which is semi-positive defined, to obtain an orthonormal basis (natural basis) [4]. We diagonalize then the Hamiltonian in this basis to obtain the ground-state energy of the nucleus. The second process can lead to numerical divergence, because some states in the natural basis might be linearly dependent to each other. We solve this with a truncation of the natural basis, selecting only those eigenvalues in the overlap matrix bigger than a certain cutoff (typically 10^{-10}) [3].

III. RESULTS AND ANALYSIS

A. Nuclear shell model results

The NSM $0\nu\beta\beta$ NMEs are presented in Table I. For half-filled valence spaces, D# takes its biggest value, as the number of possible many-body states is maximal.

Table I indicates that ^{42}Ca isotope has the largest NME. This is so because the initial state (^{42}Ca) and the final state (^{42}Ti) are mirror nuclei, resulting in a favorable transition. On the other hand, the ^{60}Ca decay has the lowest NME value. This is because this isotope has a full valence space for neutrons and is magic for protons. The ^{60}Ca is very stable as a result.

TABLE I: Ground-state energy, number of Slater determinants ($D\#$) forming the nuclear wave functions and NMEs for calcium and isotopic chain using NSM. A is the number of nucleons of the calcium and titanium isotopes.

A	Ca		Ti		$M^{GT}_{0\nu}$	$M^{F}_{0\nu}$	$M^{T}_{0\nu}$	$M_{0\nu}$
	E(MeV)	$D\#$	E(MeV)	D#				
42	-2.69	4	-2.69	4	4.76	-1.43	-0.11	6.08
44	-4.96	28	-13.79	158	1.69	-0.22	-0.07	1.83
46	-6.66	137	-19.96	2343	1.19	-0.19	-0.07	1.30
48	-7.75	347	-24.23	14177	0.91	-0.15	-0.06	1.01
50	-2.85	468	-27.16	39899	1.04	-0.16	0.003	1.19
52	3.46	347	-25.03	55944	0.82	-0.12	-0.002	0.94
54	14.04	137	-20.60	39899	1.20	-0.14	0.03	1.34
56	26.17	28	-13.54	14177	1.20	-0.14	0.03	1.36
58	39.62	4	-4.22	2343	0.83	-0.13	0.06	1.03
60	54.29	1	-6.69	158	0.61	-0.11	0.06	0.78

B. Generator coordinate method results

With the GCM, we study the $0\nu\beta\beta$ decay of ^{44,48,52,56}Ca using the Fortran code Taurus [9].

1. *Hartree-Fock-Bogoliubov functions*

Fig.2 shows the nuclear energy surfaces as a function of the deformation (coordinates γ and β used in the HFB states), for ^{48}Ca as an example. The energy is minimal in the spherical region, both for the unprojected and projected HFB states. Fig.2 shows the effect of the projection to good quantum numbers in the GCM state (9). The energies are lowered, making the state's energy deeper. The position of the absolute minimum might change slightly in the projection, but always keeping the original form (oblate, prolate or spherical), where prolate corresponds to a bean shape and oblate to a lentil shape. All calcium isotopes show a minimum in the spherical region and titanium isotopes in the prolate region.

2. *Energy and NME convergence*

We study the energy convergence resulting from the second diagonalization in (10) to determine the ground-state energy of the nucleus. The top panels of Fig.3 show the convergence as a function of the number of states of the natural basis for ^{48}Ca and ^{48}Ti. The GCM energy must be higher than the NSM one, because the energy given by the variational principle is always higher than the exact value [6]. For this purpose, Fig.3 shows the NSM exact value as well.

In the determination of the ground-state energy of a nucleus, we only need to take one natural basis into account. However, $0\nu\beta\beta$ transitions involve two nuclei, and therefore two natural bases. This results in a difficulty when choosing the natural basis, because the basis affects differently the energy and the NME. We prioritize the convergence of the NME over the energy convergence, since the former is our target of study. This means that, in some cases, the ground-state energy could be lowered and closer to the NSM value, but we choose a smaller natural basis because the NME already diverges. In the study of the NME convergence, we use the GT element, for it is the biggest of the three parts (2) (Table II).

Fig.3 is an example of how we check the convergence of the energy and NME for each transition. We find where the NME element is more stable when changing the number of states in the natural bases of the initial (Ca) and final state (Ti). In Fig.3 c), when changing the number of states in the ^{48}Ca natural basis, with the ^{48}Ti

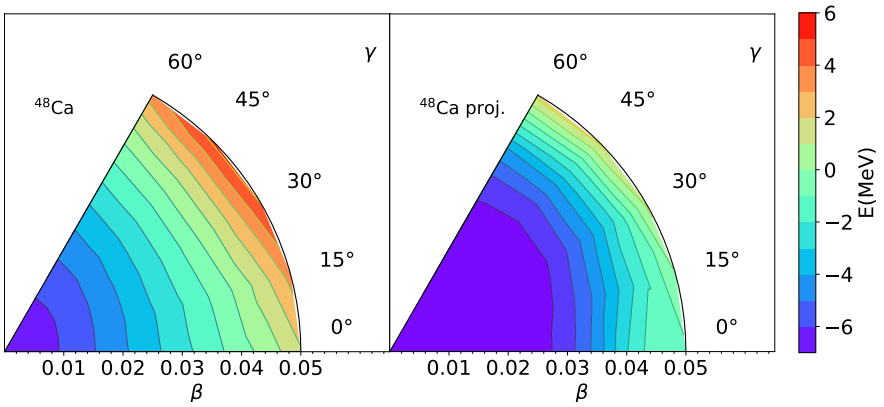

FIG. 2: **Energy surface for the HFB states of ^{48}Ca**. The nucleus shows a spherical shape with minimum energy at $\beta = 0$. Left panel: unprojected HFB states. Right panel: projected HFB states to good quantum numbers for J, N and Z.

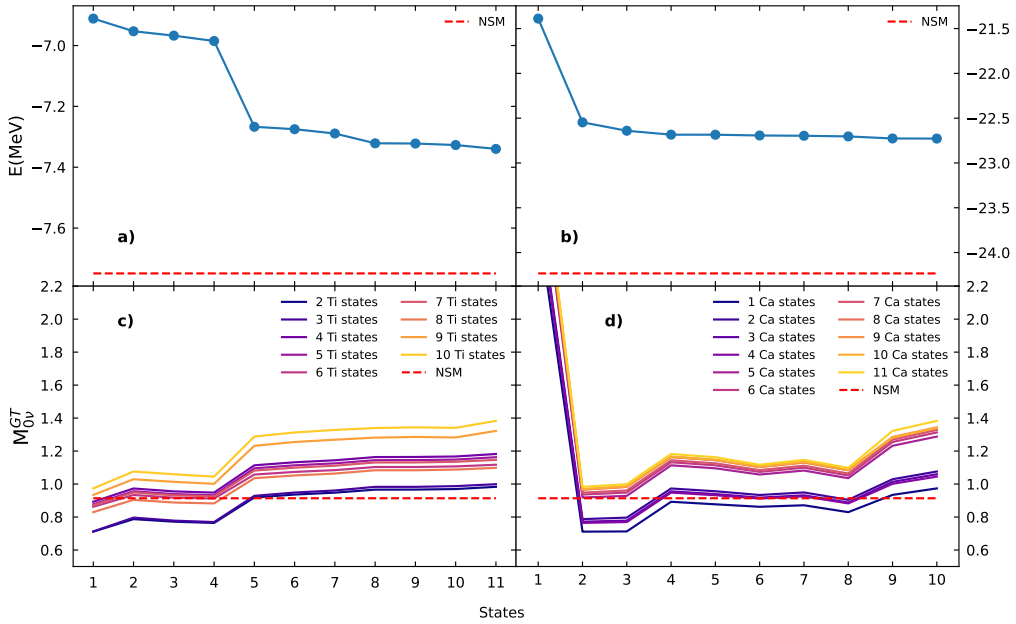

FIG. 3: **Ground-state energy and $0\nu\beta\beta$ decay Gamow-Teller matrix element convergence for ^{48}Ca** . Top panels correspond to the energy convergence and the bottom panels to the GT element convergence. a): ^{48}Ca ground-state energy convergence. b): ^{48}Ti ground-state energy convergence. c): the number of states in the Ti natural basis is fixed and the number of states in the Ca natural basis is varied. d): the number of Ti states in the natural basis is varied. The red dashed-lines show NSM exact values both for the ground-state energy and the NME.

natural basis fixed, the NME is quite stable between 5 and 10 states (plateau of 6 states). On the other hand, when changing the number of states in the ^{48}Ti natural basis, with number of states in the ^{48}Ca basis fixed (panel 3 d)), there is stability between 4 and 8 states. Panel 3 d) shows that the values that are closer to each other in the y-axis are those with the number of Ca states fixed between 5 and 10. These are precisely the number of states in the Ca natural basis that give us stability in panel 3 c), so panels 3 c) and 3 d) are easily related to each other. Lastly, we check that the energy is converged in the selected region and that its value is higher than the NSM one. Ground-state energies are usually between 1 and 2 MeV higher in the GCM calculation of the final state. On the other hand, the energy of the initial state is much closer to the NSM value (panels 3 a) and 3 b)).

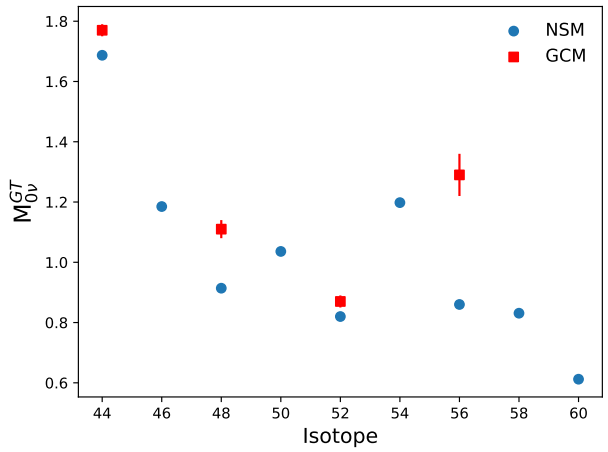

FIG. 4: **Gamow-Teller NME for Ca isotopes**. Comparison of NSM and GCM results. The GCM results are presented with error bars given by the standard deviation.

TABLE II: NME mean value for each computed isotope. Each result is presented with its standard deviation. A is the number of nucleons of the calcium and titanium isotopes.

A	$M^{GT}_{0\nu}$	$M^{F}_{0\nu}$	$M^{T}_{0\nu}$	$M_{0\nu}$
44	1.77±0.02	-0.280±0.007	-0.082±0.001	1.97±0.03
48	1.11±0.03	-0.277±0.011	-0.053±0.003	1.33±0.04
52	0.87±0.02	-0.141±0.003	-0.012±0.001	0.99±0.02
56	1.36±0.07	-0.135±0.009	0.079±0.004	1.57±0.08

Panels 3 c) and 3 d) show the typical behavior for the NME convergence. When changing the number of Ca states, firstly we have oscillations for few states and a big plateau for a bigger number of states until there is divergence to bigger values. On the other hand, when changing the number of Ti states, the plateaus of stability are shorter and there are some oscillations. The NME presents more stability to changes in the natural basis of the initial state, rather than changes in the final state basis.

We follow this same procedure for other three isotopes, ^{44,52,56}Ca. We calculate the NME for each decay in the stability region, as the average value of the considered plateaus, and give an error to our calculations with the standard deviation. Table II summarizes the GCM NMEs we have found. Fig.4 compares the NSM and GCM results for the NMEs of ^{44,48,52,56}Ca. The GCM is pretty close to the NSM values for ^{44}Ca, ^{48}Ca and ^{52}Ca isotopes, but not so much in the ^{56}Ca decay. Table II indicates that the error in ^{56}Ca calculation is larger, because we choose two different plateaus of stability in this case, and only one for the other isotopes. We choose these two plateaus because both have a three-state extension and show equally good stability, so it is not possible to choose between them. The NME discrepancies between NSM and GCM in ^{44}Ca, ^{48}Ca, ^{52}Ca and ^{56}Ca are 7%, 24%, 5% and 34%, respectively.

IV. CONCLUSIONS

We have shown that the GCM can approximately reproduce some NSM $0\nu\beta\beta$ NME results, but that some improvements are needed. The ground-state energies are closer to the NSM ones for the initial state and between 1 and 2 MeV higher for the final state.

For the NME we have also always obtained bigger values with the GCM. Our best result was the NME for the ^{44}Ca and ^{52}Ca isotopes. These have a similar situation in the final state. ^{44}Ti has 2 neutrons and 2 protons in partially filled shells. ^{52}Ti has a full $1f_{7/2}$, two neutrons in the $2p_{3/2}$ and two protons in the $1f_{7/2}$ shell. Partially filled shells have two nucleons in both cases.

Still, the ^{48}Ca and ^{56}Ca isotopes NME calculation needs improvement. Pairing correlations could be used in the determination of the HFB states. In [5] it is shown that isoscalar-pairing correlation improves the NME values calculated with GCM, getting them closer to the NSM ones. This addition would considerably increase the complexity of the GCM calculations of the corresponding symmetry-projected Hamiltonian and overlap kernels.

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