Improvements of the Shell Model Method for Calculations of the Two-Body Matrix Elements of the Transition Operators in Neutrinoless Double Beta Decay

A. Neacsu[1,2]

[1] IFIN-HH, Magurele Bucharest
[2] "Horia Hulubei" Foundation, Magurele Bucharest

Seminar DFT 2012

Summary

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Introduction - $\beta\beta$ decay

The $\beta\beta$ - a transition among isobaric isotopes that transforms an e-e nucleus into another e-e nucleus with **Z** modified by two units and **A** unchanged.

$2\nu\beta\beta$ (exp. observed and in agreement to SM)

$(Z, A) \rightarrow (Z+2, A) + 2e^- + 2\bar{\nu}_e, \quad \left(T^{2\nu}_{1/2}\right)^{-1} = G^{2\nu}(Q, Z) \mid M^{2\nu}_{GT} \mid^2,$

$G^{2\nu}$-phase space, Q-transition energy and $M^{2\nu}_{GT}$ the MNE

$M^{2\nu}_{GT} = \sum_j \frac{\left\langle 0^+_f \mid t_- \sigma \| 1^+_j \right\rangle \left\langle 1^+_j \| t_- \sigma \mid o^+_i \right\rangle}{E_j + Q/2 + m_e - E_i}$.

We observe that in the half life expression, the sum is only over 1^+ states.

$0\nu\beta\beta$ (th. predicted by theories beyond SM)

When considering only the exchange of light SM ν between nucleons. $(Z, A) \rightarrow (Z+2, A) + 2e^-$,

$\left(T^{0\nu}_{1/2}\right)^{-1} = F^{0\nu}_1 \mid M^{0\nu} \mid^2 \left(\frac{\langle m_\nu \rangle}{m_e}\right)^2$,

$M^{0\nu} = M^{0\nu}_{GT} - \left(\frac{g_V}{g_A}\right)^2 \cdot M^{0\nu}_F + M^{0\nu}_T \qquad M^{0\nu}_\alpha = \sum_{m,n} \left\langle 0^+_f \| t_{-m} t_{-n} O^\alpha_{mn} \| 0^+_i \right\rangle$,

where O^α_{mn} are transition operators and $\alpha = GT, F, T$

The $\langle m_\nu \rangle$ ν mass parameter could be extracted if we have an accurate evaluation of the NME.

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- $0\nu\beta\beta$ decay
  - occurs by violationg the conservation of the total lepton number
  - is a beyond Standard Model process
  - fundamental for the study of nutrino propreties:
    - ν mass
    - nature of the ν: Dirac or Majorana
- calculation of NME for the $0\nu\beta\beta$ decay halflives
  - Shell Model ShM
  - Quasi Random Phase Approximation QRPA
  - Interacting Boson Approach IBA
  - Angular Momentum Projected Hartree-Fock-Bogoliubov PHFB
  - Energy Density Functional EDF

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The Shell Model approach:

- advantages : incorporates all types of correlations and uses effective nucleon-nucleon interactions which are checked with other spectroscopic calculations for nuclei from the same region.
- disadvantages : the problem of the large model spaces which requires the transition operator to be modified.

J. Engel and G. Hagen, Phys. Rev. C 79, 064317 (2009) analyzed for the $0\nu\beta\beta$ decay of ^{82}Se in the *jj*44 model space consisting of the $f_{5/2}, p_{3/2}, p_{1/2}, g_{9/2}$ orbitals.
Computations have to be performed in up to 8 major harmonic oscillator shells (MHOS) and one needs all two body matrix elements of the $0\nu\beta\beta$ transition operator in these large spaces.

Recent proposals to investigate the modifications of the transition operator in increasingly larger shell model spaces for a fictitious $0\nu\beta\beta$ decay of a $p-$shell nucleus:

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Our previous work

In previous works,
M. Horoi and S. Stoica, Phys. Rev. **81**, 024321 (2010),
M. Horoi, S. Stoica, B.A. Brown, Phys Rev C **75** 034303 (2007)
our group started to develop an efficient nuclear ShM approach to accurately calculate the NMEs for both $2\nu\beta\beta$ and $0\nu\beta\beta$ decay modes. The approach used to calculate the two-body matrix elements (TBME) of the transition operator that includes higher order terms in the nucleon current needs to calculate two-dimensional integrals, on the relative momentum and the relative coordinate. This approach was sufficiently fast for calculating the two-body matrix elements in a single major shell, such as *pf*-shell. However, calculations of these two-body matrix elements in 8-12 major shells would be intractable with this approach.

Our present status

We have created a new improved (fast, efficient) ShM code which reduces substantially the computing time of calculation of the two-body matrix elements of the transition operators for the $0\nu\beta\beta$ decay.

- a simpler version similar to E. Caurier, A.P. Zuker, A. Poves, G. Martinez-Pinedo, Phys. Rev. C **50**, 225 (1994); J. Retamosa, E. Caurier and F. Nowacki, Phys. Rev. C **51**, 371 (1995), does not include finite nucleon size (FNS) and higher order nucleon currents correction (HOC) effects because the the integrals over the neutrino potentials can be performed only in the coordinate space
- then, the full version of the code, where these effects and the short range correlations (SRC) effects are included, normally two-dimensional integrations need to be done, one in the coordinate space and one in momentum space.

Well, what's new?
The main improvement in this code is a rearrangement of the two-body matrix elements that allows us to do the radial integrals (the integrals in coordinate space) analytically when harmonic oscillator (HO) single particle wave functions are used. Therefore, only the integration over the momentum remains to be performed numerically.

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Details of the calculations

Due to the two-body nature of the transition operator, the matrix elements are reduced to sum of products of two-body transition densities (TBTD) and matrix elements for two-particle states (TBME),

$$M_{\alpha}^{0\nu} = \sum_{j_p j_{p'} j_n j_{n'} J_\pi} TBTD\left(j_p j_{p'}, j_n j_{n'}; J_\pi\right) \left\langle j_p j_{p'}; J_\pi \| \tau_{-1}\tau_{-2} O_{12}^{\alpha} \| j_n j_{n'}; J_\pi \right\rangle ,$$

The two-body transition operators O_{12}^{α} can be expressed in a factorized form as:

$$O_{12}^{\alpha} = N_\alpha S_\alpha^{(k)} \cdot R_\alpha^{(k)}$$

where N_α is a numerical factor including the coupling constants, and $S_\alpha^{(k)}$ and $R_\alpha^{(k)}$ are operators acting on the spin and relative wave functions of two-particle states. Thus, the calculation of the matrix elements of these operators can be decomposed into products of reduced matrix elements within the two subspaces. The expressions of the two-body transition operators are:

$$O_{12}^{GT} = \sigma_1 \cdot \sigma_2 H(r) , \quad O_{12}^{F} = H(r) .$$

The neutrino potential

A neutrino potential of Coulomb type, depending weakly on the intermediate states.
This potential is defined by integrals of momentum carried by the virtual neutrino exchanged between the two nucleons.

$$H_\alpha(r) \quad = \quad \frac{2R}{\pi}\int_0^\infty j_0(qr)\frac{h_\alpha(q)}{\omega}\frac{1}{\omega+\langle E\rangle}q^2dq \quad \equiv \quad \int_0^\infty j_0(qr)V_\alpha(q)q^2dq\ ,$$

where $R = 1.2A^{1/3}$, $\omega = \sqrt{q^2+m_\nu^2}$ neutrino energy and $j_0(qr)$ spherical Bessel function. $\langle E\rangle$ average excitation energy of the states in the intermediate odd-odd nucleus, that contribute to the decay. $h_\alpha(\alpha = F, GT)$

$$h_F = G_V^2(q^2) \quad \text{and}$$

$$h_{GT}(q^2) = \frac{G_A^2(q^2)}{g_A^2}\left[1-\frac{2}{3}\frac{q^2}{q^2+m_\pi^2}+\frac{1}{3}\left(\frac{q^2}{q^2+m_\pi^2}\right)^2\right]+\frac{2}{3}\frac{G_M^2(q^2)}{g_A^2}\frac{q^2}{4m_p^2}\ ,$$

where m_π pion mass, m_p proton mass and $G_M(q^2) = (\mu_p-\mu_n)G_V(q^2)$, with $(\mu_p-\mu_n) = 4.71$.

$$G_A\left(q^2\right) = g_A\left(\frac{\Lambda_A^2}{\Lambda_A^2+q^2}\right)^2,\ G_V\left(q^2\right) = g_V\left(\frac{\Lambda_V^2}{\Lambda_V^2+q^2}\right)^2$$

$g_V = 1$, $g_A = 1.25$, $\Lambda_V = 850MeV$ and $\Lambda_A = 1086MeV$.

Short range corellations

When computing the radial matrix elements
$\langle nl|H_\alpha|n'l'\rangle$ we use the harmonic oscillator wave functions $\psi_{nl}(r)$ and $\psi_{n'l'}(r)$ corrected by a factor $[1 + f(r)]$, which takes into account the nuclear interaction short range correlations:

$$\psi_{nl}(r) \to [1 + f(r)]\, \psi_{nl}(r) \ .$$

For the correlation function we take the functional form

$$f(r) = -c \cdot e^{-ar^2} \left(1 - br^2\right) \ ,$$

where a, b and c are constants which have particular values for in different parameterizations.
In the simple version of our code, in the limit $m_\nu = 0 \to \omega = q$ and when HOC and FNS effects are neglected, the integral over q can be easily done and the expression of the neutrino potential becomes

$$H_\alpha \propto \frac{1}{r} \left[\sin(\langle E\rangle\, r)\ Ci(\langle E\rangle\, r) - \cos(\langle E\rangle\, r)\ Si(\langle E\rangle\, r)\right]$$

where $Si(z)$ and $Ci(z)$ are the sine and cosine integral functions.
Then, the calculation of the radial integrals over the neutrino potential reduces to a single integral in the coordinate space, which can give a hint about the magnitude of the NMES within an error of about 25-35%.

Including HOC and FNS effects the radial matrix elements of the neutrino potentials become:

$$\langle nl \mid H_\alpha(r) \mid n'l' \rangle = \int_0^\infty r^2 dr \psi_{nl}(r)\psi_{n'l'}(r)\,[1+f(r)]^2 \times \int_0^\infty q^2 dq V_\alpha(q) j_0(qr)\ ,$$

where ν is the oscillator constant.
This requires the computation of two integrals, one over the coordinate space and the other over the momentum space.
We rearranged the expression of the radial integral in coordinate space as a sum of terms with the same power of r. The dependence of r appears from the product of the *HO* wave functions, the correlation function and Bessel functions. First, one can write the product of two *HO* wave functions as a sum over the terms with the same power in r:

$$\psi_{nl}(r)\psi_{n'l'}(r) = \sum_{s=0}^{n+n'} A_{l+l'+2s}(nl, n'l') \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \times (2\nu)^{\frac{l+l'+2s+3}{2}} e^{-\nu r^2} r^{l+l'+2s},$$

This leads us to perform integrals of the form:

$$\mathcal{I}_\alpha(\mu; m) = \int_0^\infty q^2 dq\ V_\alpha(q) \times \left(\frac{2}{\pi}\right)^{\frac{1}{2}} (2\nu)^{\frac{m+1}{2}} \int_0^\infty dr\ e^{-\mu r^2} r^m j_0(qr)$$

where $\mu = \nu, \nu + a, \nu + 2a$ and m is integer.

The analytic integration over r

The integration over r can be done analytically and one gets:

$$\left(\frac{2}{\pi}\right)^{\frac{1}{2}}(2\nu)^{\frac{m+1}{2}}\int_0^\infty dr\; e^{-\mu r^2} r^m j_0(qr) =$$

$$\left(\frac{2\nu}{2\mu}\right)^{\frac{m+1}{2}} \times (m-1)!! \sum_{k=0}^{\frac{m}{2}-1}(-1)^k \binom{\frac{m}{2}-1}{k} \frac{e^{-\frac{q^2}{4\mu}}}{(2k+1)!!(2\mu)^k} q^{2k}$$

Thus, $\mathcal{I}_\alpha(\mu; m)$ becomes:

$$\mathcal{I}_\alpha(\mu; m) = \left(\frac{2\nu}{2\mu}\right)^{\frac{m+1}{2}} (m-1)!! \times \sum_{k=0}^{\frac{m}{2}-1}(-1)^k \binom{\frac{m}{2}-1}{k} \mathcal{J}_\alpha(\mu; k)$$

where $\mathcal{J}_\alpha(\mu; k)$ are integrals over momentum:

$$\mathcal{J}_\alpha(\mu; k) = \frac{1}{(2k+1)!!}\frac{1}{(2\mu)^k} \times \int_0^\infty exp\left(-\frac{q^2}{4\mu}\right) q^{2k+2} V_\alpha(q) dq$$

So, the radial matrix element can be expressed as a sum of integrals over the momentum space:

$$\langle nl \mid H_\alpha(r) \mid n'l' \rangle = \sum_{s=0}^{n+n'} A_{l+l'+2s}(nl, n'l') \mathcal{K}_\alpha(m)$$

where $\mathcal{K}_\alpha(m)$ is a sum of six $\mathcal{I}_\alpha(\mu; m)$ integrals over momentum.

Numerical results and discussions

In order to obtain the $M^{0\nu}$ nuclear matrix element, the two-body transition densities are calculated as described in M. Horoi and S. Stoica, Phys. Rev. **81**, 024321 (2010). For ^{48}Ca we used GXPF1A effective interaction in the full *pf* model space, and for ^{82}Se we used JUN-45 effective interaction in the *jj*44 model space.

Our code enables us to include in a flexible manner the nuclear effects, such as SRC of Jastrow type with Miller-Spencer and coupled cluster model (CCM) with Argonne V18 and CD-Bonn parameterizations, FNS, and HOC.

For comparison, we used in our calculation the same nuclear effects as those used in the corresponding references.

$M^{0\nu}$	^{48}Ca	^{82}Se
$^{(*)}$ present work	0.573	2.47
[1] (2010 ShM)	0.57	
[2] (2008 ISM)	0.59	2.11
[3] (2009 ISM)	0.61	2.18
[4] (2007 QRPA)		2.77

Table: Comparison between the results of the present work $^{(*)}$ and other similar results from the references indicated. In the calculation we used SRC of Jastrow type, FNS and HOC.

[1] M. Horoi and S. Stoica, Phys. Rev. **81**, 024321 (2010)

[2] E. Caurier, J. Menendez, F. Nowacki, and A. Poves, Phys. Rev. Lett. **100**, 052503 (2008)

[3] J. Menendez, A. Poves, E. Caurier, F. Nowacki, and A. Poves, Nuclear Physics **A 818** 139-151 (2009)

[4] Markus Kortelainen and Jouni Suhonen, Phys. Rev. C **75** 051303(R) (2007)

How fast did we get?

We have analyzed the performance of our code in getting an improved computing speed.

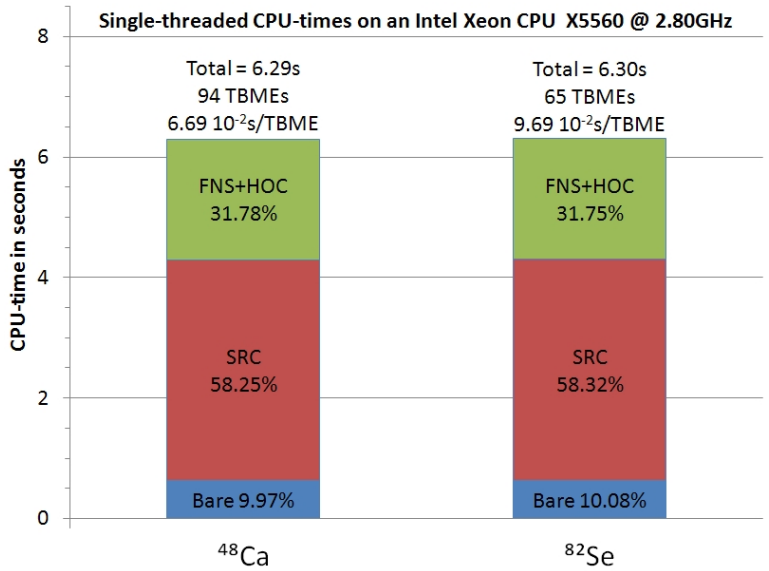

Figure: CPU-times for the computation of the TBMEs

With our new method and code, we obtain an improvement in speed by a factor of about 30, as compared to the previous code used, where more than three minutes where needed instead of 6.3 seconds.
The performance of the new code makes us confident that it is now possible to rapidly, accurately and efficiently compute TBMEs for many nuclear shells. For example, if one wants to investigate the effective transition operator in only 8 MHOS, J. Engel and G. Hagen, Phys. Rev. C **79**, 064317 (2009), one needs to calculate about 434k TBMEs (*GT* plus *F*).

Thank you!