Generator Coordinate Method framework for Double Beta Decay

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Abstract. We propose a consistent prescription for the derivation of the particle number and angular momentum projected QRPA (PQRPA) equation in the Generator Coordinate Method (GCM) framework for calculation of NME’s of double-beta decay of axially deformed nuclei. We derive closed formulae for the calculation of excitation energies and wave functions of the intermediate nucleus.

PACS numbers: 23.40.Bw, 21.60.Cs, 23.40.Hc, 14.60.Pq

Submitted to: Phys. Scr.

1. Introduction

Neutrinoless double beta decay $0\nu\beta\beta$, if observed experimentally, would provide unique information on the neutrino properties \cite{1,2,3}. The $0\nu\beta\beta$ decay process and the associated nuclear matrix elements (NME), necessary to extract these properties from experimental data, were investigated up to now using several approaches, including the quasiparticle random phase approximation (QRPA) \cite{1}, the interacting shell model \cite{4,5}, the interacting boson model \cite{6,7}, and the projected Hartree-Fock Bogoliubov model \cite{8}. Although the Generator Coordinate Method (GCM) has been applied previously in the context of double beta decay \cite{9}, it has been used solely over PHFB calculations to account for configuration mixing effects. In the present work we propose the GCM framework to deliver consistent number- and angular momentum projected QRPA (PQRPA) approach for calculation of NME’s of double-beta decay of axially deformed nuclei.
2. Projection method

Nuclear states with well-defined angular momentum quantum numbers in the laboratory frame can be constructed by projecting the corresponding components of the nuclear states, defined in the intrinsic frame of the nucleus [11]:

$$P_{JM} = \frac{2J+1}{8\pi^2} \int d\Omega D_{JM}^{*} R(\Omega),$$

(1)

where $R(\Omega) = e^{-i\alpha J_3} e^{-i\beta J_2} e^{-i\gamma J_3}$ is the rotation operator and $\Omega$ represents Euler angles $\alpha$, $\beta$ and $\gamma$ ($d\Omega = d\alpha d\gamma d\beta$).

In the case of axial symmetry of the nucleus, this operator reduces to the form:

$$P_{JM} = (J + \frac{1}{2}) \int_0^\pi d\beta \sin \beta d_d^J \langle \beta \rangle R(\beta),$$

(2)

with $R(\beta) = e^{-i\beta J_2}$, where $d_d^J(\beta)$ are the so-called "small" (reduced) real-valued Wigner matrices. The particle number projector for protons and neutrons can be expressed in the similar form:

$$P_{Z,N} = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\zeta \int_0^{2\pi} d\eta e^{i(\zeta Z_0 + \eta N_0)} R_Z(\zeta) R_N(\eta),$$

(3)

where $R_Z(\zeta) = e^{-i\zeta Z}$ and $R_N(\eta) = e^{-i\eta N}$. From now on we will use the shorthand notation $R = R(\beta) R_Z(\zeta) R_N(\eta)$ and $P = P_{JM} P_{Z,N}$.

To obtain the excited states in the intermediate nucleus we need to construct the charge-changing operator, that creates a pair of quasi-nucleons. Because for a deformed nucleus with axial symmetry, the conserved quantum numbers are the $z$-component of the angular momentum projection on the symmetry axis of the nucleus ($K$) and the spatial parity ($\pi$), this operator can be expressed in the form:

$$B_{{(pm)K}}(H - E_P^P)P_0|\Phi_0\rangle$$

for the ground-state $|\Phi_0\rangle$ and the (projected) ground-state energy, given by:

$$E_P^P = N_0^{-1}\langle \Phi_0|HP_0|\Phi_0\rangle,$$

(6)

with the norm $N_0 = \langle \Phi_0|P_0|\Phi_0\rangle$. Please note, that $P_0$ in the above expressions is the projected operator on the corresponding quantum numbers for the ground state of the initial/final nuclei and not the excited states in the intermediate nucleus. In our approach we not only project out the non-physical components in the ground states of the initial and final nuclei but in the intermediate states as well.
To construct these states within the PQRPA framework we use the derivation proposed in [14], where they are obtained as trial functions in the form, given by the GCM ansatz:

\[ |\Psi\rangle = \int dz \, f(z) \, P|\Phi(z^*)\rangle, \tag{7} \]

where

\[ |\Phi(z)\rangle = P \, \exp \left( \sum_{pn} z_{pn} \beta_p^I \beta_n^I \right) |\Phi_0\rangle. \tag{8} \]

This leads to the well-known integral Hill-Wheeler equation [15], that using the so-called gaussian overlap approximation (GOA) can be cast in the differential form. Within this approximation the norm overlap can be expressed as:

\[ N(z, z') = N_0 \exp \left\{ (s^*, s) \left( \frac{z'}{z} \right) + \frac{1}{2} (z, z^*) \left( \begin{array}{cc} M & T \\ T^* & M^* \end{array} \right) \left( \begin{array}{c} z' \\ z \end{array} \right) \right\} \tag{9} \]

with the coefficients \( s_\kappa, M_{\kappa\lambda} \) and \( T_{\kappa\lambda} \) given by:

\[ s_\kappa = \frac{\partial}{\partial z_\kappa} \ln N|_{z = z' = 0} = N_0^{-1} \langle \Phi_0 | \beta_n \beta_p P | \Phi_0 \rangle \tag{10} \]

\[ M_{\kappa\lambda} = \frac{\partial^2}{\partial z_\kappa \partial z_\lambda^*} \ln N|_{z = z' = 0} = N_0^{-1} \langle \Phi_0 | \beta_n \beta_p P \beta_{p'}^I \beta_{n'}^I | \Phi_0 \rangle - s_\kappa s_\lambda^* \tag{11} \]

\[ T_{\kappa\lambda} = \frac{\partial^2}{\partial z_\kappa \partial z_\lambda} \ln N|_{z = z' = 0} = N_0^{-1} \langle \Phi_0 | \beta_n \beta_p \beta_{p'} \beta_{n'} P | \Phi_0 \rangle - s_\kappa s_\lambda, \tag{12} \]

where \( \kappa = \{p, n\} \) and \( \lambda = \{p', n'\} \) are combination of proton/neutron indices, fulfilling condition \( m_p + m_n = K, (-1)^{l_p + l_n} = \pi \).

Following [12] to calculate the contractions, we can now obtain explicit expressions for these coefficients, i.e.:

\[ s_\kappa = \frac{J + \frac{1}{2}}{(2\pi)^2 N_0} \int_0^\pi \int_0^{2\pi} \int_0^{2\pi} d\omega \, \rho(\omega) \sqrt{\det U(\omega)} \frac{1}{e^{-i(\Omega_\omega + \eta N_0)}} B_{\omega n\omega n' P} \tag{13} \]

\[ M_{\kappa\lambda} = \frac{J + \frac{1}{2}}{(2\pi)^2 N_0} \int_0^\pi \int_0^{2\pi} \int_0^{2\pi} d\omega \, \rho(\omega) \sqrt{\det U(\omega)} e^{-i(\Omega_\omega + \eta N_0)} \]

\[ \times (B_{\omega n\omega n' P} A_{\omega n' P} - C_{\omega n' P} C_{\omega n P} + C_{\omega n P} C_{\omega n' P}) - s_\kappa s_\lambda^* \tag{14} \]

\[ T_{\kappa\lambda} = \frac{J + \frac{1}{2}}{(2\pi)^2 N_0} \int_0^\pi \int_0^{2\pi} \int_0^{2\pi} d\omega \, \rho(\omega) \sqrt{\det U(\omega)} e^{-i(\Omega_\omega + \eta N_0)} \]

\[ \times (B_{\omega n\omega n' P} B_{\omega n' P} - B_{\omega n P} B_{\omega n' P} + B_{\omega n P} B_{\omega n' P}) - s_\kappa s_\lambda \tag{15} \]

with \( \omega = \{\beta, \zeta, \eta\} \) and \( \rho(\omega) = \sin \beta d^I_{MK}(\beta) d e^{-i(\Omega_\omega + \eta N_0)} \) and the \( A, B, C \) and \( U \) matrices given by:

\[ U_{\omega n' P} (\omega) = (u_{\nu n'} e^{i\varphi} + v_{\nu} v_{\nu'} e^{-i\varphi}) W_{\omega n' P} (\beta) \tag{16} \]

\[ V_{\omega n' P} (\omega) = (u_{\nu n'} e^{i\varphi} - v_{\nu} u_{\nu'} e^{-i\varphi}) W_{\omega n' P} (\beta) \tag{17} \]

\[ C(\omega) = U^{-1}(\omega), \quad A(\omega) = V^*(\omega) C(\omega), \quad B(\omega) = C(\omega) V(\omega) \tag{18} \]
In the above expressions, $\Omega_Z$ ($\Omega_N$) is the total number of proton (neutron) levels and $\varphi = \zeta$ ($\varphi = \eta$) for protons (neutrons). This means that these matrices are block diagonal, e.g.:

$$U = \begin{pmatrix} U^{(p)} & 0 \\ 0 & U^{(n)} \end{pmatrix}, \quad \det U(\omega) = \det U^{(p)}(\beta, \zeta) \cdot \det U^{(n)}(\beta, \eta). \quad (19)$$

It should be noted, that the integrals $\int_{-\infty}^{\infty} x^{i(m - \Omega)} e^{x^{(\alpha - \beta)}} dx$ can be evaluated numerically exactly with a relatively small number of integration points, using formulae given in [12] and [16]. Moreover, since the intermediate nucleus is an odd-odd nucleus it is more convenient in practice (albeit equivalent) to project not onto $Z$ and $N$, but onto $A/2 = (N + Z)/2$ and $T_3 = (N - Z)/2$, that are both integers.

In the above expressions $u$ and $v$ are the HFB transformation coefficients and $W_{\nu\nu'}(\beta)$ are the matrix elements of the $R(\beta)$ operator between the single-particle states in the deformed basis. They can be calculated as follows:

Matrix elements of the $J_2$ component of the (intrinsic frame) angular momentum in the axially-symmetric deformed basis $|am\rangle$ ($a$ denotes all the other quantum numbers except $m$) can be found by expanding the states of this basis on the eigenstates $|nljm\rangle$ of the spherical harmonic oscillator. We get:

$$\langle a'm'|J_3|am \rangle = \delta_{a'a} \delta_{mm'} \cdot m \quad (20)$$

$$\langle a'm'|J^2|am \rangle = \delta_{mm'} \cdot \sum_{nlj} C_{nlj}^a (C_{nlj}^{a'})^* \cdot j(j + 1), \quad (21)$$

where $C_{nlj}^a$ expansion coefficients of the states $|am\rangle$ on the spherical states:

$$|am\rangle = \sum_{nlj} C_{nlj}^a |nljm\rangle. \quad (22)$$

We define in the usual way "ladder" operators of the angular momentum:

$$J_\pm = J_1 \pm i J_2. \quad (23)$$

Because $J_+ = J_1^\dagger$, we get:

$$J_+ |am \rangle = \lambda_{am} |a, m + 1 \rangle \quad \mbox{(24)}$$

$$J_\mp |a, m + 1 \rangle = (\lambda_{am})^* |am \rangle \quad (25)$$

One can easily show that $J_+ J_+ = J_2^2 = J_3^2 - J_3$, thus, keeping Condon and Shortley phase convention ($\lambda_{am} > 0$) we get:

$$\lambda_{am} = \sqrt{\langle j(j + 1) \rangle_a - m(m + 1)}, \quad (26)$$

where $\langle j(j + 1) \rangle_a = \sum_{nlj} |C_{nlj}^a|^2 \cdot j(j + 1)$ is the expectation value of the $J_2$ operator in the $a$ shell. Resolving (23) we obtain matrix elements of $J_2$:

$$\langle a'm'|J_2|am \rangle = \frac{i}{2} \delta_{aa'} (\delta_{m',m-1} - \delta_{m',m+1}) \sqrt{\langle j(j + 1) \rangle_a - mm'}. \quad (27)$$

Matrix elements of the rotation operator $R(\beta) = e^{-i\beta J_2} = e^{r(\beta)}$ can be found, using corresponding algorithms for calculation of exponent of real antisymmetric matrices [17], since the matrix of the $r(\beta)$ operator is block-wise antisymmetric:

$$r_{am,am'}(\beta) = \frac{\beta}{2} \delta_{aa'} (\delta_{m',m-1} - \delta_{m',m+1}) r_{mm'}, \quad (28)$$
where \( r_{amm'} = \frac{\beta}{2} \sqrt{(j(j+1))_{a} - mm'} \). Let primed indices enumerate columns of the \( r = \text{diag}(r_a) \) matrix and let quantum numbers \( m \) run values from \(-m_{\text{max}}\) up to \( m_{\text{max}}\) for each block \( N_a \times N_a \). Blocks \( r_a \) take then the form:

\[
\begin{pmatrix}
0 & -r_{amm'} & 0 & \cdots & \cdots \\
r_{amm'} & 0 & -r_{amm'} & 0 & \cdots \\
0 & r_{amm'} & 0 & -r_{amm'} & \cdots \\
\vdots & 0 & r_{amm'} & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots \\
\end{pmatrix},
\]

that allows us easily express \( R = e^r \) as \( \text{diag}(e^{r_a}) \).

### 3. Derivation of the PQRPA equations

For the derivation of projected QRPA (PQRPA) equations we follow the procedure, described by Federschmidt and Ring [14], with several hints on the resolution of the integral equation and determination of the wave function (7), cast by Jancovici and Schiff [18]. In the spirit of the GOA, if we stop after second order in \( z, z^{*} \) in the approximation of the ratio of the Hamiltonian and the norm kernels:

\[
h(z, z^{*}) = \frac{H(z, z^{*})}{N(z, z^{*})},
\]

we obtain an equation, that resembles already the well-known QRPA form:

\[
h(z, z^{*}) = E_0^P + \frac{1}{2}(z, z^{*}) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} z^* \\ z \end{pmatrix}
\]

with the generalized PQRPA matrices:

\[
A_{\kappa\lambda} = N_0^{-1} \langle \Phi_0 | \beta_{\kappa} \beta_{\mu} (H - E_0^P) \beta_{\mu}^{\dagger} \beta_{\lambda}^{\dagger} | \Phi_0 \rangle
\]

\[
= N_0^{-1} \langle \Phi_0 | \beta_{\kappa} \beta_{\mu} H \beta_{\mu}^{\dagger} \beta_{\lambda}^{\dagger} | \Phi_0 \rangle - E_0^P (M_{\kappa\lambda} + s_{\kappa}s_{\lambda})
\]

\[
B_{\kappa\lambda} = N_0^{-1} \langle \Phi_0 | \beta_{\kappa} \beta_{\mu} \beta_{\mu}^{\dagger} \beta_{\lambda} (H - E_0^P) \beta_{\mu}^{\dagger} | \Phi_0 \rangle
\]

\[
= N_0^{-1} \langle \Phi_0 | \beta_{\kappa} \beta_{\mu} \beta_{\mu}^{\dagger} \beta_{\lambda} H \beta_{\mu} | \Phi_0 \rangle - E_0^P (T_{\kappa\lambda} + s_{\kappa}s_{\lambda}),
\]

that can be calculated using the recursive formula for the antisymmetrized sum of products of contractions, of the type given by Hara and Iwaski [12], analogous to the ordinary Wick theorem. Actually, we use this relation to avoid explicit writing of \((8-1)!! = 105\) terms and simply treat this recursion numerically.

The hermitian matrix \( M \) can be then decomposed into \( WW^\dagger \) and boson operators can be introduced:

\[
B_{\kappa} = \sum_{\lambda} W_{\lambda\kappa} z_{\lambda}, \quad B_{\kappa} = \sum_{\lambda} (W^{-1})_{\lambda\kappa} \frac{\partial}{\partial z_{\lambda}},
\]

which allows the Hill-Wheeler equation [15] to be transformed into differential equation. Defining the PQRPA phonon operators:

\[
A_{\mu}^\dagger = \sum_{\kappa} (X_{\kappa\mu} B_{\kappa} - Y_{\kappa\mu} B_{\kappa})
\]
we end up with the projected QRPA (PQRPA) equation ($\Omega_\mu$ is the phonon energy):

\[
\begin{pmatrix}
A & B \\
B^* & A^*
\end{pmatrix}
\begin{pmatrix}
X \\
Y
\end{pmatrix}_\mu = \Omega_\mu
\begin{pmatrix}
M & 0 \\
0 & -M^*
\end{pmatrix}
\begin{pmatrix}
X \\
Y
\end{pmatrix}_\mu
\]  

(36)

for the forward- and backward-going amplitudes $X$ and $Y$, respectively. One should note, that without the projection, this equation reduces to the usual QRPA equation, since then coefficients $s_\kappa$ and $T_{\kappa\lambda}$ vanish and $M_{\kappa\lambda}$ becomes an unity matrix.

In practice, one more step has to be done, because due to overcompleteness of the basis, the coefficients $X$ and $Y$ do not fulfill usual orthogonality relations and removal of zero-energy (spurious) excitation modes is necessary. This step is done along with the decomposition of the matrix $M = WW^\dagger$ by using only those components with non-vanishing eigenvalue, which makes the (effective) $W$ matrix rectangular in principle and reduces the dimension of the PQRPA equation. Finally, the (orthogonalized) boson operators read:

\[
C_\mu^\dagger = \sum_\kappa (W_\mu^\dagger X^\kappa B_\kappa^\dagger - (W^T Y)^\kappa B_\kappa)
\]  

(37)

and the redefined PQRPA matrices gain the form:

\[
\tilde{A} = W^\dagger A W, \quad \tilde{B} = W^T B W^*
\]  

(38)

giving the usual shape of the PQRPA equation:

\[
\begin{pmatrix}
\tilde{A} & \tilde{B} \\
-\tilde{B}^* & -\tilde{A}^*
\end{pmatrix}
\begin{pmatrix}
\tilde{X} \\
\tilde{Y}
\end{pmatrix}_\mu = \Omega_\mu
\begin{pmatrix}
\tilde{X} \\
\tilde{Y}
\end{pmatrix}_\mu
\]  

(39)

where $\tilde{X} = W^\dagger X$ and $\tilde{Y} = W^T Y$.

4. Determination of the wave function

To determine the wave function (7) of the excited intermediate nucleus, we first introduce the transformed weight function:

\[
g(z) = \int d z' \exp \left( \sum_\mu z_\mu z'_\mu \right) f(z')
\]  

(40)

that allows us to transform the Hill-Wheeler equation into a differential equation for $g(z)$ [13]. Since, from (34) we see, that $B_\mu$ should annihilate the phonon vacuum, the function $G(z)$, which corresponds to the ground-state solution should fulfill the condition

\[
B_\mu G(z) = 0
\]  

(41)

that give us a solution of the form:

\[
G(z) = \exp \left( -\frac{1}{2} \sum_{\kappa\lambda} Z_{\kappa\lambda} z_\kappa z_\lambda \right)
\]  

(42)

‡ Similar problem arises when one concerns the so-called second-order QRPA or extended QRPA with inclusion of scattering terms.
where $Z_{\kappa\lambda}$ is the solution of the system of linear equations:

$$
\sum_{\mu} X_{\kappa\mu} Z_{\mu\lambda} = Y_{\kappa\lambda}.
$$

(43)

The excited states can then be constructed by applying the phonon creation operators $B_{\mu}^\dagger$ to the ground-state $G$ function.

However, because $f(z)$ is a function of real and imaginary parts of $z$ separately, it cannot be determined uniquely. It comes from the fact, that states $|\Phi(z)\rangle$ form an overcomplete set. This is actually of an advantage, because we can use the freedom of choice of $f(z)$ to put some convenient condition on it. Indeed, if we use the identity:

$$
g(z) = \frac{1}{\pi^N} \int dz' \exp \left( \sum_{\mu} z_{\mu} z'_{\mu}^{*} - \sum_{\mu} |z'_{\mu}|^2 \right) g(z'),
$$

(44)

where $N$ is the dimension of the PQRPA problem, a possible solution for $f(z)$ reads:

$$
f(z) = \frac{1}{\pi^N} \exp \left( - \sum_{\mu} |z'_{\mu}|^2 \right) g(z).
$$

(45)

Finally, the excited state wave function (after replacement of each $z_{\mu}$ by $\beta_{\mu}^1 \beta_{\mu}^1$) takes the form:

$$
|\Psi\rangle = g(\beta_{\mu}^1 \beta_{\mu}^1) |\Phi_0\rangle.
$$

(46)

Acknowledgments

This work was supported by the Polish National Science Centre under the decision number DEC-2011/01/B/ST2/05932.

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