SHELL-MODEL AND QRPA TREATMENTS OF DOUBLE BETA DECAY

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The double beta decay of a model f-shell nucleus designed to simulate real, heavier, double-beta decay candidates is calculated exactly and in the Quasiparticle Random Phase Approximation (QRPA). Several features present in QRPA treatments of real nuclei are found in the exact solution, including sensitivity to neutron–proton particle–particle and quadrupole–quadrupole forces, and to short-range nucleon–nucleon repulsion. The two-neutrino double beta decay $^{46}$Ca$\rightarrow$ $^{46}$Ti is then calculated in both the shell model and QRPA; a qualitative agreement between these two very different treatments is noted.

Double beta decay is the process by which a nucleus with neutron and proton numbers $(N, Z)$ undergoes a transition to the nucleus $(N-2, Z+2)$ when the single beta decay to the intermediate nucleus $(N-1, Z+1)$ is energetically forbidden or highly retarded. There are two modes of double beta decay, one involving the emission of two antineutrinos and two electrons (2ν mode) and another (0ν mode) in which only electrons are emitted and which requires for its occurrence the existence of lepton-number-violating massive Majorana neutrinos.

Calculations of the nuclear matrix elements needed to understand these processes have recently been performed [1–3] in the context of the quasiparticle random phase approximation [4]. In refs. [1,2], the nucleon–nucleon potential was taken to be a delta-function with independent strengths in the particle–hole (p–h) and particle–particle (p–p) channels; these were determined by fitting to the energies of giant Gamow–Teller and isobar analog resonances, and to positron decay rates in neutron-deficient nuclei. Because of an extreme sensitivity to model parameters, it is important to understand whether significant errors are introduced by the crudeness of this procedure. One unrealistic ingredient in the calculations is the delta-function form for the nucleon–nucleon interaction. Previous work has indicated, for example [5,6], that the inclusion of quadrupole–quadrupole forces reduces 2ν matrix elements, and the results of ref. [3], which employed a G-matrix interaction, differ in quantitative detail from those of ref. [1]. Another possible source of error is the use of the QRPA as an approximation to an exact solution of the nuclear many-body problem; it is often remarked that the RPA overestimates ground-state correlations [7], and the QRPA results of ref. [2] show unexpectedly large reductions in 0ν decay rates from two-body correlations induced by short-range nucleon–nucleon repulsion. To better understand these aspects of the calculations, we will address several issues here: How large are the effects introduced by the delta-force and by the approximations inher-
ent in the QRPA, and can they be at least partly compensated for by renormalizing the parameters of the delta-function interaction? Are the substantial reductions in 0ν decay rates produced by short-range correlations real or are they an artifact of the QRPA? We discuss these questions via a simple yet partially realistic model in which the relevant nuclear quantities can be calculated exactly. After the issues have been clarified, we compare shell-model [8–12] and QRPA calculations of 2ν decay in 48Ca, with an eye to an improved understanding of the relation between the two approaches in real nuclei.

Our model space consists of a single 1-shell \( (j=l+1/2, l-1/2) \) for both neutrons and protons. As a compromise between our desires to minimize computation time and maximize the number of particles treated, we have chosen the f-shell, so that the model contains the levels \( 0^+_7/2 \) and \( 0^+_5/2 \). Since such a space is invariant under the action of the operator \( \sigma \), the 2ν decay amplitude

\[
M_{2T} = \sum_k \langle 0^-_m | \sum_l \sigma(k) \tau^+(k) | 1^+_m \rangle \times \langle 1^+_m | \sum_l \sigma(l) \tau^+(l) | 0^+_n \rangle \times [E_m - (M_i + M_f)/2]^{-1}
\]

may be calculated without ignoring contributions from intermediate state outside the model space. In this respect, the calculations here differ significantly from those of ref. [6] which, while similar in style, involve only the \( f_{7/2} \) level.

All further remarks will refer to the model decay in which the initial (final) nucleus contains 2(4) valence protons and 14(12) valence neutrons in the f-shell. This configuration was chosen to represent the situation in heavy nuclei large neutron excesses, such as those treated in refs. [1,2]. We have also carried out calculations in an initial (final) nucleus with 0(2) protons and 4(2) neutrons, and found our conclusions unchanged. In constructing and diagonalizing our hamiltonian matrices, we have made use of the OXBASH shell-model code [13].

Our starting point is the choice \( \epsilon_{f_{7/2}} = 0 \) and \( \epsilon_{f_{5/2}} = 6 \) MeV for the single-particle energies, and a two-body hamiltonian of the form

\[
H_{ij} = -A_0 P_o \delta(r_i - r_j) P_0 - A_1 P_i \delta(r_i - r_j) P_1 - B P_0 Y_2(\Omega_i) \cdot Y_2(\Omega_j) P_0 ,
\]

where \( A_0 = (14 \text{ MeV})/R, A_1 = (8 \text{ MeV})/R \) with

\[
R = \int \phi_{n}^2(r)r^2dr,
\]

and \( n=0, l=3, \phi=\text{radial wave function} \). (With the above choice for \( A_0 \) and \( A_1 \), we obtain reasonable values for the Gamow-Teller resonance energy and for the pairing gap.) \( P_o \) and \( P_i \) are projection operators onto the \( T=0 \) and \( T=1 \) channels respectively, and \( B \) is a parameter that will be varied to test the effects of quadrupole forces on the double beta decay. In addition, the above hamiltonian contains a hidden parameter, \( g_{pp} \), that multiplies the \( J^T=1^+, T=0 \) two-body matrix elements coming from the delta-function. The value \( g_{pp}=0 \) corresponds to no strength in that channel and the value \( g_{pp}=1 \) to the unaltered delta-function.

The QRPA results of refs. [1,2] indicate that as the \( J^T=1^+, T=0 \) particle–particle matrix elements vary (with the particle–hole matrix elements fixed), the 2ν amplitude \( M_{2T} \) decreases in magnitude, eventually crossing zero and changing sign. By changing our parameter \( g_{pp} \) here, we are varying essentially the same quantity as in refs. [1,2]. To see this, note that the particle–hole matrix elements are related to their two-body (particle–particle) counterparts by

\[
\langle j_1 j_2^- | V | j_3 j_4 \rangle_{J^T} = - \sum_{J^T'} (2J'+1)(2T'+1)
\]

\[
\times \left\langle \frac{j_1}{J_1} j_4 J' \right| \left\langle \frac{j_3}{J_3} j_2 J \right| \left\langle \frac{1}{1/2} \frac{1/2}{1} \frac{1}{T'} \right| \left\langle j_1 j_4 | V | j_3 j_2 \rangle_{J^T} .
\]

Since the particle–hole matrix elements receive contributions from all two-body particle–particle matrix elements, they will be affected only slightly by changes that are restricted to the \( J^T=1^+, T=0 \) multipole in the p–p channel, and will remain almost constant as \( g_{pp} \) varies.

To test the role of the quadrupole–quadrupole interaction, we have computed \( M_{2T} \) exactly as a function of \( g_{pp} \), for three values of the quadrupole strength parameter \( B \). The first, \( B = -14 \text{ MeV} \), precisely cancels the \( T=0 \) quadrupole–quadrupole component in the multipole expansion of the delta-function, so that no such term remains in the hamiltonian. The second
value is $B=0$ and the third is $B=14$ MeV, which effectively doubles the quadrupole strength ordinarily present in the delta-function. The results are plotted in fig. 1a. Two features of the figure are immediately apparent: (i) the amplitudes $M^\beta_{GT}$ do indeed pass through zero as $g_{pp}$ varies (at a value close to $g_{pp}=1$ for $B=0$) and (ii) the addition or substitution of quadrupole forces has a substantial effect on the amplitudes for all values of $g_{pp}$.

In refs. [1,2], a pure delta-function nucleon–nucleon interaction was used as an ingredient in the QRPA. The results obtained here and elsewhere suggest that the decay rate is sensitive to changes in the quadrupole–quadrupole component of the two-body interaction and experience leads us to suspect that other variations in the force can also produce large effects. However, the value of $g_{pp}$ used in refs. [1,2] was obtained by fitting the delta-function predictions to experimental $\beta^+$ strengths. It is appropriate to ask here whether such a procedure might compensate for deficiencies in the Hamiltonian. In the context of our model, the question becomes: By using a delta-function only as our Hamiltonian, can we reproduce the decay rate obtained from the Hamiltonian that includes quadrupole forces if we renormalize the value of $g_{pp}$ by fitting to $\beta^+$? As an answer, we plot in fig. 1b the amplitude $M^\beta_{GT}$ versus the total $\beta^+$ strength

$$\beta^+ = \sum_m |<0^+| \sum_I \sigma(l) \tau^+ (l) |1^+_m> |^2,$$

for the three values of $B$; to the extent that the three curves are the same, the correct amplitude can be obtained with any of the Hamiltonians by fitting to $\beta^+$. While not perfect, the agreement is better than in fig. 1a, particularly in the vicinity of the zero in $M^\beta_{GT}$. The errors made by using a delta-function only can therefore be reduced from their “naive” values via a renormalization of $g_{pp}$.

The second issue we wish to address is the quality of the QRPA as an approximation. Though this was explored in refs. [1,2] through an algebraic SO(8) model, the calculation presented there was restricted to degenerate single-particle levels and space-independent interactions. Our f-shell model, while not fully realistic, does incorporate those elements ignored by SO(8).

The neutron–proton QRPA was first used in ref. [4] and is described in detail in ref. [2]. Here, because we are approximating an exact solution with a delta-function Hamiltonian ($B=0$), the particle–hole and particle–particle parameters of ref. [2] have values $\alpha_0=\alpha_0'=A_1$, $\alpha_1=\alpha_1'=A_0$ if $g_{pp}=1$. When $g_{pp}$ is not 1, the parameter $\alpha_1'$ is modified to $g_{pp}A_0$. The pairing delta-function introduced into the BCS part of the calculation has strength $A_1$. In thus assigning the parameters, we are erring only in ignoring the deviation of $g_{pp}$ from 1 when calculating the form of the particle–hole force; since the $J^T=1^+, T=0$ multipole is only one of many that contribute in eq. (4), the error is a small one. In refs. [1,2] and ref. [3], matrix elements in the particle–hole and particle–parti-

![Fig. 1. Effects of quadrupole–quadrupole forces. The amplitude $M^\beta_{GT}$ is plotted in (a) versus $g_{pp}$ and in (b) versus the $\beta^+$ strength. The solid line corresponds to $B=0$, the dashed line to $B=-14$ MeV, and the dot–dashed line to $B=14$ MeV.](image)
cle channels were specified separately. While this complete independence cannot be achieved within the context of a two-body shell-model Hamiltonian, it can be approximated by adding terms to the interaction that concentrate strength in a particular particle–hole multipole. We have not done so here simply because we were able to obtain reasonable values for p–h-relevant quantities like the energy of the giant Gamow–Teller resonance without introducing additional multipole–multipole strength.

Because in the QRPA, the wave-functions of states in the intermediate nucleus must be based on ground state wave-functions in either the initial or final nucleus, there is a some arbitrariness in the way the calculation is performed. In refs. [1,2], we chose to average the results obtained by using the ground states of the initial and final nuclei on the supposition that they do not differ much if there are many valence neutrons and protons. Here, that assumption is obviously not true; the initial nucleus in fact has all its neutron single-particle levels filled, and therefore cannot undergo β⁺ transitions at all. Thus, we have chosen to follow the approach outlined in ref. [3] (eqs. (2)–(4); see also ref. [5]), taking the β⁻ matrix elements from the initial-nucleus QRPA, the β⁺ matrix elements from the final nucleus, and using a particular prescription for the overlap of the intermediate states based on the initial and final nuclei. Fig. 2a shows the exact solution for \( M^{GT}_{\gamma\nu} \) as a function of \( g_{pp} \), alongside the QRPA results. While the qualitative behavior of the two curves is the same, they do differ from each other, and at first sight, one would seem to be making significant errors by using the QRPA. However, it is possible to pose the same question here we asked earlier in the context of quadrupole effects: namely, can we do better by renormalizing \( g_{pp} \) through a fit to the \( β^+ \) strength? Fig. 2b shows the exact and approximate \( β^+ \) strengths plotted versus \( M^{GT}_{\gamma\nu} \). One again, we see that the agreement is better, especially in the region of suppression.

To illustrate the effect of the nucleon–nucleon repulsion, we have calculated \( M^{GT}_{\nu\nu} \), the Gamow–Teller portion of the quantity relevant to neutrinoless double beta decay. It is given by

\[
M^{GT}_{\nu\nu} = R_0 \langle 0^+ | \sum_k H(E, r_{kd}) \sigma(k) \cdot \sigma(l) \times \tau^+(k) \tau^+(l) | 0^+ \rangle,
\]

where \( R_0 \) is the nuclear radius, \( H(E, r_{kd}) \) is a complicated function approximated as \( \exp(-\frac{1.5E_{kd}}{r_{kd}}) \), and \( E \) is a “typical” nuclear excitation energy, taken here to be the energy of the giant Gamow–Teller state. The correlations due to short-range repulsion are accounted for by multiplying \( H(E, r_{kd}) \) by the square of the function \( f(r_{kd}) \):

\[
f = 1 - \exp(-a r_{kd}) (1 - b r_{kd})^2,
\]

with \( a = 1.1 \text{ fm}^{-2}, b = 0.68 \text{ fm}^{-2} \). The results of the exact calculation with and without the short-range correlations appear in fig. 3. These results very much resemble the QRPA tables in ref. [2]; the roughly constant vertical distance between the two curves

Fig. 2. Comparison of exact and QRPA solutions for \( \beta = 0 \). The amplitude \( M^{GT}_{\gamma\nu} \) is plotted in (a) versus \( g_{pp} \) and in (b) versus the \( \beta^+ \) strength.
Fig. 3. Effects of short-range correlations. The amplitude $M_{2F}^{T}$ is plotted versus $g_{pp}$. The solid line corresponds to the results with short-range correlations included, the dashed line to those without them.

translates near the crossing point into a substantial relative effect. Thus, the extra suppression produced by the correlations noted in ref. [2] appears to be a real effect and not a QRPA artifact.

A final note about the QRPA: because it is a "collective state" approximation, its quality should improve as more levels and nucleons are added. A test with 16 particles (and only a few holes) in the f-shell is therefore probably overly pessimistic in its results. These facts, combined with the improvement that is obtained by judiciously fixing $g_{pp}$ lead us to conclude that a QRPA calculation of double beta decay rates may be sensible. To illustrate the basic adequacy of the QRPA (cum delta-function), we turn now to the 2v decay of a real f-shell nucleus, $^{48}$Ca, for which elaborate shell-model calculations involving the entire f-p shell have already been performed.

Because the double beta decay $^{48}$Ca→$^{48}$Ti has one of the largest $Q$-values known, it has attracted considerable interest among both experimentalists and theorists [8–12]. In these relatively light nuclei, shell-model calculations perhaps include enough configurations to provide an accurate value for the 2v decay rate. The double beta decay of $^{48}$Ca was not calculated in refs. [1,2], whether heavier nuclei in which pairing correlations are well developed were considered. However, encouraged by the f-shell results reported above, we wish now to understand the role played by $g_{pp}$ in this real decay, and to examine further the correspondence between shell-model and QRPA calculations.

Our shell-model calculations make use of the entire f-p shell, allowing all configurations in which at most two particles are promoted out of the $f_{7/2}$ level. We take as a hamiltonian the single particle energies and modified Kuo–Brown two-body interaction used in ref. [11], and test the effects of the particle–particle force by multiplying all $J^T=1^+, T=0$ matrix elements by a parameter $g_{pp}$ as described above; the presumably realistic rate is obtained with $g_{pp}=1$. (We must note that there is a discrepancy of about 7% between our results with $g_{pp}=1$, and those of ref. [11]; the source of the difference is unknown to us.) The QRPA calculation uses standard Woods–Saxon single particle energies and the full s, d and p, f shells, with the deltaforce interaction specified by the p–h constants in ref. [2], $\alpha_1=-1010$ MeV fm$^3$, $\alpha_0=-890$ MeV fm$^3$. The p–p parameter $\alpha'$ is varied, like $g_{pp}$ above. The method of refs. [3,5] mentioned previously is used to evaluate overlaps between states in the initial and final nuclei. In both the shell-model and QRPA treatments (and in ref. [11]), the
excitation energy of the first strongly excited \(1^+\) state is taken from experiment rather than from the calculation.

The results are shown in figs. 4a, b, where we plot \(M_{\text{MCT}}^\text{\(1\)}}, eq. (1), and the corresponding closure matrix element

\[
M_{\text{close}} = \langle 0^+_\text{\(1\)} | \sum_{k, l} \sigma(k) \cdot \sigma(l) \tau^+ (k) \tau^+ (l) | 0^+_\text{\(1\)} \rangle ,
\]

(8)
as a function of the \(\beta^+\) strength from the final nucleus \({^{48}\text{Ti}}\); our previous discussion demonstrated that this strength should be used in fixing p–p parameters and therefore properly belongs on the x-axis. The two sets of curves are in relatively close agreement, particularly near the crossing. It is important to note, however, that the “real” shell model result occurs at \(g_{\text{pp}} = 1\), corresponding in the figure to a \(\beta^+\) strength of 1.47. At this value, the closure matrix element is only moderately suppressed from its \(g_{\text{pp}} = 0\) value, and \(M_{\text{MCT}}^\text{\(1\)}\) is essentially completely unsuppressed. Even here though, the QRPA, based on a different model

\[
\text{space and interaction, reproduced the shell model result to within a factor of } 2. \text{ The value of } \alpha'_1 \text{ that yields the "correct" (i.e., shell-model) } \beta^+ \text{ strength is } -330 \text{ MeV fm}^3, \text{ outside the window } 390-430 \text{ determined in ref. } [2], \text{ but not terribly far so. That the parameter should be different here is not surprising because, unlike the situation in all the heavier } \beta \beta \text{ decay candidates, } \beta^+ \text{ transitions are not blocked.}
\]

One interesting and complicating fact is that the experimental lower limit for the half-life of 2\(v\) decay in \({^{48}\text{Ca}}\) [15] translates into an upper limit (with an effective \(g_4 = 1\) on \(M_{\text{MCT}}^\text{\(1\)}\)) of 0.08 MeV \(-\) \(\text{MeV}\), a value smaller than the shell model result with \(g_{\text{pp}} = 1\). This discrepancy has been attributed by Brown [2] to the truncation of the f–p configuration space to two-particle two-hole states mentioned above. In any event, there is still disagreement between currently feasible shell-model calculations and experimental data, and final word on the role of the particle–particle force in suppressing the decay in calcium awaits further study. An (n, p) experiment to measure the \(\beta^+\) distribution from \({^{48}\text{Ca}}\) would help clarify matters.

Our conclusion is that the QRPA provides a good way of calculating \(\beta\beta\) decay if the \(\beta^+\) strength is used to fix particle–particle parameters in the hamiltonian. We close by mentioning one more item that increases our faith in the method. A recently reported measurement of the (n, p) reaction \({^{54}\text{Fe}}\) [14] allows us to test our determination of the QRPA p–p coupling constant in a nucleus near \({^{48}\text{Ca}}\) in mass. The measured strength (suppressed by \(\approx 3\) from single particle value) is a consistent with a value \(\alpha'_1\) between \(-260\) and \(-460 \text{ MeV fm}^3\). Though this window is large due to a slow dependence of the strength on \(\alpha'_1\), it is consistent with the values extracted both in ref. [2] and from the shell-model calculation in \({^{48}\text{Ca}}\). It is encouraging, though not entirely surprising given the results presented above, that the QRPA is able to postdict this strength.

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References