Atomic corrections for the β decay of neutrino mass measurement candidates

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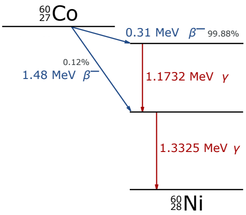
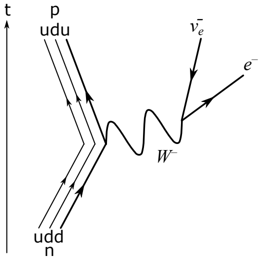
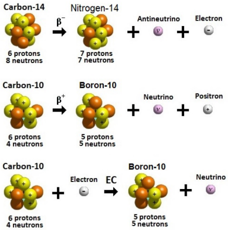
Outlook

Nuclear β decay and EC process





$$H_\beta(x) = \frac{G_\beta}{\sqrt{2}} \overline{e}(x)\gamma_\mu(1-\gamma^5)\nu_e(x)j^\mu(x)$$

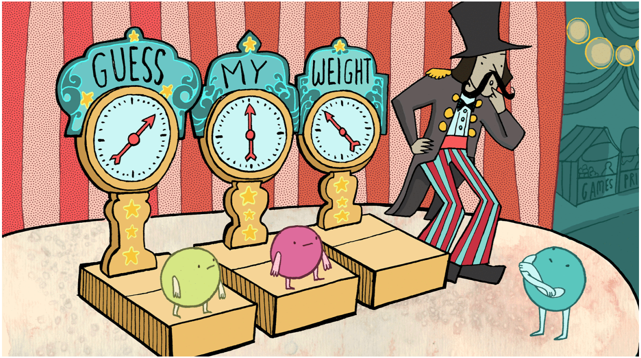


Transition	L	$\lvert\Delta J\rvert$	$\Delta\pi$
allowed	0	0,1	0
first-forbidden	1	0,1,2	1
second-forbidden	2	1,2,3	0
third-forbidden	3	2,3,4	1
fourth-forbidden	4	3,4,5	0

	L	$\lvert\Delta J\rvert$	$\Delta\pi$	S
Fermi	0	0	0	0
Gamow-Teller	0	0,1 ($0 \nrightarrow 0$)	0	1

Why precise β and EC theoretical predictions?

- neutrino mass determination: (ultra-)low Q value β and EC transitions
  KATRIN, Project-8, ECHo, HOLMES, PTOLEMY, NuMECS



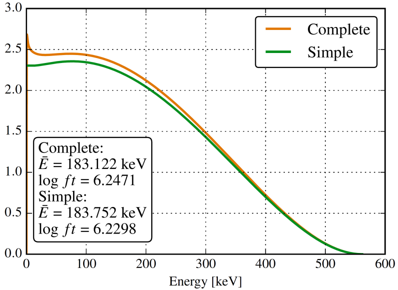
- unavoidable background sources in liquid xenon experiments searching for WIMPs: XENON, LUX, PandaX, XMASS, DarkSide CEνNS: XENONnT, LUX-ZEPLIN, DARWIN
- new physics parameters constrains from the shape analysis of β spectrum

Corrected analytical spectrum of the allowed β^- decay:

$$\frac{d\Gamma}{dE_e} = \frac{G_F^2 V_{ud}^2}{2\pi^3} p_e E_e (E_e^0 - E_e)^2 F_0(Z, E_e) L_0(Z, E_e) U(Z, E_e) D_{FS}(Z, E_e, \beta_2) R(E_e, E_e^0)$$

$$\times R_N(E_e, E_e^0, M) Q(Z, E_e) S(Z, E_e) X(Z, E_e) r(Z, E_e) C(Z, E_e) D_C(Z, E_e, \beta_2)$$

Rev. Mod. Phys. ***90****, 015008 (2018)*

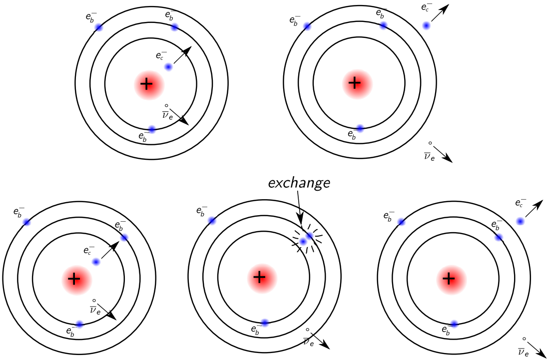


(^{67}Cu) Comput. Phys. Commun. ***240****, 152-164 (2019)*

point-like nucleus, finite nuclear size,

diffuse nuclear surface, deformation, radiative corrections, nuclear recoil, atomic screening, atomic exchange, etc.

Atomic exchange correction in β^- decay



$$\frac{d\Gamma}{dE_e} \Rightarrow \frac{d\Gamma}{dE_e} \times \left[1 + \eta^T(E_e)\right]$$

$$\eta^T(E_e) = f_s(2T_s + T_s^2) + (1 - f_s)(2T_{\bar{p}} + T_{\bar{p}}^2) = \eta_s(E_e) + \eta_{\bar{p}}(E_e)$$

$$T_s = \sum_{(ns)'} T_{ns} = -\sum_{(ns)'} \frac{\left\langle \psi'_{E_e s} \middle| \psi_{ns} \right\rangle}{\langle \psi'_{ns} | \psi_{ns} \rangle} \frac{g'_{n,-1}(R)}{g'_{-1}(E_e, R)}, \quad f_s = \frac{g'^2_{-1}(E_e, R)}{g'^2_{-1}(E_e, R) + f'^2_{+1}(E_e, R)}.$$

DHFS self-consistent method

The relativistic wave function of the bound electron

$$\psi_{n,\kappa}(\boldsymbol{r}) = \sum_{\kappa m} \begin{pmatrix} g_{n,\kappa}(r)\Omega_{\kappa,m}(\hat{\boldsymbol{r}}) \\ i f_{n,\kappa}(r)\Omega_{-\kappa,m}(\hat{\boldsymbol{r}}) \end{pmatrix},$$

where the large- and small-component radial functions obey the radial Dirac equation

$$\left(\frac{d}{dr} + \frac{\kappa+1}{r}\right) g_{n\kappa} - (E_{n\kappa} - V(r) + m_e) f_{n\kappa} = 0,$$

$$\left(\frac{d}{dr} - \frac{\kappa-1}{r}\right) f_{n\kappa} + (E_{n\kappa} - V(r) - m_e) g_{n\kappa} = 0.$$

Bound states ($E_e < m_e$): discrete energy levels (n, κ, $t_{n\kappa}$, $E_{n\kappa} = m_e - |t_{n\kappa}|$), $\langle \psi_{n\kappa} | \psi_{n'\kappa'} \rangle = \delta_{nn'}\delta_{\kappa\kappa'}$ and

$$V(r) \equiv V_{\mathrm{DHFS}}(r) = V_{\mathrm{nuc}}(r) + V_{\mathrm{el}}(r) + V_{\mathrm{ex}}(r)$$

The nuclear potential is obtained from a Fermi distribution for the proton density

$$\rho_p(r) = \frac{\rho_0}{1 + e^{(r - c_{\mathrm{rms}})/a}}, \qquad V_{\mathrm{nuc}}(r) = -\alpha \int \frac{\rho_p(r')}{|\boldsymbol{r} - \boldsymbol{r}'|} d\boldsymbol{r}'.$$

DHFS self-consistent method

The electronic potential is

$$V_{\text{el}}(r) = \alpha \int \frac{\rho(r')}{|\mathbf{r} - \mathbf{r'}|} d\mathbf{r'}.$$

The local exchange potential with correct asymptotic behavour is

$$V_{\text{ex}}(r) = \begin{cases} V_{\text{ex}}^{\text{Slater}}(r) = -\frac{3}{2}\alpha\left(\frac{3}{\pi}\right)^{1/3}[\rho(r)]^{1/3} & r < r_{\text{Latter}}, \\ -\frac{\alpha(Z-N+1)}{r} - V_{\text{nuc}}(r) - V_{\text{el}}(r) & r \geq r_{\text{Latter}}. \end{cases}$$

- start from an approximate electron density (Molière parametrization of the Thomas-Fermi potential)
- solve the Dirac equation
- update the electron density from the obtained wave functions

$$\rho(r) = \sum_{n\kappa} \psi_{n\kappa}^{\dagger}(r)\psi_{n\kappa}(r)$$

- repeat and stop when the atomic binding energy is not changing (ϵ tolerance)

Exchange correction calculation: current status

The overlap between final continuum and initial bound states,

$$\left\langle \psi'_{E_e\kappa} \middle| \psi_{n\kappa} \right\rangle = \int_0^\infty r^2 \left[g'_\kappa(E_e, r) g_{n,\kappa}(r) + f'_\kappa(E_e, r) f_{n,\kappa}(r) \right] dr$$

- good knowledge of the continuum w.f. over large distances
- integration method
- orthogonal continuum and bound w.f. for the same atomic system

Phys. Rev. A ***45***, *6282 (1992)*

$$\left\langle \psi'_{E_e\kappa} \middle| \psi'_{n\kappa} \right\rangle = 0$$

Standard calculations (true DHFS)

$|\psi_{n\kappa}\rangle$, $|\psi'_{n\kappa}\rangle$: $V_{\text{nuc}}(r) + V_{\text{el}}(r) + V_{\text{ex}}(r)$

$|\psi'_{E_e s}\rangle$: $V_{\text{nuc}}(r) + V_{\text{el}}(r)$

Phys. Rev. A ***90***, *012501 (2014)*
Rev. Mod. Phys. ***90***, *015008 (2018)*
Phys. Rev. C ***102***, *065501 (2020)*
Phys. Rev. D ***102***, *072004 (2020)*
Appl. Radiat. Isot. ***185***, *110237 (2022)*

Our calculations (modified DHFS)

$|\psi_{n\kappa}\rangle$, $|\psi'_{n\kappa}\rangle$ and $|\psi'_{E_e s}\rangle$:

$V_{\text{nuc}}(r) + V_{\text{el}}(r) + V_{\text{ex}}^{\text{Slater}}(r)$

Phys. Rev. C ***107***, *025501 (2023)*

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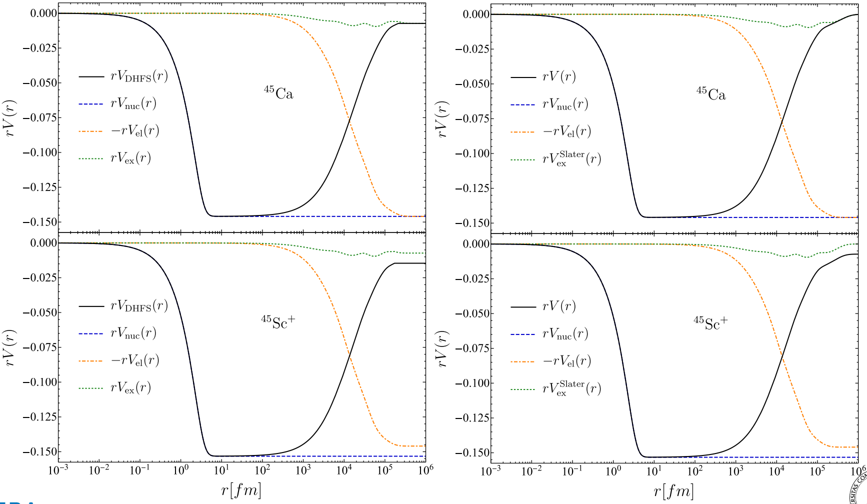
True DHFS vs Modified DHFS

The β-decay of $^{45}Ca \rightarrow {}^{45}Sc^{+} + e^{-} + \overline{\nu}_e$



true DHFS

modified DHFS

Binding Energies (eV)

^{187}Re neutral atom

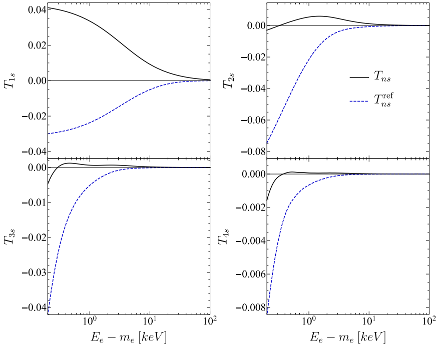
Orbital $(n\ell_j)$	$\epsilon_e^{n\kappa}$ (true)	$\epsilon_e^{n\kappa}$ (modified)	$\epsilon_e^{n\kappa}$(exp)
$1s_{1/2}$	-71857.5	-71857.5	-71681 ± 2
$2s_{1/2}$	-12508.4	-12508.4	-12532 ± 2
$2p_{1/2}$	-11993.7	-11993.7	-11963 ± 2
$2p_{3/2}$	-10537.7	-10537.7	-10540 ± 2
$3s_{1/2}$	-2911.9	-2911.9	-2937 ± 2
$3p_{1/2}$	-2677.7	-2677.7	-2686 ± 2
$3p_{3/2}$	-2360.0	-2360.0	-2371 ± 2
$3d_{3/2}$	-1961.4	-1961.4	-1953 ± 2
$3d_{5/2}$	-1891.9	-1891.9	-1887 ± 2
$4s_{1/2}$	-615.7	-615.7	-629 ± 2
$4p_{1/2}$	-516.7	-516.7	-522 ± 2
$4p_{3/2}$	-442.2	-442.2	-450 ± 2
$4d_{3/2}$	-277.8	-277.8	-278 ± 2
$4d_{5/2}$	-263.9	-263.9	-264 ± 2
$5s_{1/2}$	-91.2	-91.2	-86 ± 2
$5p_{1/2}$	-60.6	-60.6	-56 ± 2
$4f_{5/2}$	-55.0	-55.0	-47 ± 2
$4f_{7/2}$	-52.3	-52.3	-45 ± 2
$5p_{3/2}$	-49.0	-49.0	-45 ± 2
$5d_{3/2}$	**-9.28**	**-9.24**	-9.6 ± 1
$5d_{5/2}$	**-8.24**	**-8.20**	-9.6 ± 1
$6s_{1/2}$	**-7.98**	**-7.67**	-7.9 ± 1

^{45}Ca neutral atom

Orbital $(n\ell_j)$	$\epsilon_e^{n\kappa}$(true)	$\epsilon_e^{n\kappa}$(modified)	$\epsilon_e^{n\kappa}$(exp)
$*1s_{1/2}$	-4015.1	-4015.1	-4041 ± 2
$*2s_{1/2}$	-434.1	-434.1	-441 ± 2
$*2p_{1/2}$	-359.1	-359.1	-353 ± 2
$2p_{3/2}$	-355.2	-355.2	-349 ± 2
$*3s_{1/2}$	-53.2	-53.2	-46 ± 2
$*3p_{1/2}$	-34.0	-34.0	-28 ± 2
$3p_{3/2}$	-33.6	-33.6	-28 ± 2
$*4s_{1/2}$	**-5.45**	**-5.08**	-6.113 ± 0.01

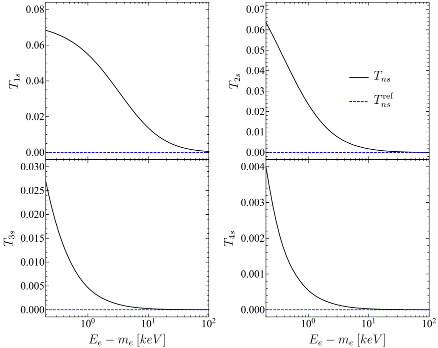
The β-decay of $^{45}\mathrm{Ca} \rightarrow {}^{45}\mathrm{Sc}^{+} + e^{-} + \overline{\nu}_e$

$$T_{ns} = -\frac{\left\langle \psi'_{E_e s} \middle| \psi_{ns} \right\rangle}{\langle \psi'_{ns} | \psi_{ns} \rangle} \frac{g'_{n,-1}(R)}{g'_{-1}(E_e, R)} \qquad T^{\mathrm{ref}}_{ns} = -\frac{\left\langle \psi'_{E_e s} \middle| \psi'_{ns} \right\rangle}{\langle \psi'_{ns} | \psi_{ns} \rangle} \frac{g'_{n,-1}(R)}{g'_{-1}(E_e, R)}$$



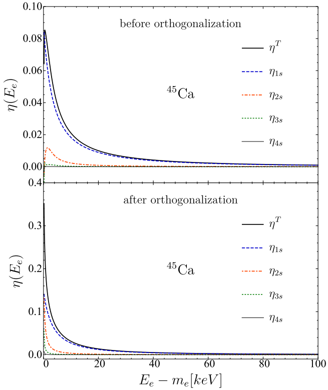
ψ_{ns}, ψ'_{ns}: true DHFS

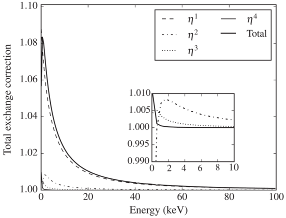
$\psi'_{E_e s}$: $V_{\mathrm{nuc}}(r) + V_{\mathrm{el}}(r)$

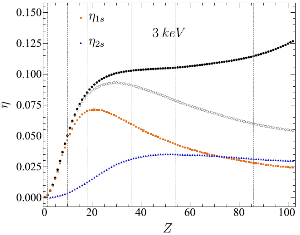


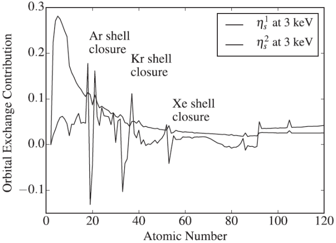
ψ_{ns}, ψ'_{ns}: modified DHFS

$\psi'_{E_e s}$: modified DHFS


before orthogonalization
after orthogonalization
^{45}Ca
η^T
η_{1s}
η_{2s}
η_{3s}
η_{4s}
$\eta(E_e)$
$E_e - m_e[keV]$


η^1
η^2
η^3
η^4
Total
Total exchange correction
Energy (keV)

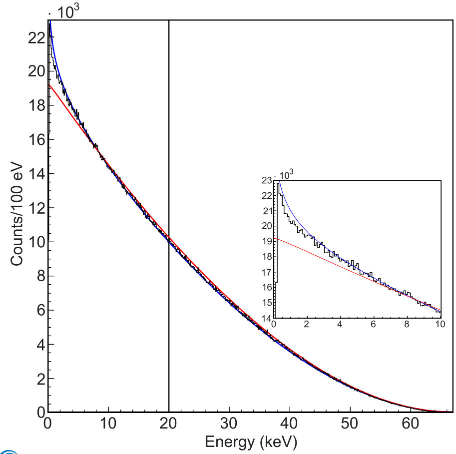

η_{1s}
η_{2s}
3 keV
η
Z


η_s^1 at 3 keV
η_s^2 at 3 keV
Ar shell closure
Kr shell closure
Xe shell closure
Orbital Exchange Contribution
Atomic Number

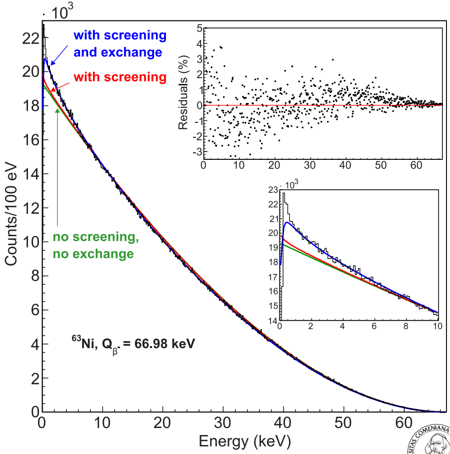
Experiment vs Theory

$$^{63}\text{Ni} \rightarrow {}^{63}\text{Cu}^{+} + e^{-} + \overline{\nu}_e \qquad Q = 66.945 \text{ keV}$$

our result: Phys. Rev. C ***107****, 025501 (2023)*

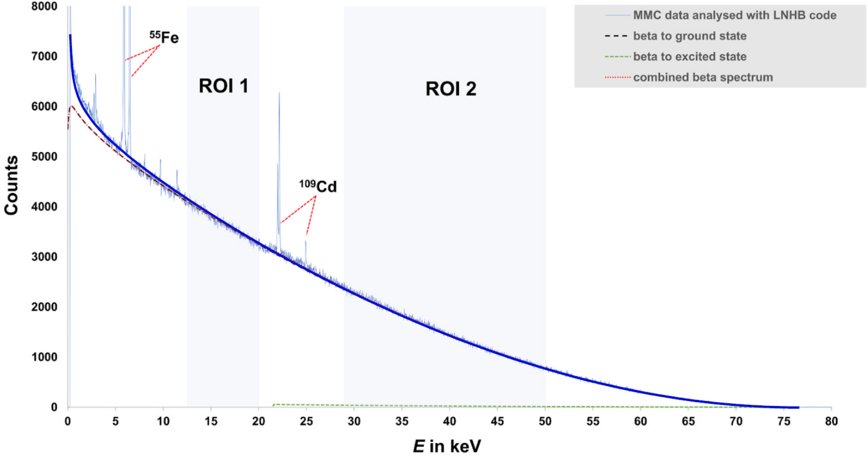


Phys. Rev. A ***90****, 012501 (2014)*



Experiment vs Theory

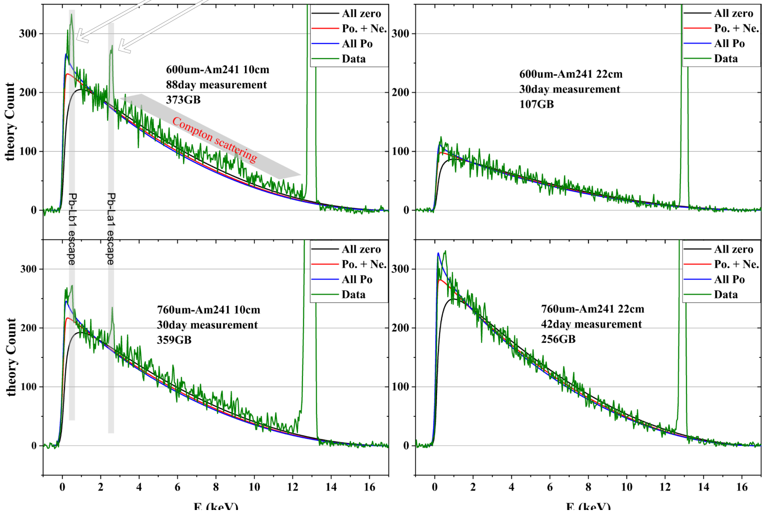
$^{151}\text{Sm} \rightarrow {}^{151}\text{Eu}^{+} + e^{-} + \overline{\nu}_e \qquad Q = 76.6 \text{ keV}$



Appl. Radiat. Isot. ***185****, 110237 (2022)*

Experiment vs Theory

$^{210}\text{Pb} \rightarrow {}^{210}\text{Bi}^{*} + e^{-} + \overline{\nu}_e \qquad Q = 16.96\ \text{keV}$

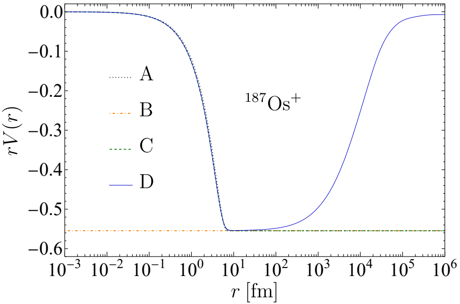


arXiv:2307.16276 (2023)

Atomic corrections for β decay of ^{187}Re

$$^{187}\mathrm{Re} \rightarrow {}^{187}\mathrm{Os}^{+} + \mathrm{e}^{-} + \overline{\nu}_{\mathrm{e}} \qquad \Delta \mathrm{J}^{\pi} = 2^{-} \quad (\Delta \mathrm{L} = 1, \Delta \mathrm{S} = 1)$$

- lowest g.s. to g.s. Q-value in nature ($\sim$ 2.4 keV) $\rightarrow$ perfect candidate for neutrino mass determination (MANU, MIBETA and MARE experiments)



- A: uniform charge sphere for nucleus + approximated w.f.
- B: point-like nucleus + exact w.f.
- C: realistic proton distribution for nucleus + exact w.f.
- D: C + realistic screening (from DHFS) + exact w.f.

Editors' Suggestion

PDF HTML

Atomic corrections for the unique first-forbidden β transition of ^{187}Re

O. Niţescu, R. Dvornický, and F. Šimkovic

Phys. Rev. C **109**, 025501 (2024) – Published 13 February 2024

CIFRA

The decay rate of ^{187}Re

- for 1 electron emitted in $s_{1/2}$-state, 10^4 are emitted in $p_{3/2}$-state

$$\frac{d\Gamma}{dE_e} = \frac{d\Gamma^{p_{3/2}}}{dE_e} + \frac{d\Gamma^{s_{1/2}}}{dE_e} = \sum_{k=1}^{3} |U_{ek}|^2 \frac{G_F^2 V_{ud}^2}{2\pi^3} \; B \; R^2 \; p_e \; E_e \; (E_0 - E_e)$$

$$\times \quad \frac{1}{3}\left[F_1(Z,E_e)p_e^2 + F_0(Z,E_e)((E_0-E_e)^2 - m_k^2)\right]\sqrt{(E_0-E_e)^2 - m_k^2} \quad \theta(E_0 - E_e - m_k)$$

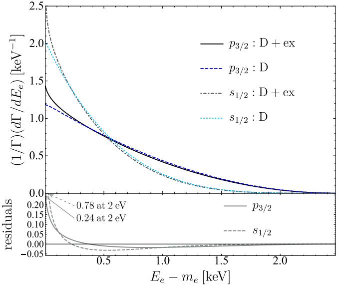
- including exchange correction for $s_{1/2}$- and $p_{3/2}$-state emission

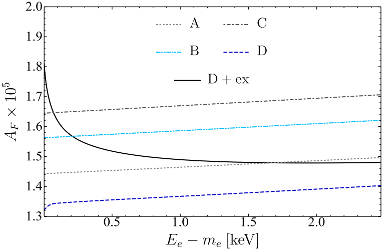
$$\frac{d\Gamma^{s_{1/2}}}{dE_e} \Rightarrow \frac{d\Gamma^{s_{1/2}}}{dE_e} \times (1 + \eta_1^T(E_e)), \qquad \frac{d\Gamma^{p_{3/2}}}{dE_e} \Rightarrow \frac{d\Gamma^{p_{3/2}}}{dE_e} \times (1 + \eta_2^T(E_e)).$$

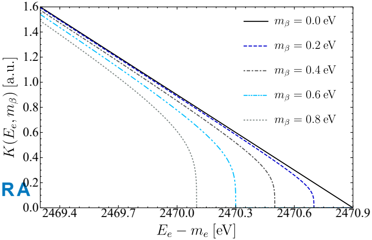
w. f.	$\frac{10^{41}}{B} \times \Gamma^{s_{1/2}}$ [MeV]	$\delta^{s_{1/2}}$ %	$\frac{10^{37}}{B} \times \Gamma^{p_{3/2}}$ [MeV]	$\delta^{p_{3/2}}$ %	$B \times 10^4$
A	9.30	-	9.19	-	3.63
B	8.33	-10.41	8.92	-2.95	3.74
C	7.88	-15.23	8.88	-3.35	3.76
D	7.58	-18.48	6.98	-24.02	4.78
D+ex	9.46	1.75	7.92	-13.84	4.22

Spectrum modification and Kurie plot of ^{187}Re

$$\frac{d\Gamma}{dE_e} = \frac{G_F^2 V_{ud}^2}{2\pi^3} B p_e E_e F_0^{\mathrm{I}}(Z, E_e)(E_0 - E_e)^2 A_F^{\mathrm{I}}$$







$$K(E_e, m_\beta) = \sqrt{\frac{d\Gamma/dE_e}{p_e E_e (p_e R)^2 F_1(Z, E_e)(1 + \eta_2^{\mathrm{T}}(E_e))}}$$

$$= G_F V_{ud} \sqrt{\frac{B}{6\pi^3}} (E_0 - E_e) \sqrt[4]{1 - \frac{m_\beta^2}{(E_0 - E_e)^2}}$$

$$\times \left[1 + \frac{p_\nu}{p_e} \frac{F_0(Z, E_e)}{F_1(Z, E_e)} \frac{(1 + \eta_1^{\mathrm{T}}(E_e))}{(1 + \eta_2^{\mathrm{T}}(E_e))}\right]^{1/2}$$

Conclusions

Exchange correction in allowed β decay:

- For the atomic structure calculation we have used standard and modified self-consistent DHFS framework.
- Imposing the orthogonality condition, i.e. $\left\langle \psi'_{E_e\kappa} \middle| \psi'_{n\kappa} \right\rangle = 0$, is the most important ingredient in the atomic exchange correction.
- Our model is in agreement with the experimental β decay spectra.

Atomic corrections for UFF β decay of ^{187}Re:

- spectrum shape: considerable modification due to exchange correction for $s_{1/2}$ and $p_{3/2}$ emissions
- decay rate: 14% decrease for $p_{3/2}$ emission and 2% increase for $s_{1/2}$ emission
- redefinition of the Fermi-Kurie function to maintain the linearity for $m_\beta = 0$

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$2\nu\beta\beta$-decay rate via Taylor expansion

We get a more accurate expression of the $2\nu\beta\beta$ decay rate

$$\left[T^{2\nu}_{1/2}(\xi_{31},\xi_{51})\right]^{-1} = G^{2\nu}_0 \left(g_A^{\text{eff}}\right)^4 \left|M^{2\nu}_{GT}\right|^2 \times \left\{1 + \xi_{31}\frac{G^{2\nu}_2}{G^{2\nu}_0} + \frac{1}{3}\xi^2_{31}\frac{G^{2\nu}_{22}}{G^{2\nu}_0} + \left(\frac{1}{3}\xi^2_{31} + \xi_{51}\right)\frac{G^{2\nu}_4}{G^{2\nu}_0}\right\},$$

by performing in the matrix elements the following Taylor expansion

$$M^{K,L}_{F,GT} = m_e \sum_n M_{F,GT}(n)\frac{E_n - (E_i - E_f)/2}{[E_n - (E_i - E_f)/2]^2 - \epsilon^2_{K,L}}$$
$$= m_e \sum_n M_{F,GT}(n)\frac{1}{E_n - (E_i - E_f)/2} \times \left\{1 + \left(\frac{\epsilon_{K,L}}{E_n - (E_i - E_f)/2}\right)^2 + \left(\frac{\epsilon_{K,L}}{E_n - (E_i - E_f)/2}\right)^4 + \dots\right\}$$

F.Šimkovic, R. Dvornický, D. Štefánik, and A. Faessler, Phys. Rev. C 97, 034315 (2018)

CIFRA

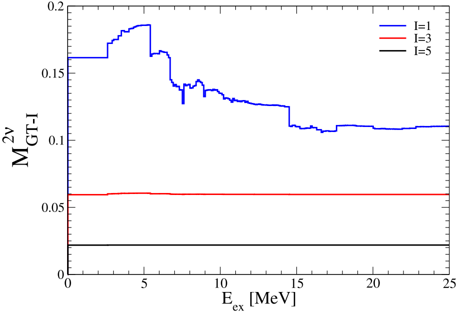
$2\nu\beta\beta$-decay rate via Taylor expansion

$$\xi_{31} = \frac{M^{2\nu}_{GT-3}}{M^{2\nu}_{GT}}, \qquad \xi_{51} = \frac{M^{2\nu}_{GT-5}}{M^{2\nu}_{GT}}.$$

$$M^{2\nu}_{GT-1} \equiv M^{2\nu}_{GT} = \sum_n M_{GT}(n) \frac{m_e}{E_n(1^+) - (E_i + E_f)/2},$$

$$M^{2\nu}_{GT-3} = \sum_n M_{GT}(n) \frac{4\ \ m_e^3}{[E_n(1^+) - (E_i + E_f)/2]^3},$$

$$M^{2\nu}_{GT-5} = \sum_n M_{GT}(n) \frac{16\ \ m_e^5}{[E_n(1^+) - (E_i + E_f)/2]^5},$$



$$M_{GT}(n) = \langle 0_f^+ \| \sum_m \tau_m^+ \sigma_m \| 1_n^+ \rangle \langle 1_n^+ \| \sum_m \tau_m^+ \sigma_m \| 0_i^+ \rangle,$$

Adding exchange and radiative corrections to $2\nu\beta\beta$ decay

O. Nițescu, S. Stoica, R. Dvornický and F.Šimkovic, Universe 2021, 7(5), 147

$$G_N^{2\nu} = \frac{m_e (G_\beta m_e^2)^4}{8\pi^7 \ln 2} \frac{1}{m_e^{11}} \int_{m_e}^{E_i - E_f - m_e} dE_{e_1} \int_{m_e}^{E_i - E_f - E_{e_1}} dE_{e_2}$$
$$\times p_{e_1} E_{e_1} \left[1 + \eta^T(E_{e_1})\right] R(E_{e_1}, E_i - E_f - m_e) p_{e_2} E_{e_2} \left[1 + \eta^T(E_{e_2})\right]$$
$$\times R(E_{e_2}, E_i - E_f - E_{e_1}) F_{ss}(E_{e_1}) F_{ss}(E_{e_2}) \mathscr{I}_N$$

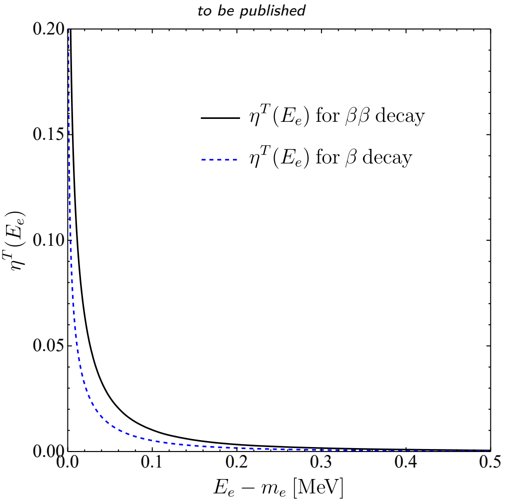
with $N = \{0, 2, 22, 4\}$.

$$R(E_e, E_e^{\max}) = 1 + \frac{\alpha}{2\pi} g(E_e, E_e^{\max})$$

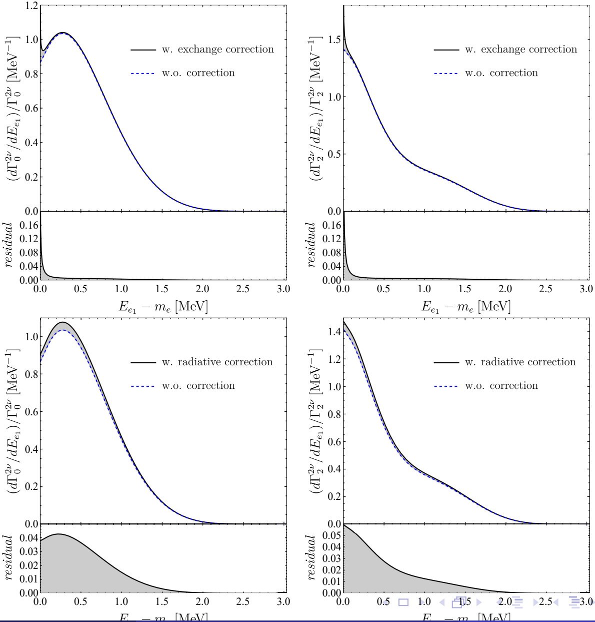
$$g(E_e, E_e^{\max}) = 3\ln(m_p) - \frac{3}{4} - \frac{4}{\beta}\mathrm{Li}_2\left(\frac{2\beta}{1+\beta}\right)$$
$$+ \frac{\tanh^{-1}\beta}{\beta}\left[2\left(1+\beta^2\right) + \frac{(E_e^{\max} - E_e)^2}{6E_e^2} - 4\tanh^{-1}\beta\right]$$
$$+4\left(\frac{\tanh^{-1}\beta}{\beta} - 1\right)\left\{\frac{E_e^{\max} - E_e}{3E_e} - \frac{3}{2} + \ln\left[2\left(E_e^{\max} - E_e\right)\right]\right\}$$

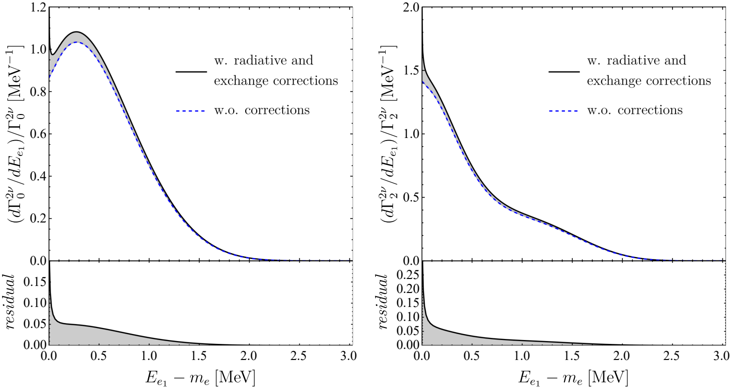
where $\beta = p_e / E_e$.

Exchange correction for β and $\beta\beta$ decay



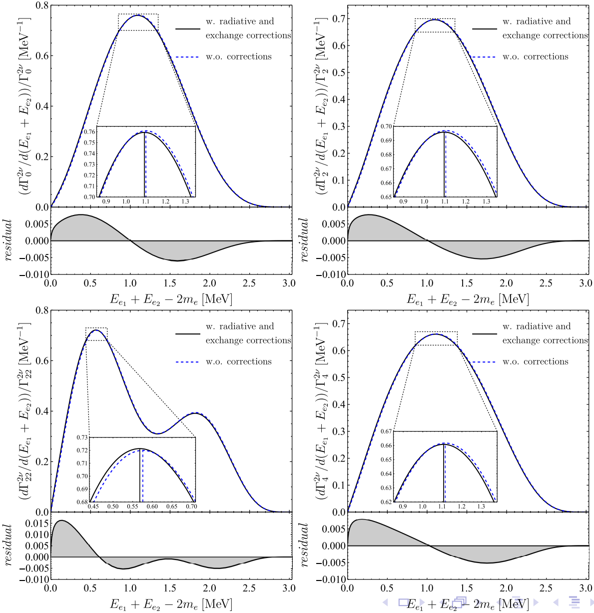
Single Electron Spectra





Nucleus	Correction(s)	$G_0^{2\nu}$	$G_2^{2\nu}$	$G_{22}^{2\nu}$	$G_4^{2\nu}$
^{100}Mo	DHFS	3.307×10^{-18}	1.511×10^{-18}	1.989×10^{-19}	8.652×10^{-19}
	Exchange	3.343×10^{-18}	1.536×10^{-18}	2.031×10^{-19}	8.835×10^{-19}
	Radiative	3.432×10^{-18}	1.568×10^{-18}	2.066×10^{-19}	8.974×10^{-19}
	Radiative and Exchange	3.470×10^{-18}	1.593×10^{-18}	2.109×10^{-19}	9.164×10^{-19}
	δ	4.91%	5.42%	5.97%	5.92%

Summed Electron Spectra



Remarks for corrections in $2\nu\beta\beta$ decay

Radiative and exchange corrections in $2\nu\beta\beta$ decay:

- shape modifications in the single electron spectrum due to exchange corrections
- around 5% deviations in the decay rate for ^{100}Mo due to radiative correction
- a shift of $\sim$10 keV in the summed electron spectrum which may be important for SM and BSM experimental investigations