Use of summation methods in the calculation of nuclear double beta decay processes

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The use of summation methods, to deal with the calculation of matrix elements involved in the microscopic description of nuclear double beta decay processes, is discussed. The analysis focuses on the accuracy of a procedure which formally expresses the matrix elements of the standard current-current weak interaction, starting from the second-order perturbation treatment of the standard weak Lagrangian, as divergent power series of energy denominators. It is shown that, when properly treated, the summation method leads to results which coincide with the numerical sum of contributions due to virtual intermediate states.

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The nuclear structure component of the double beta decay mode with the emission of two neutrinos ($2\nu\beta\beta$) [1–3] has been carefully examined during the last years [4,5]. Theoretical results for the $2\nu\beta\beta$ mode, obtained by using different models and/or approximations, have been reported [6–11] and the existence of a suppression mechanism has been established. This suppression mechanism [8,9] has been explained in terms of the competition between different channels of the residual two-body interaction, regardless of the method used to treat the interactions [6–11]. A review of the existing literature and of the status of the theory including comparison with data [12–14] can be found in Refs. [4,5] and can be summarized in the following.

(i) The nuclear matrix elements which are needed to describe the experimental half-lives of several double beta decay candidates, are strongly suppressed as compared with single-particle values. The suppression mechanism can be explained in terms of the competition between repulsive and attractive channels of the residual two-body proton-neutron interaction [8,9].

(ii) The quasiparticle random-phase approximation (QRPA) method [9,10] does indeed yield to results which reproduce the data [12–14]. A highly selective test of the QRPA wave functions and $2\nu\beta\beta$ matrix elements is the ratio between half-lives for the decay of ^{128}Te and ^{130}Te, where the QRPA model [10] is able to predict the recent experimental number very well [14].

(iii) Shell-model calculations, for the few cases which can be computed in this fashion, do show that QRPA results are qualitatively correct and that they are also comparable in magnitude with the shell-model ones [11].

Finding new methods, other than the QRPA, to compute nuclear double beta decay observables is a matter of utmost interest. Recently a new technique has been reported [15–17] which, if it can be proved to be correct, greatly changes the situation since it yields matrix elements which are apparently not sensitive to the microscopic description of the virtual states which are an essential ingredient of the QRPA calculations.

Unfortunately, as we are going to show next, this cannot be the case if the mathematical assumptions upon which the new technique, the operator expansion method (OEM) of Ref. [15], is based are reexamined. Since the OEM has been explained in detail in Ref. [15], we shall assume that the reader is already familiar with the formalism of Refs. [15–17]. We will show that, contrary to what it is claimed by the OEM, the dependence of the nuclear matrix elements on the intermediate states remains even if the matrix elements are written as a series.

To start with let us introduce the nuclear matrix element which is relevant for the description of $2\nu\beta\beta$ transitions; it can be written as

$$M_{\rm GT}^{2\nu}=\sum_N \frac{\langle 0_F^+\|\tau^+\sigma\|1_N^+\rangle\langle 1_N^+\|\tau^+\sigma\|0_I^+\rangle}{E_0+E_N-E_I}\ , \qquad (1)$$

where E_0 is half of the total energy released $E_0=\frac{1}{2}Q_{\beta\beta}+m_ec^2$; $|0_I^+\rangle$, $|0_F^+\rangle$, and $|1_N^+\rangle$ are the initial, final, and virtual intermediate states, respectively; and E_N and E_I are intermediate and initial energies, respectively. In the derivation of Eq. (1) it is assumed that the decay involves only left-handed currents and that energy denominators, which explicitly contain leptonic energies, are already approximated by the denominator of Eq. (1) [2,5]. The information about leptonic wave function is given by the factor $F_{2\nu}$, the phase-space factor, to be included in the definition of the half-life: $(\tau_{1/2}^{2\nu})^{-1}=F_{2\nu}|M_{\rm GT}^{2\nu}|^2$. Therefore, one has to perform a sum over all intermediate states in order to compute Eq. (1).

The OEM expansion aims at elimination of the sum over intermediate states by using an analytic continuation of the sum and be replacing it by an expansion in terms of commutators of the nuclear Hamiltonian with the transition operator $\hat{O}_{1\mu}=\tau^+\hat{\sigma}_{1\mu}$. In Ref. [15] the summation is performed by (a) Taylor expanding the energy denominator of (1), and (b) commuting the transition operator with a bare two-body interaction.

Concerning approximation (a) the divergent nature of

the series expansion of the OEM is not enough to guarantee that the techniques of Hardy [18,19] can be safely applied. Rather, if the behavior of a series is dominated by few terms, then the analytic continuation of it past the circle of convergence does not always yield to meaningful results and more often it yields to meaningless results [19,20]. The drawback of (b) is discussed in Ref. [21]. In the following we shall show (i) that a summation method can be used which does not require the Taylor expansion of the OEM and (ii) that this method leads to the same result as the brute-force sum over intermediate states, when applied to (1), contrary to the results of Ref. [15].

In order to show that the advantages pointed out in Refs. [15–17], concerning the independence on the intermediate states, are only apparent let us compute (1) in a slightly different fashion.

Since the energy denominator of Eq. (1) and the quantity $x_N=(E_N-E_I)/E_0$ are always positive, one can write Eq. (1) as

$$M_{\rm GT}^{2\nu}=\frac{1}{E_0}\sum_N \langle F|\hat{O}|N\rangle\langle N|\hat{O}|I\rangle \int_0^\infty dt\, e^{-t(1+x_N)} . \tag{2}$$

By changing the variable of integration t by $\omega=t/E_0$, which is allowed since $E_0>0$, by replacing $e^{-\omega E_N}|N\rangle$ by $e^{-\omega\hat{H}}|N\rangle$ and $e^{\omega E_I}|I\rangle$ by $e^{\omega\hat{H}}|I\rangle$, which is allowed since the intermediate states $|N\rangle$ and the initial state $|I\rangle$ are eigenstates of the nuclear Hamiltonian $\hat{H}$, one has after summing over all intermediate states:

$$M_{\rm GT}^{2\nu}=\int_0^\infty d\omega\langle F|\hat{O}e^{-\omega\hat{H}}\hat{O}e^{\omega\hat{H}}|I\rangle e^{-\omega E_0} . \tag{3}$$

By using the Baker-Hausdorff lemma the operator $e^{-\omega\hat{H}}\hat{O}_{1\mu}e^{\omega\hat{H}}$ can be expanded in terms of multiple commutators

$$e^{-\omega\hat{H}}\hat{O}e^{\omega\hat{H}}=\hat{O}+\sum_{l=1}^{\infty}\frac{(-1)^l\omega^l}{l!}\times[\hat{H},[\hat{H},[\ldots,[\hat{H},\hat{O}]]\cdots]]^{(l\text{ times})} . \tag{4}$$

The integral (3) can now be performed and the result for $M_{\rm GT}^{2\nu}$ can be written:

$$M_{\rm GT}^{2\nu}=\frac{\langle F|\hat{O}\hat{O}|I\rangle}{E_0}+\delta M , \tag{5}$$

where

$$\delta M=\sum_{l=1}^{\infty}(-1)^l\frac{C^{(l)}}{E_0^{l+1}} \tag{6}$$

and

$$C^{(l)}=\langle F|\hat{O}[\hat{H},\ldots[\hat{H},\hat{O}]]\ldots]^{(l\text{ times})}|I\rangle . \tag{7}$$

The above equations have been obtained without performing the Taylor expansion of (1). Therefore, they cannot be compared with a modified version of the OEM presented in Ref. [17] [Eq. (12)].

Since the Hamiltonian $\hat{H}$ entering in Eq. (4) is the effective nuclear Hamiltonian, namely, a single-particle term plus a residual two-body interaction term, all terms of the series will contribute. That Eq. (5) should give the same result as the brute-force sum of Eq. (1) can be easily shown by computing it for the following cases.

(1) Single-particle Hamiltonian: We can write for $\hat{H}$ and $\hat{O}$ in second quantization

$$\hat{H}=\sum_k \epsilon_k a_k^\dagger a_k+\text{const} \tag{8}$$

and

$$\hat{O}_{1\mu}=\sum_{p,n}\sigma(p,n)A^\dagger(p,n,1\mu) , \tag{9}$$

where

$$\sigma(p,n)=\frac{\langle p\|\sigma\|n\rangle}{\sqrt{3}}$$

and

$$A^\dagger(p,n,1\mu)=[a_p^\dagger\tilde{a}_n]_{1\mu} ,$$

$$\tilde{a}_{j_n,m_n}\equiv(-1)^{j_n+m_n}a_{j_n,-m_n} .$$

For this case the l-times commutator gives

$$[[\hat{H},\ldots[\hat{H},\hat{O}_{1\mu}]]\ldots]^{(l\text{ times})}=\sum_{p,n}\sigma(p,n)(\epsilon_p-\epsilon_n)^lA^\dagger(p,n,1\mu) , \tag{10}$$

and the corresponding series can be written as

$$M_{\rm GT}^{2\nu}=\sum_{p,n,p',n'}\sigma(p,n)\sigma(p',n')\times\frac{\langle F|A^\dagger(p,n)A^\dagger(p',n')|I\rangle}{E_0}F(p',n') . \tag{11}$$

The factor

$$F(p',n')=1+\sum_{l=1}^{\infty}(-1)^l\frac{(\epsilon_{p'}-\epsilon_{n'})^l}{E_0^l} \tag{12}$$

represents the divergent series expansion of $E_0/[E_0+(\epsilon_p-\epsilon_n)]$ thus the matrix element $M_{\rm GT}$ is, for this case, given by

$$M_{\rm GT}^{2\nu}=\sum_{p,n}\sum_{p',n'}\sigma(p,n)\sigma(p',n')\times\frac{\langle F|A^\dagger(p,n)A^\dagger(p',n')|I\rangle}{E_0+\epsilon_{p'}-\epsilon_{n'}} , \tag{13}$$

which is the correct result, namely, it is the result given by the brute-force summation of terms in Eq. (1) when the intermediate states N are replaced by uncorrelated proton-neutron pairs.

(2) Tamm-Dancoff treatment of $\hat{H}$: In this case the intermediate states $|N\rangle$ are described by correlated proton-neutron pairs

$$\Gamma_{1\mu}^\dagger(s)=\sum_{p,n}X(p,n,s)A^\dagger(p,n,1\mu) , \tag{14}$$

and $\hat{H}$ has the form

$$\hat{H}=\text{const}+\sum_s \hbar\omega_s \Gamma^\dagger(s)\Gamma(s) ,$$

where $\hbar\omega_s$ is the energy of the sth correlated intermediate virtual state. In the same basis the transition operator $\hat{O}_{1\mu}$ has the form $\hat{O}=\sum_s \Lambda_s \Gamma^\dagger(s)$, with

$$\Lambda_s=\sum_{p,n} X(p,n,s)\sigma(p,n) ,$$

and the multiple commutator of Eq. (7) can be written as

$$[[\hat{H},\ldots[\hat{H},\hat{O}]]\ldots]^{(l \text{ times})}=\sum_s \Lambda_s(\hbar\omega_s)^l\Gamma^\dagger(s) . \quad (15)$$

Thus the matrix element of Eq. (7) is readily obtained and then Eq. (5) gives

$$M^{2\nu}_{\text{GT}}=\sum_{s,s'} \Lambda_s\Lambda_{s'}\frac{\langle F|\Gamma^\dagger(s)\Gamma^\dagger(s')|I\rangle}{E_0}F(\hbar\omega_{s'}) , \quad (16)$$

where $F(\hbar\omega_{s'})$ is the divergent series expansion of $E_0/(E_0+\hbar\omega_{s'})$ which is again what one would obtain by explicitly performing the sum of Eq. (1) in the Tamm-Damcoff approximation for the intermediate states.

(3) The QRPA treatment [9,10]: In this case, the Hamiltonian $\hat{H}$ and the transition operator $\hat{O}_{1\mu}$ can be expanded in the QRPA phonon basis

$$\Gamma^\dagger_{1\mu}(s)=\sum_{p,n}[X(p,n,s)A^\dagger(p,n,1\mu) - Y(p,n,s)\tilde{A}(p,n,1\mu)] , \quad (17)$$

where

$$\tilde{A}(p,n,1\mu)=(-1)^{1+\mu}A(p,n,1,-\mu) .$$

In this representation

$$\hat{H}=\text{const}+\sum_s \hbar\omega_s\Gamma^\dagger(s)\Gamma(s)$$

and

$$\hat{O}_{1\mu}=\sum_{p,n}[\sigma(p,n)A^\dagger(p,n,1\mu)+\sigma'(p,n)\tilde{A}(p,n,1\mu)] ,$$

where the proton-neutron pair configurations are expressed in quasiparticle basis and where the reduced matrix elements $\sigma(p,n)$ and $\sigma'(p,n)$ include the BCS occupation factors u_pv_n and v_pu_n, respectively. The multiple commutator of Eq. (7) now yields

$$[[\hat{H},\ldots[\hat{H},\hat{O}]]\ldots]^{(l \text{ times})} = \sum_s(\hbar\omega_s)^l[\Lambda_s\Gamma^\dagger(s)+\Lambda'_s\tilde{\Gamma}(s)] , \quad (18)$$

where

$$\tilde{\Gamma}_{1\mu}(s)=(-1)^{1+\mu}\Gamma_{1,-\mu}(s) ,$$

$$\Lambda_s=\sum_{p,n}[X(p,n,s)\sigma(p,n)+Y(p,n,s)\sigma'(p,n)] ,$$

and

$$\Lambda'_s=\sum_{p,n}[X(p,n,s)\sigma'(p,n)+Y(p,n,s)\sigma(p,n)] .$$

The matrix element M_{GT} is finally given by

$$M^{2\nu}_{\text{GT}}=\sum_{s,s'}\frac{\langle F|[\Lambda_s\Gamma^\dagger(s)+\Lambda'_s\tilde{\Gamma}(s)][\Lambda_{s'}\Gamma^\dagger(s')+\Lambda'_{s'}\tilde{\Gamma}(s')]|I\rangle}{E_0+\hbar\omega_{s'}} , \quad (19)$$

which agrees with the result given by a direct computation of Eq. (1).

In the above-discussed examples, both Eqs. (1) and (5) give the same result for the matrix element M_{GT}. Therefore, when the summation, both in the brute-force approach and in the fashion of Eq. (5), is properly done, the result for M_{GT} is always dependent on the structure of the intermediate states, as well as on their energies. It means that in going back and forth from one expression to the other, namely, from Eq. (1) to Eq. (5), the relevant information is always represented by the structure of the virtual intermediate states and that no terms are missing. Then, why do the OEM results [15–17] claim to be so different from those presented above, particularly from the QRPA results? The answer can be as follows: The expansion of the series $1/(1+x)$, as is performed in the OEM in order to bring the energies on the numerator of (1), does not coincide with the expansion of the series e^{-x}, which is obtained from the use of the integral representation (2) and from the use of the Baker-Hausdorff lemma (4)—except for the first two terms even inside the resion of convergence $|x|=1$.

Concerning Eqs. (1) and (5), we have shown that both equations contain the same information and that the independence of Eq. (5) on the structure of the intermediate states is only apparent. The same must be true with any other summation method. Otherwise, one can end up with results which are not necessarily of physical meaning and which are produced by a mismatching between series expansions. In view of the examples which we have shown in this paper, we think that this is the case with the OEM results of Refs. [15–17]. Similar conclusions have been reported in Ref. [21].

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