Project PCE 3-0318-2011
Title: “Development of advanced computer codes for double beta decay calculations”

Synthetic scientific report
throughout the period of execution

Period: January 2012 – December 2016

Introduction
Double beta decay (DBD) is a nuclear process by which an even-even nucleus decays into another even-even nucleus with the same mass but with the electric charge changed by two units. It is the rarest decay process ever measured until present with lifetimes of $10^{19} - 10^{24}$ years.

Its importance is mainly related to the search of the neutrinoless DBD mode, whose discovery would bring important information to clarify several fundamental issues such as: i) lepton number conservation; ii) absolute mass of neutrino; iii) neutrino mass hierarchy; neutrino character, namely if they are identical or not with their anti-particles (Majorana or Dirac neutrinos?); iv) number of neutrino flavors, etc.

Clarification of these issues would be of crucial importance for understanding the formation, structure and evolution of the universe. This explains the great interest for the study of DBD process. DBD experiments are carried out worldwide in underground laboratories. In the next future these experiments will reach lifetime limits of $10^{26} - 10^{27}$ years, which is equivalent with the measurement of neutrino masses of 0.2 – 0.1 eV. In theory, precise methods of calculation of the nuclear matrix elements (NMEs) and phase spaces factors (PSFs) are continuously developing in order to derive accurately neutrino mass parameters. This will help experimentalists to interpret their measured data and plan performance and costs of their future experiments.

For the neutrinoless DBD ($0\nu\beta\beta$) process to occur, it is necessary that neutrino be a massive Majorana particle. Neutrinos with these properties are not allowed within the Standard Model (SM), but are allowed within more general theories, GUTs. The discovery of $0\nu\beta\beta$, would lead to the extension of the SM. The same information, about the neutrino character and masses are also investigated now by the LHC experiments CERN. The discovery that neutrinos have nonzero mass, by measurements of the neutrino oscillation experiments, has stimulated the studies on DBD process. However, in these neutrino oscillating experiments one can measure only squared mass differences, thus the absolute masses and character of the neutrinos, as well as the conservation of the lepton number remain unaddressed issues in
these experiments. Hence, DBD still remains the most sensitive process to check these fundamental neutrino properties.

Theoretically, the DBD lifetimes, both for the $2\nu\beta\beta$ and $0\nu\beta\beta$ decay modes can be expressed as a product of specific factors, as follows:

\[
[T^{2\nu}]^{-1} = G^{2\nu}(Q_{\beta\beta}, Z) g_A^4 |m_e c^2 M^{2\nu}|^2 \quad (A, Z) \rightarrow (A, Z+2) + 2e^- + 2(\text{anti})\nu
\]

\[
[T^{0\nu}]^{-1} = G^{2\nu}(Q_{\beta\beta}, Z) g_A^4 |M^{0\nu}|^2 <\eta> \quad (A, Z) \rightarrow (A, Z+2) + 2e^- \]

$G^{2\nu}$ and $G^{0\nu}$ represent the PSFs for the decay modes $2\nu\beta\beta$ and $0\nu\beta\beta$, respectively, $M^{2\nu}$ and $M^{0\nu}$ are the corresponding NMEs and $<\eta>$ is the neutrino mass parameter.

From these formulas one can see that the precise calculation of both PSFs and NMEs allows the correct estimation of the lifetimes and, in corroboration with experimental results, allows verification of the nuclear structure models and extraction of the neutrino parameters. Hence, the theoretical investigations on DBD process help a lot the experimentalists in planning their DBD experiments and interpreting their results, and save important costs.

Within this project we proposed ourselves to develop advanced computational methods for calculation of the PSF and NME quantities, which appear in the DBD lifetimes. Particularly, we built new, performant numerical codes with which we have re-calculated these quantities for several decay modes and many nuclei, of experimental interest. Specifically, we did the following activities and obtained the following results:

1) **Building of a fast, efficient numerical code for the NME computation of $0\nu\beta\beta$.**

We developed a performant code based on the Shell Model (ShM) approximation for the NME computation. The main steps and ingredients of this code are:

- Obtaining formulas for $M^{0\nu}$ in a new form, which allowed the reduction of the CPU time of calculation. $M^{0\nu}$ can be written as a sum of three components: a) a component that represents the contribution of the Gamow-Teller (GT) nuclear transitions; b) a component that represents the contribution of the Fermi (F) nuclear transitions and c) a tensorial component (T).

- The most difficult is the computation of the radial part of NMEs, that contain the neutrino potentials. Normally, it is necessary to perform double integrals over coordinates and momenta, which are not easy to calculate and, that require long CPU times, when the nuclear model space has huge dimensions. However, by obtaining new formulas of the $M^{0\nu}$ radial part, we succeeded, by using appropriate recurrence formulas, to perform the integral over coordinates analytically and hence, to reduce the
numerical computation to only one integral. In this way the computation becomes simpler and the CPU time is significantly reduced. The procedure is described in detail in ref. [1].

- The use of effective nucleon-nucleon (NN) interactions which reproduce well other spectroscopic properties of the nuclei under investigation. They were first identified the most suitable NN interactions from literature, for the nuclei $^{48}$Ca, $^{76}$Ge and $^{82}$Se. Thus, we performed calculations with GXPF1A (for $^{48}$Ca) and JUN-45 (for $^{76}$Ge and $^{82}$Se) effective NN interactions. The use of tested NN effective interactions is very important in getting of precise values for $M_{\beta\beta}^{0\nu}$.

- Building of a flexible numerical code that allows the alternative/cumulative inclusion of different nuclear ingredients, as: short range correlations (SRCs) between nucleons in different parametrizations, finite nuclear size (FNS) effect, inclusion of the tensor component, due to the higher order contributions in nuclear currents (HOC), etc. The influence of all these ingredients on the NME results is much discussed in literature.

Results obtained: i) getting a performant numerical code about 30 times than similar codes from literature; ii) testing it on several cases (decays and nuclei) and getting very good results as compared with other ones from literature.

The results described above have been published in a paper appeared in Phys. Rev. C [1] and presented in conferences [3], [5]–[6].

2. Computation of the NMEs.

Using numerical code developed in the first phase of the project, we calculated NMEs related to the $0\nu\beta\beta$ for two mechanisms of decay: a) exchange of light Majorana neutrinos between two nucleons in the nucleus and b) exchange of heavy Majorana neutrinos between two nucleons the nucleus.

a) NME computation for $0\nu\beta\beta$ through exchange of light Majorana neutrinos

Using numerical code developed in the first phase of the project, we calculated NMEs for $0\nu\beta\beta$ for 3 nuclei of experimental interest: $^{48}$Ca, $^{76}$Ge and $^{82}$Se. The aim was: i) to test the new code, faster than the existing ones, reporting new values for $M_{0\nu}$ and comparing them with other results existing in literature; ii) to make a detailed analysis of the nuclear effects included in the calculation; iii) analysis of results obtained with various nuclear ingredients/parameters of model taken into account in calculation; iv) to clarify the importance of inclusion of the tensor part in calculation, a subject still under debate.

The conclusions, in short, are the following:

We completed the code previously developed with the inclusion of the tensor contribution in the $M_{\beta\beta}^{0\nu}$ calculation. We compared our results with other results from literature, obtained with similar methods (based ShM) or with different methods, getting either a good agreement or expected differences, which are due to specific features of each method. Our results, thus, completes the results from literature. The
common effect of these ingredients included in calculations, is a significant decrease (of ~ 50%) of the M⁰ν “bare” values. Inclusion of the HOC component leads to a 4-9% decrease of the NME values, which can be justifiably neglected in non-rigorous calculations. Using of different effective NN interactions can influence the results with ~ 17%. We also notice a significant effect on the M⁰ν results, when “quenched” or “unquenched” values of the gA coupling constant, are used. The results are published in J. Phys. G[10] and presented in conferences [15]-[16]. Also, they appeared in J. Phys.

a) NME computation for 0νββ through exchange of heavy Majorana neutrinos

We also calculated M⁰ν through the heavy Majorana neutrinos exchange mechanism. This alternative mechanism to the common one, the exchange of light neutrinos, is approached more and more at present. The motivation is related to the fact that this mechanism could provide us with additional information about the possible existence of “sterile” massive neutrinos, which differ from the “active” ones, discovered until present, which can be searched in high energy experiments, for example LHC experiments. Our results complete those existing in literature. Details can be found in ref. [12].

3. Computation of the phase space factors (PSFs).

PSFs are also important in the lifetime calculations, as shown above. Until recently it was considered that they were calculated with good approximation, so the theorists effort has focused on precise calculation of the NMEs only. However, very recently in Ref. Kotila & Iachello, PRC 85, 2012 using a more accurate method, the authors obtained PSF values that differ significantly from the older calculations, especially for heavier nuclei, and positron emitting and electron capture DBD modes. To check this, we developed an improved method for the PSF calculation, particularly a new numeric code. Within this method we used wave functions for description the motion of the relativistic electrons in the Coulomb field of the nucleus obtained by solving a Dirac equation. In the procedure we took into account both the screening and finite nucleon size effects. In addition to other previous methods, our Coulomb potential was obtained from a realistic distribution of protons inside the nucleus daughter. In addition, our routines have a more accurate precision and we improved the method of identification of the bound eigenstates of the Dirac equation. With this code based we calculated the PSFs for the decay modes 2νββ and 0νββ for double beta transitions to ground states and excited 2⁺ and 0⁺ states of the daughter nuclei.

The results can be summarized as follows: significant differences were obtained for the PSF values in comparison with older methods, especially for the 2νββ, β⁺ β⁺ and EC decay modes. The differences between our results and other ones from literature, may originate from two sources: i) the use of a more realistic Coulomb potential; ii) improvement of the numerical precision in our routines; iii) new method of identification of the bound states in the numerical procedure of solving the Dirac equation. Differences
obtained by us will determine the lifetime recalculation of DBD and, further, the review of the neutrino mass parameters. These results are reported in refs. [9], [13] and presented in the conference [16]. Encouraged by the results obtained for double beta transitions $\beta^-\beta^-$ and $\beta^+\beta^+$, we have improved the accuracy of numerical calculation of the PSFs, for these transitions. Then, we developed numerical codes to calculate PSFs for DBD modes involving electron capture, $2\nu$EC/$\beta^-$, $0\nu$EC/$\beta^+$ and $2\nu$ECEC. For the latter calculations we developed a procedure for an appropriate identification of the “bound” eigenvalues obtained by solving the Dirac equation for these electron capture decay modes. We also showed that the previous PSF results were based on a numerical procedure that could lead to an incorrect choice of the eigenvalues and, hence, leads to erroneous results. It is also one of the explanations for the significant differences, in several cases, between our PSF values and those found in literature, for electron double beta transitions. Thus, we calculated a complete set of PSFs for all decay modes and possible double beta transitions. The results were published in Refs. [13], [25] and were presented in the conference MEDEX'15 [26].

**Calculation of beta transitions in stellar environments**

We began in stage 1 of the project, a program to develop an advanced numerical code, alternative to the ShM, based on approximation pnQRPA, for DBD calculations. First, we developed this code to calculate transitions GT and beta decay rates in stellar environments, in which were included transitions "unique first forbidden" (U1F). We reported decay rates and lifetimes for beta and forbidden beta decays of isotopes Ni (72-78), calculated for the first time for a stellar environment, with a code based on pnQRPA. It was shown that estimating rates of beta decay with inclusion of the U1F transitions, can lead to a better understanding of the composition of the nuclear core of the star, before the collapse stage and also the r processes, which are essential for the synthesis of heavy elements in astrophysical sites. Detailed presentation of these results can be found in ref. [11].

Then, in 2015, we continued the beta decay study in stellar environments with transitions "first forbidden" (FF). They were calculated beta-type transitions FF and GT in stellar environments for Zn and Ge isotopes. Our calculations performed with a QRPA-based method adapted to such transitions are in good agreement with experimental measurements, and show the increasing of the contribution of FF transitions to the total beta decay rate, as the number of protons in the nuclei increases. Details on these results can be found in Ref. [24].

5. **Investigation of the high-energy processes that violate lepton number conservation**

They were investigated the decay processes without neutrino emission, similar to DBD, but which can occur at high energies. Their study opens a new research direction in the LHC experiments at CERN. The search for such processes, in parallel with the DBD study brings advantages to both directions of research and could provide complementary information on the neutrino parameters. We have described
and proposed a number of channels to be investigated in the LHCb experiment at CERN. Details of these results are found in Refs. [2], [8], [14], [17].

6. Constraints on the light and heavy neutrino mass parameters and coupling strength of SUSY particles from $0\nu\beta\beta$ analysis.

Double beta decay without neutrino emission can take place, in principle, through several mechanisms, each of which may contribute to the decay rate. The lifetime expressions of this process can be written therefore as a sum of contributions from several mechanisms. We choose in the following the hypothesis that $0\nu\beta\beta$ can take place through the contribution of four mechanisms: the exchange of light LH neutrinos between nucleons ($<\eta_\nu>$), through the exchange of heavy RH neutrinos between nucleons ($<\eta_N>$), the exchange of SUSY particles (gluino ($<\eta_\lambda>$) and squark ($<\eta_q>$)) between nucleons:

$$\left( T^{0\nu}_{1/2} \right)^{-1} = G^{0\nu}(Q_{\beta\beta}, Z) \left( | M^{0\nu}_\nu | <\eta_\nu> + | M^{0\nu}_N | <\eta_N> + | M^{0\nu}_N | <\eta_N> + | M^{0\nu}_q | <\eta_q> \right)^2$$

In the absence of an experimental signal regarding the discovery of $0\nu\beta\beta$, we can put constraints on these parameters if we have precise theoretical calculations of NMEs and PSFs, and experimental lifetime limits. Taking the newest experimental lifetime results and using the NME and PSF values from our calculations, we extracted new limits for the mass parameters described above. Up-dated values of these parameters are very useful in the study of these processes, which may occur beyond the current Standard Model. The results are listed in the Tables and were published in Adv. High En. Phys. (refs. [14], [15]), and presented in the conferences ISCHIA2014, Italy 12 - 16 May 2014 and ISPUN14 3-8 November, 2014, HoChiMinh, Vietnam.
Phase space factor calculations for beta decay and electron capture

The phase space factors (PSFs) for beta decay have been calculated since long time (see for example Martin&Blichert-Toft, ADNDT A8, 1 (1970); Gove&Martin, ADNDT A10, 3 (1971); Wilkinson&Macefield, NPA 232, 58 (1974)) and have been used to evaluate beta and electron capture rates. Encouraged by the results obtained for the calculations of PSF for double-beta decay, where we have gotten significant differences as compared with previous reported

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<tbody>
<tr>
<td>$Q_{\beta\beta}[MeV]$</td>
<td>$T_{\text{exp}}^{\beta\beta}[yr]$</td>
<td>$G_{\text{exp}}^{0\beta\beta}[yr^{-1}]$</td>
<td>$M_0^{0\beta\beta}$</td>
<td>$\langle m_0 \rangle [eV]$</td>
<td></td>
</tr>
<tr>
<td>$^{48}\text{Ca}$</td>
<td>4.272</td>
<td>&gt; 5.8 $10^{22}[52]$</td>
<td>2.46E-14</td>
<td>0.81-0.90</td>
<td>&lt; [15.0 - 16.7]</td>
</tr>
<tr>
<td>$^{76}\text{Ge}$</td>
<td>2.039</td>
<td>&gt; 2.1 $10^{25}[38]$</td>
<td>2.37E-15</td>
<td>2.81-6.16</td>
<td>[0.37 - 0.82]</td>
</tr>
<tr>
<td>$^{82}\text{Se}$</td>
<td>2.995</td>
<td>&gt; 3.6 $10^{23}[53]$</td>
<td>1.01E-14</td>
<td>2.64-4.99</td>
<td>&lt; [1.70 - 3.21]</td>
</tr>
<tr>
<td>$^{98}\text{Zr}$</td>
<td>3.350</td>
<td>&gt; 9.2 $10^{21}[54]$</td>
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<td>2.19-5.65</td>
<td>&lt; [6.59 - 17.0]</td>
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<td>1.57E-14</td>
<td>3.93-6.07</td>
<td>&lt; [0.64 - 0.99]</td>
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<td>$^{116}\text{Cd}$</td>
<td>2.814</td>
<td>&gt; 1.7 $10^{23}[56]$</td>
<td>1.66E-14</td>
<td>3.29-4.79</td>
<td>&lt; [2.00 - 2.92]</td>
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<td>&gt; 2.8 $10^{24}[57]$</td>
<td>1.41E-14</td>
<td>2.65-5.13</td>
<td>&lt; [0.50 - 0.97]</td>
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<tr>
<td>$^{136}\text{Xe}$</td>
<td>2.458</td>
<td>&gt; 1.6 $10^{23}[39]$</td>
<td>1.45E-14</td>
<td>2.19-4.20</td>
<td>&lt; [0.25 - 0.48]</td>
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<tr>
<td>$^{150}\text{Nd}$</td>
<td>3.371</td>
<td>&gt; 1.8 $10^{22}[55]$</td>
<td>6.19E-14</td>
<td>1.71-3.16</td>
<td>&lt; [4.84 - 8.95]</td>
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</table>

Table 2 Majorana neutrino mass parameters together with the other components of the $0\nu\beta\beta$ decay halflife: the $Q_{\beta\beta}$ values, the experimental lifetimes limits, the phase space factors and the nuclear matrix elements.

<table>
<thead>
<tr>
<th></th>
<th>$T_{\text{exp}}^{0\nu}[yr]$</th>
<th>$G_{\text{exp}}^{0\nu}[yr^{-1}]$</th>
<th>$M_0^{0\nu}$</th>
<th>$M_N^{0\nu}$</th>
<th>$M_Y^{0\nu}$</th>
<th>$\langle \eta_N \rangle$</th>
<th>$\langle \eta_Y \rangle$</th>
<th>$\langle \eta_q \rangle$</th>
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<tr>
<td>$^{48}\text{Ca}$</td>
<td>5.8 $10^{22}[43]$</td>
<td>2.46E-14</td>
<td>70.3</td>
<td>548.2</td>
<td>70</td>
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<td>4.83-10^{-8}</td>
<td>3.78-10^{-7}</td>
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<tr>
<td>$^{48}\text{Ca}$</td>
<td>5.8 $10^{22}[43]$</td>
<td>2.46E-14</td>
<td>82.8</td>
<td>641.7</td>
<td>78.6</td>
<td>3.20-10^{-7}</td>
<td>4.12-10^{-8}</td>
<td>3.37-10^{-7}</td>
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<tr>
<td>$^{76}\text{Ge}$</td>
<td>2.1 $10^{25}[44]$</td>
<td>2.37E-15</td>
<td>199.2</td>
<td>1509.4</td>
<td>296.8</td>
<td>0.22-10^{-7}</td>
<td>0.30-10^{-8}</td>
<td>0.15-10^{-7}</td>
</tr>
<tr>
<td>$^{82}\text{Se}$</td>
<td>3.6 $10^{23}[45]$</td>
<td>1.01E-14</td>
<td>184.5</td>
<td>1393.5</td>
<td>268.1</td>
<td>0.90-10^{-7}</td>
<td>1.19-10^{-8}</td>
<td>0.62-10^{-7}</td>
</tr>
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</table>

* denotes GXPFI A [40] effective interaction and † KB3G [41] effective interaction.

7. Phase space factor calculations for beta decay and electron capture

The phase space factors (PSFs) for beta decay have been calculated since long time (see for example Martin&Blichert-Toft, ADNDT A8, 1 (1970); Gove&Martin, ADNDT A10, 3 (1971); Wilkinson&Macefield, NPA 232, 58 (1974)) and have been used to evaluate beta and electron capture rates. Encouraged by the results obtained for the calculations of PSF for double-beta decay, where we have gotten significant differences as compared with previous reported
results, we developed a similar method for PSF calculations for single beta decays and electron
capture. For beta decay cases we also used a relativistic formalism where the electron/positron
wave functions for free and bound states are solutions of Dirac equations in a Coulomb-type
potential. This potential was obtained from a realistic distribution of protons in the decaying
nuclei. The corrections to these wave functions have been introduced through methods that differ
from those used in previous similar calculations. For example, the screening effect was taken
into account by multiplying the Coulomb potential with a scalar function, solution of a Thomas-
Fermi equation, resolved with the Majorana method. The numerical accuracy imposed to the new
developed algorithms is superior to that used in old algorithms, previously used in similar
calculations. We also used the most recent Q-values reported in literature. For beta decay with
positron emission, we find that our results are in good agreement with previous results for the
majority of nuclei, but there are also relevant differences in many cases. We also observed a
notable influence of the screening effect. Our PSF calculations may be useful for more precise
evaluation of the beta decay and electron capture rates for nuclei far from the beta stability line
and, further for a better understanding of the stellar evolution. Some of the results are presented
in Tables 1 and 3. More details and results can be find in ref. [30].
Table 1: Calculated phase space of $\beta^+$-decay (BP) compared with previous calculations. The value of maximum $\beta$-decay energy is taken from [15] for pure Fermi transitions. The last two columns show our calculated results.

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<td>$^{10}$C</td>
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<td>2.361</td>
<td>2.325</td>
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<td>$^{14}$O</td>
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<td>43.398</td>
<td>43.378</td>
<td>42.822</td>
<td>42.814</td>
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<td>$^{18}$Ne</td>
<td>2.383</td>
<td>136.83</td>
<td>136.83</td>
<td>135.19</td>
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<td>$^{22}$Mg</td>
<td>3.109</td>
<td>427.02</td>
<td>426.88</td>
<td>422.19</td>
<td>421.51</td>
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<td>$^{26}$Al</td>
<td>3.211</td>
<td>483.84</td>
<td>483.68</td>
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<td>1035.9</td>
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<td>2014.7</td>
<td>2013.4</td>
<td>1993.13</td>
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<td>5.021</td>
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<td>3383.8</td>
<td>3351.58</td>
<td>3339.85</td>
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<td>5.028</td>
<td>3346.9</td>
<td>3344.9</td>
<td>3312.82</td>
<td>3300.54</td>
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<tr>
<td>$^{38}$Ca</td>
<td>5.620</td>
<td>5515.9</td>
<td>5510.3</td>
<td>5457.95</td>
<td>5449</td>
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<tr>
<td>$^{42}$Sc</td>
<td>5.409</td>
<td>4533.5</td>
<td>4531.7</td>
<td>4490.19</td>
<td>4462.21</td>
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<td>5.964</td>
<td>7025.4</td>
<td>7024.1</td>
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<td>6853.74</td>
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<td>6.032</td>
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<td>7091.9</td>
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<td>15956</td>
<td>15951</td>
<td>14988.470</td>
<td>14412.5</td>
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</table>
Other results:

1) Following the results obtained in the field, project members were invited to give oral presentations and invited lectures at international conferences mentioned in the bibliography.

2) The project helped to develop international collaborations. Two foreign researchers visited Horia Hulubei Foundation: prof. Jameel Un- Nabi Jameel, dean at the GIK Institute, Pakistan and dr. Javier...
Menendez from Darmstadt, Germany, with which we started collaborations on topics related to the project theme.

(3) Completion of a PhD thesis in the project domain, double beta decay. A. Neacsu, a project team member, included part of the above described results in his doctoral thesis: "Charge-exchange exotic reactions". He defended his thesis in a public session, on October 24, 2013.

(4) A remarkable result is the receipt of our group, its leader (S. Stoica) with HHF affiliation as associate member of the SuperNEMO prestigious international collaboration, which aims to build a new generation detector for measuring a DBD in the underground laboratory in Modane, France. The receipt was made after the presentation of our achievements in SuperNEMO meeting, from Paris, 22-25 October 2012.

(5) S. Stoica and M. Horoi, were among the four organizers (S. Stoica main organizer) of the Workshop "Towards a resolution of the DBD problem", held at "European Centre Theoretical Physics in Nuclear Physics and Related Areas" (ECT*), Trento, September 3-7, 2012. (www.ectstar.eu). It was one of the most important conferences on DBD topic and was attended by major figures in the field.

(6) S. Stoica was invited to join the conference program committee MANPP13 (http://www.engii.org/workshop/manpp2013august/).

(7) With these results we consider, the appropriate objectives of the project have been fulfilled.

References
Articles and Conferences
2012


8. S. Stoica, Neutrino properties probed by LNV at low and high energies, Workshop of the SEE UNESCO network, on Quantum Field Theory and Hamiltonian Systems Craiova, 19-22 September; Rom. J. Phys., 58, no. 5-6, 665 (2013). ISSN 1221-146X.

2013-2014


Seminarii, conferințe
17. S. Stoica, Motivation for the search of LNV processes at high energy, seminar CERN, January, 2013.

2015 Articles


Conferences
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