Nuclear structure input to low-energy precision tests of the Standard Model via superallowed $0^+ \to 0^+$ Fermi β decay

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Outline

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6. Radial mismatch correction
7. Standard-Model implications

Aims

- To investigate isospin-symmetry breaking within the shell-model framework, and its impact on weak interaction tests

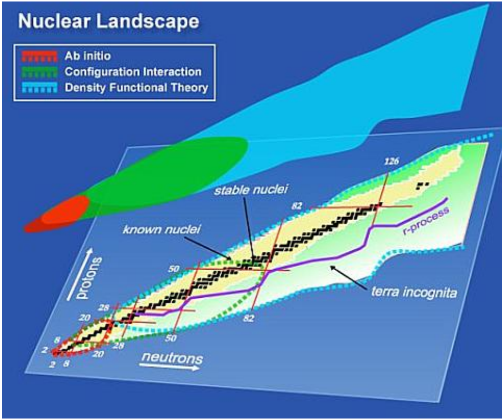
1) Improve isospin-nonconserving effective interactions (Coulomb, nuclear charge-dependent forces)
2) Implement realistic bases (Woods-Saxon, Hartree-Fock)
3) Explore theoretical uncertainty quantification by examining parameter-(fitting) dependence

Typical nuclear many-body approaches

- General nuclear Hamiltonian

$$H = \sum_i^A \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j}^A V_{ij}^{NN} + \mathcal{O}(V^{3N})$$

1) Ab-initio methods (typically up to the lower part of the *sd* shell)
2) Configuration interaction (can reach the Sn region within an inert core)
3) DFT (the whole nuclear landscape)



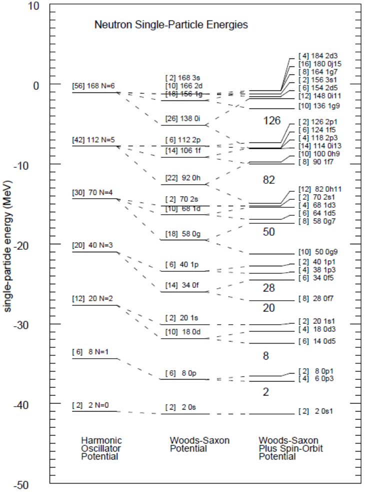
Each approach has its pros and cons, depending on the nature of the state/observable to be calculated.

- **Major ingredients for the shell-model :**

1) Valence space (defined by magic numbers)
2) Basis functions (oscillator, Woods-Saxon, Hartree-Fock, ...)
3) Effective nuclear interactions optimized for the model spaces,

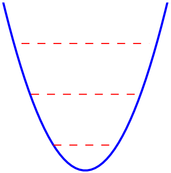
$$H_{eff} = PHP, \quad QH_{eff}P = 0, \quad P + Q = 1$$

where various choices are available for H.



http://nucleartalent.github.io/Course2ManyBodyMethods/doc/pub/intro/html/intro.html

How the shell model works



1) Choosing a suitable basis (spherically symmetric HO)

$$\phi_{nljm}(\boldsymbol{r}) = R_{nlj}(r) \sum_{m_l m_s} \langle l \frac{1}{2} m_l m_s | jm \rangle \, Y^l_{m_l}(\boldsymbol{\Omega}) \chi^{\frac{1}{2}}_{m_s}(\boldsymbol{\sigma}$$

$$\Phi_x(\boldsymbol{r}_1, ..., \boldsymbol{r}_A) = \frac{1}{\sqrt{A!}} \sum_{\alpha \in S_A} sgn(\alpha) \prod_{i=1}^{A} \phi_{\alpha_i}(\boldsymbol{r}_i)$$

2) Configuration-mixing wave functions

$$\Psi_x = C_{x1}\Phi_{x1} + C_{x2}\Phi_{x2} + C_{x3}\Phi_{x3} + ...$$

3) Solving the secular equation

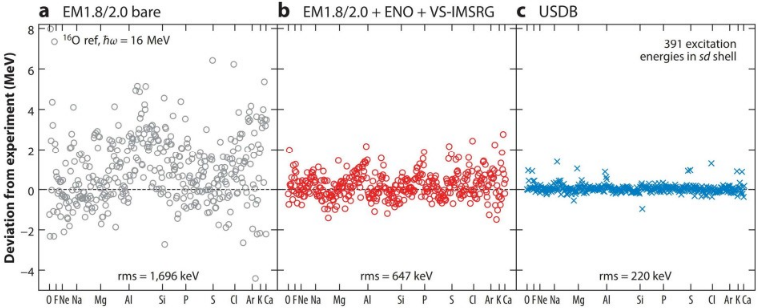
$$\begin{pmatrix} \langle \Phi_{x1}|H_{eff}|\Phi_{x1}\rangle & \langle \Phi_{x1}|H_{eff}|\Phi_{x2}\rangle & \cdots & \langle \Phi_{x1}|H_{eff}|\Phi_{xn}\rangle \\ \langle \Phi_{x2}|H_{eff}|\Phi_{x1}\rangle & \langle \Phi_{x2}|H_{eff}|\Phi_{x2}\rangle & \cdots & \langle \Phi_{x2}|H_{eff}|\Phi_{xn}\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \Phi_{xn}|H_{eff}|\Phi_{x1}\rangle & \langle \Phi_{xn}|H_{eff}|\Phi_{x2}\rangle & \cdots & \langle \Phi_{xn}|H_{eff}|\Phi_{xn}\rangle \end{pmatrix} \begin{pmatrix} C_{x1} \\ C_{x2} \\ \vdots \\ C_{xn} \end{pmatrix} = E_x \begin{pmatrix} C_{x1} \\ C_{x2} \\ \vdots \\ C_{xn} \end{pmatrix}$$

This is a large but sparse matrix. Computational price :

$$Dim = \begin{pmatrix} D_N \\ N \end{pmatrix} \times \begin{pmatrix} D_Z \\ Z \end{pmatrix}$$

Precision hierarchy of the shell model

- Construction of effective interaction is essential for valence-space shell model. Three-body force is often necessary, if higher precision is required.



Stroberg, ARNPS69, 307 (2019)

Phenomenological effective interactions typically provide the highest precision.

Superallowed $0^+ \to 0^+$ Fermi β decay

- **Superallowed $0^+ \to 0^+$ Fermi β decay of $T = 1$ (isotriplet) nuclei**

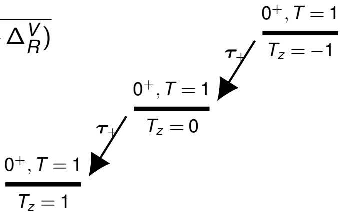
1) The cleanest probe of the Standard Model (weak sector)

$$\mathscr{F}t = ft(1+\delta_R')(1-\delta_C+\delta_{NS}) = \frac{K}{2G_F^2 V_{ud}^2(1+\Delta_R^V)}$$

ft ~experimental input,

δ_C ~nuclear structure correction,

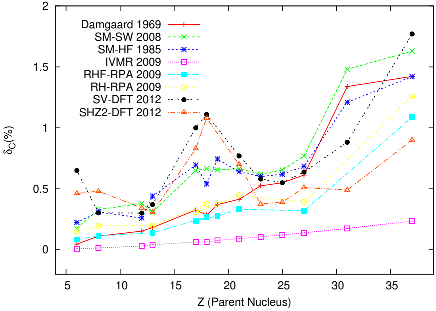
$(\delta_R', \delta_{NS}, \Delta_R^V)$ ~radiative corrections.



2) Experimental error~ 0.1% or better. **It is challenging for any theoretical models to meet this precision requirement**.

Hardy and Towner, PRC102, 045501 (2020)

- Divergence of δ_C



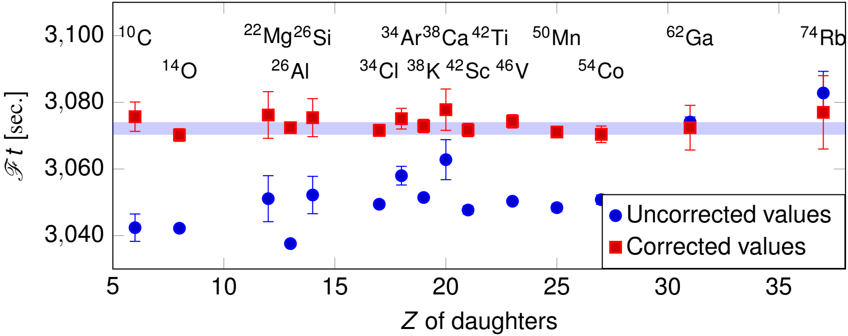
1) Damgaard: harmonic oscillator
2) RHF-RPA/RH-RPA: relativistic mean field + RPA
3) SV-DFT/SHZ2-DFT: density functional theory with JT projections
4) IVMR: isovector monopole resonances
5) SM-WS: shell model with WS basis
6) SM-HF: shell model with HF basis

- Considering all these variations, the uncertainties in δ_C reach nearly 100 %.
- **Only the shell-model results are consistent with CVC. However, a significant discrepancy persists between SM-WS and SM-HF**.

Towner and Hardy, PRC82, 065501 (2010)

Superallowed $0^+ \to 0^+$ Fermi β decay

- 15 cases with sub-percent exp. precision (δ_C from SM-WS)



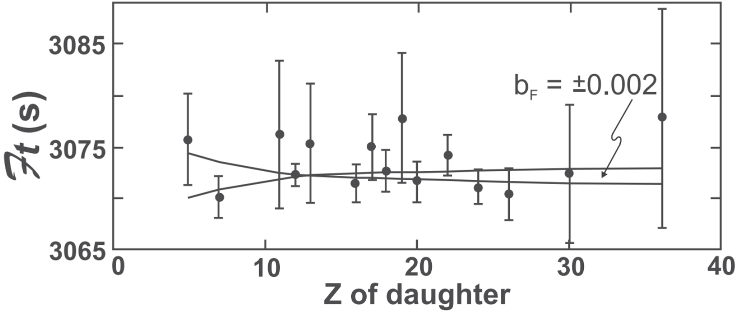
1) Good agreement with CVC : $\overline{\mathscr{F}t} = 3072.24 \pm 0.57_{stat} \pm 0.36_{\delta'_R} \pm 1.73_{\delta_{NS}}$ sec with $\chi^2/\nu = 0.47$. **The theoretical corrections are primary contributor to the uncertainties**.

Hardy and Towner, PRC102, 045501 (2020)

- Constraining the scalar current (δ_C from SM-WS)

$$\mathscr{F}t = \frac{K}{2G_F^2 V_{ud}^2(1+\Delta_R^V)} \frac{1}{1+b_F\gamma\langle 1/W\rangle}$$

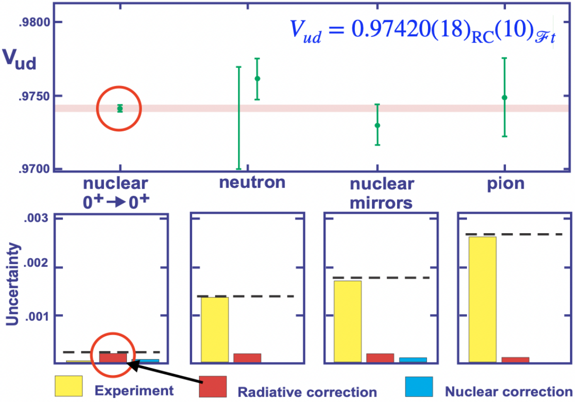
where $b_F = 2C_S/C_V$ and $\gamma = \sqrt{1-\alpha^2 Z^2}$



As W increases with A, the scalar contribution is expected to be largest in light nuclei, in particular ^{10}C and ^{14}O. **Improving theo. uncertainties in these two cases is priority !**.

Hardy and Towner, PRC102, 045501 (2020)

- Comparison of $|V_{ud}|$ data (δ_C from SM-WS)



Based on data from superallowed $0^+ \to 0^+$ Fermi β decay, **the CKM top-row unitarity is found to be violated by more than two standard deviations**.

Hardy and Towner, PRC102, 045501 (2020)

Formalism

- Fermi matrix element in realistic basis

$$M_F = \sum_{k_\alpha k_\beta} \langle \alpha || \tau_\pm || \beta \rangle \, \mathrm{OBTD}(\alpha \beta i f \lambda) = \sum_{k_\alpha k_\beta} \langle \alpha || \tau_\pm || \beta \rangle \frac{\langle \Psi_f || [c_\beta^\dagger \otimes \tilde{c}_\alpha]^{(\lambda)} || \Psi_i \rangle}{\sqrt{2\lambda + 1}}$$

where $\lambda = 1$. The SPME can be decomposed as, $\langle \alpha || \tau_\pm || \beta \rangle = \xi_{\alpha\beta} \theta_{\alpha\beta} \Omega_{\alpha\beta}$ with

$$\begin{aligned} \xi_{\alpha\beta} &= \langle \tau_\alpha | \tau_\pm | \tau_\beta \rangle \\ \theta_{\alpha\beta} &= \sqrt{2j_\alpha + 1}\, \delta_{l_\alpha l_\beta} \delta_{j_\alpha j_\beta} \\ \Omega_{\alpha\beta} &= \int_0^\infty R_\alpha(r) R_\beta(r) r^2 dr \end{aligned}$$

- The correction δ_C is defined as

$$M_F^2 = M_0^2 (1 - \delta_C)$$

where $M_0^2 = T(T+1) \pm T_{zi} T_{zf}$. For isotriplet $M_0^2 = 2$.

Isospin-symmetry breaking affects M_F in two different ways : 1) isospin mixing in many-body states, 2) mismatch between proton and neutron wave functions

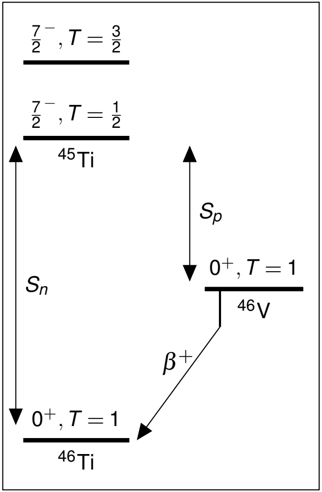
Formalism

- Essentially, we expand OBTDs in terms of intermediate states

$$\mathrm{OBTD}(\alpha\beta if\lambda) = \sum_{\pi} \Theta^{\pi\lambda}_{\alpha\beta if} \langle \Psi_i || c^\dagger_\beta || \pi \rangle \langle \Psi_f || c^\dagger_\alpha || \pi \rangle ,$$

where $\Theta^{\pi\lambda}_{\alpha\beta if} = (-1)^{J_f + J_\pi + j_\alpha + \lambda} \left\{ \begin{array}{ccc} J_i & J_f & \lambda \\ j_\beta & j_\alpha & J_\pi \end{array} \right\}$

- In principle, the spectroscopic amplitudes, $A(i;\pi\beta) \sim \langle \Psi_i || c^\dagger_\beta || \pi \rangle$ and $A(f;\pi\alpha) \sim \langle \Psi_f || c^\dagger_\alpha || \pi \rangle$ are measurable. Although exp. data are not precise enough, they can be used to identify significantly contributed orbitals.
- We also constraint radial wave functions with excitation energy of intermediate states.



Towner and Hardy, PRC77, 025501 (2008)

Formalism

- We break the correction into six terms, $\delta_C = \sum_{i=1}^{6} \delta_{Ci}$ where

$$
\begin{aligned}
\delta_{C1} &= \frac{2}{\sqrt{2}} \sum_{k_a k_b} \theta_{ab}\xi_{ab}[\mathrm{OBTD}_0(abif\lambda) - \mathrm{OBTD}(abif\lambda)], && \text{LO} \\
\delta_{C2} &= \frac{2}{\sqrt{2}} \sum_{k_a k_b \pi} \theta_{ab}(1-\Omega_{ab}^{\pi})\xi_{ab}\Theta_{abif}^{\pi\lambda} A_0(f\pi a)A_0(i\pi b), && \text{LO} \\
\delta_{C3} &= -\delta_{C2} + \frac{2}{\sqrt{2}} \sum_{k_a k_b \pi} \theta_{ab}(1-\Omega_{ab}^{\pi})\xi_{ab}\Theta_{abif}^{\pi\lambda} A(f\pi a)A(i\pi b), && \text{NLO} \\
\delta_{C4} &= -\frac{1}{4}(\delta_{C1}+\delta_{C2})^2, && \text{NLO} \\
\delta_{C5} &= -\delta_{C3}\sqrt{|\delta_{C4}|}, && \text{N}^2\text{LO} \\
\delta_{C6} &= -\frac{1}{4}(\delta_{C3})^2, && \text{N}^3\text{LO.}
\end{aligned}
$$

where θ_{ab}, ξ_{ab}, and $\Theta_{abif}^{\pi\lambda}$ are functions of quantum numbers. **Only the LO terms were considered in the prior calculations**.

Xayavong and Smirnova, PRC109, 014317 (2024)

Isospin-nonconserving effective interactions

Construction of INC Hamiltonian

1) Within the phenomenological approach, we start from a well-established isospin-invariant Hamiltonian H_0 ($[H_0, T] = 0$)
2) Then, we add a charge-dependent two-body interaction V_{INC} ($[V_{INC}, T] \neq 0$):

$$H = H_0 + V_{INC}$$

where V_{INC} is parametrized as

$$V_{INC} = \sum_{k=0,1,2} V_{INC}^{(k)} = \sum_{k=0,1,2} \left[C^{(k)} V_C(\boldsymbol{r}) + P^{(k)} V_\pi(\boldsymbol{r}) + R^{(k)} V_\rho(\boldsymbol{r}) \right] I^{(k)},$$

with $V_C(\boldsymbol{r})$=Coulomb, $V_\pi(\boldsymbol{r})/V_\rho(\boldsymbol{r})$=Yukawa potentials.

Lam *et al.*, PRC87, 054304 (2013)
Ormand and Brown, NPA440 (1985) 174-300

Construction of INC Hamiltonian

- Isobaric multiplet mass equation (IMME) :

$$M(\alpha, T, T_z) = a(\alpha, T) + b(\alpha, T)T_z + c(\alpha, T)T_z^2$$

Its coefficients a, b, c are determined by V_{INC} :

$$a(\alpha, T) = \frac{\langle \Psi_{TT_z} || V_{INC}^{(0)} || \Psi_{TT_z} \rangle}{\sqrt{2T+1}} - \frac{T(T+1)\langle \Psi_{TT_z} || V_{INC}^{(2)} || \Psi_{TT_z} \rangle}{\sqrt{T(2T+1)(2T+1)(T+1)(2T-1)}}$$

$$b(\alpha, T) = \frac{\langle \Psi_{TT_z} || V_{INC}^{(1)} || \Psi_{TT_z} \rangle}{\sqrt{T(2T+1)(T+1)}}$$

$$c(\alpha, T) = \frac{3\langle \Psi_{TT_z} || V_{INC}^{(2)} || \Psi_{TT_z} \rangle}{\sqrt{T(2T+1)(2T+1)(T+1)(2T-1)}}$$

With exp. data on a, b, c, the interaction's parameters can be obtained through least squares fitting which includes a wide variety of nucleus species

Lam *et al.*, PRC87, 054304 (2013)
Ormand and Brown, NPA440 (1985) 174-300

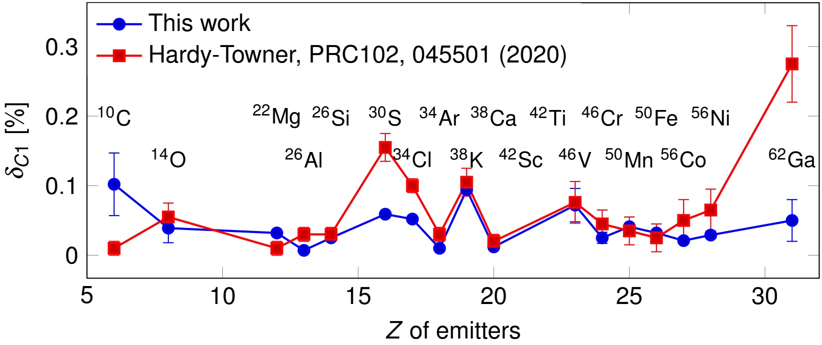
Model spaces and isospin-conserving effective interactions

- Our shell-model calculations

Nuclei	model spaces	effective interactions	Refs.
$A \leq 14$	p shell	CKPOT/CKI/CKII	Cohen-Kurath, 1965
$14 < A \leq 24$	$1p_{\frac{3}{2}}1d_{\frac{5}{2}}2s_{\frac{1}{2}}$	REWIL ZBMI/ZBMII	Rehal-Wildenthal, 1973 Zuker et al., 1969
$24 < A \leq 34$	sd shell	USD USDA/USDB	Wildenthal, 1984 Brown-Richter, 2006
$34 < A \leq 46$	$2s_{\frac{1}{2}}1d_{\frac{3}{2}}1f_{\frac{1}{2}}2p_{\frac{3}{2}}$	ZBM2	Nowacki et al., 2014
$46 < A \leq 62$	pf shell	GXPF1A KB3G FPD6	Honma et al., 2004 Poves et al., 2004 Richter et al., 1991
$62 < A$	$2p_{\frac{3}{2}}2p_{\frac{1}{2}}1f_{\frac{5}{2}}1g_{\frac{9}{2}}$	JUN45 MRG	Honma et al., 2009 Nowacki et al., 1996

Isospin-mixing correction (δ_{C1})

- Results for δ_{C1} (Preliminary !)



- Our values are too large for ^{10}C and too small for (^{30}S, ^{34}Cl, ^{62}Ga). Further investigations are in progress (Smirnova et al.)

Smirnova and Xayavong, Proceeding for NTSE-2018

Radial mismatch correction (δ_{C2})

1) Woods-Saxon potential

$$V(r) = -V_0 f(r, a_0, r_0) - \frac{V_0 \lambda \hbar^2}{4\mu^2 c^2} \frac{1}{r} \frac{d}{dr} f(r, a_s, r_s) \langle \boldsymbol{l} \cdot \boldsymbol{\sigma} \rangle + V_{coul}(r) + \frac{V_g}{r} \frac{d}{dr} f(r, a_s, r_s)$$

- $V_{coul}(r)$ ~uniformly charged sphere approximation
- V_g and r_0 constrained with separation energies and charge radii
- Finite size correction

$$\rho_{ch}(r) = \rho_{ch}^{p}(r) + \rho_{ch}^{n}(r) + \rho_{ch}^{ls}(r),$$

with

$$\rho_{ch}^{q}(\boldsymbol{r}) = \int d\boldsymbol{r}' \rho_q(\boldsymbol{r}') G_q(\boldsymbol{r} - \boldsymbol{r}'),$$

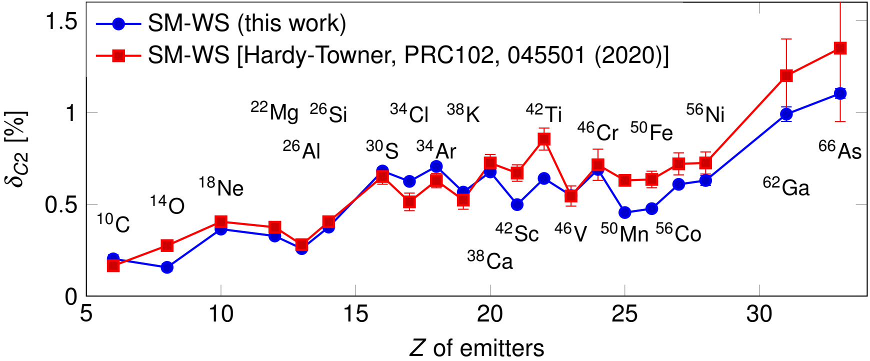
$$\rho_{ch}^{ls}(r) = -\left(\frac{\hbar}{mc}\right)^2 \sum_{\alpha,q} v_{\alpha}^{q} \langle \boldsymbol{\sigma} \cdot \boldsymbol{l} \rangle \frac{g_q'}{r^2} \frac{d}{dr}\left[r \rho_{\alpha}^{q}(r)\right],$$

the nucleon charge form factors are given by [PRC13, 245 (1976)]:

$$G_q(\boldsymbol{r}) = \sum_{i=1}^{n_q} \frac{a_q^i}{(r_q^i \sqrt{\pi})^3} \exp\left[-\frac{\boldsymbol{r}^2}{(r_q^i)^2}\right]$$

Radial mismatch correction (δ_{C2})

- Results for δ_{C2} with Woods-Saxon basis (Preliminary !)



- We obtain smaller values for ^{14}O, ^{42}Sc, ^{42}Ti, ^{50}Mn, ^{50}Fe, ^{54}Co and ^{54}Ni. This is due to difference in configuration spaces, fitting procedure and number of intermediate states included. **This should, at least, be accounted for as an uncertainty source**.

Partially published ! Xayavong and Smirnova; PRC97, 024324 (2018)

Radial mismatch correction (δ_{C2})

2) Self-consistent Skyrme-Hartree-Fock potential

$$U^L_{\alpha_q}(r,\varepsilon_{\alpha_q}) = \frac{m^*_q(r)}{m}\left\{\cdot U_q(r) + \frac{d^2}{dr^2}\frac{\hbar^2}{4m^*_q(r)} - \frac{m^*_q(r)}{2\hbar^2}\left[\frac{d}{dr}\frac{\hbar^2}{m^*_q(r)}\right]^2 + \frac{1}{2}W_q(r)\langle\boldsymbol{\sigma}\cdot\boldsymbol{l}\rangle + \delta_{qp}V_{coul}(r)\right\} + \left[1 - \frac{m^*_q(r)}{m}\right]\varepsilon_{\alpha_q}$$

- Kinetic term

$$\frac{\hbar^2}{m^*_q} = \frac{\hbar^2}{m} + \frac{1}{4}\left[t_1(2+x_1) + t_2(2+x_2)\right]\rho + \frac{1}{4}\left[t_1(1+2x_1) + t_2(1+2x_2)\right]\rho_q$$

- Central term

$$U_q = t_0\left[\left(1+\frac{x_0}{2}\right)\rho - \left(x_0+\frac{1}{2}\right)\rho_q\right] + \frac{t_1}{4}\left\{\left(1+\frac{x_1}{2}\right)\left(\tau - \frac{3}{2}\Delta\rho\right) - \left(x_1+\frac{1}{2}\right)\left(\tau_q - \frac{3}{2}\Delta\rho_q\right)\right\}$$
$$+\tfrac{t_2}{4}\left[\left(1+\tfrac{x_2}{2}\right)\left(\tau + \tfrac{1}{2}\Delta\rho\right) + \left(x_2+\tfrac{1}{2}\right)\left(\tau_q + \tfrac{1}{2}\Delta\rho_q\right)\right]$$
$$+\tfrac{t_3}{12}\left[\left(1+\tfrac{x_3}{2}\right)(2+\gamma)\rho^{\gamma+1} - \left(x_3-\tfrac{1}{2}\right)\left(2\rho^{\gamma}\rho_q + \gamma\rho^{\gamma-1}\textstyle\sum_{q'}\rho^2_{q'}\right)\right]$$
$$-\tfrac{W_0}{2}\left[\tfrac{1}{r}\left(J+J_q\right) + \tfrac{1}{2}\tfrac{d}{dr}\left(J+J_q\right)\right],$$

- Spin-orbit term

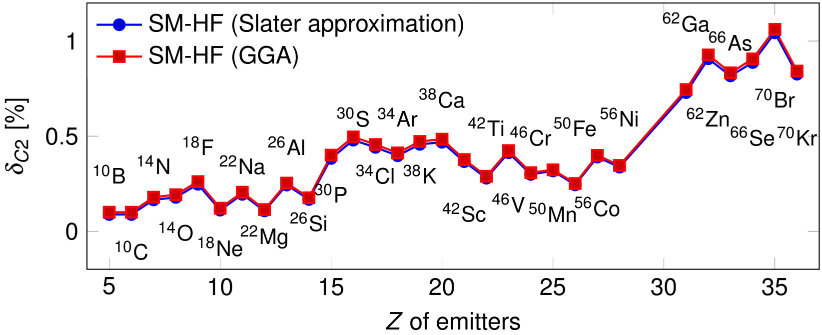
$$W_q = -\frac{1}{8}(t_1x_1 + t_2x_2)J + \frac{1}{8}(t_1 - t_2)J_q + \frac{1}{2}W_0\frac{d}{dr}(\rho+\rho_q)$$

Radial mismatch correction (δ_{C2})

- Treatment of Coulomb-exchange term using GGA

$$V_{coul}^{ex}(r) = V_{Sl}^{ex}(r)\left\{F(s) - \left[s + \frac{3}{4k_F r}\right]F'(s) + \left[s^2 - \frac{3\rho''_{ch}(r)}{8\rho_{ch}(r)k_F^2}\right]F''(s)\right\}$$

where s is the density gradient (a function of r).



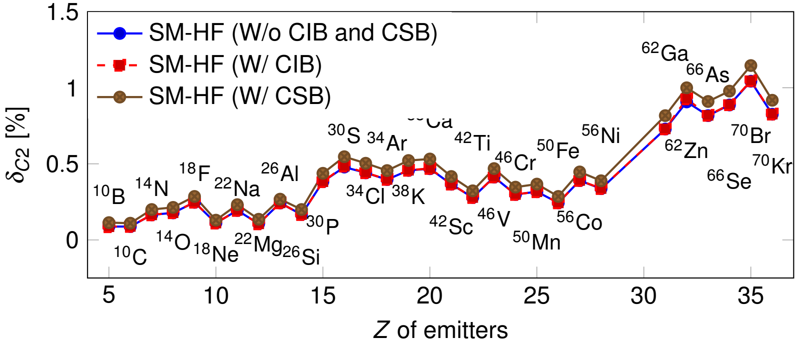
- The GGA values are 2-14 % larger than those obtained with the Slater approximation

Radial mismatch correction (δ_{C2})

- CIB and CSB forces [Suzuki *et al.*, PRL112, 102502 (1995)]

$$
\begin{aligned}
V_{CIB} &= 2t_{iz}t_{jz}\delta[u_0(1-P_\sigma)+\frac{u_1}{2}(1-P_\sigma)\left(\boldsymbol{k}^2+\boldsymbol{k}'^2\right)+u_2(1-P_\sigma)\boldsymbol{k}'\cdot\boldsymbol{k}] \\
V_{CSB} &= (t_{iz}+t_{jz})\delta[s_0(1-P_\sigma)+\frac{s_1}{2}(1-P_\sigma)\left(\boldsymbol{k}^2+\boldsymbol{k}'^2\right)+s_2(1-P_\sigma)\boldsymbol{k}'\cdot\boldsymbol{k}]
\end{aligned}
$$

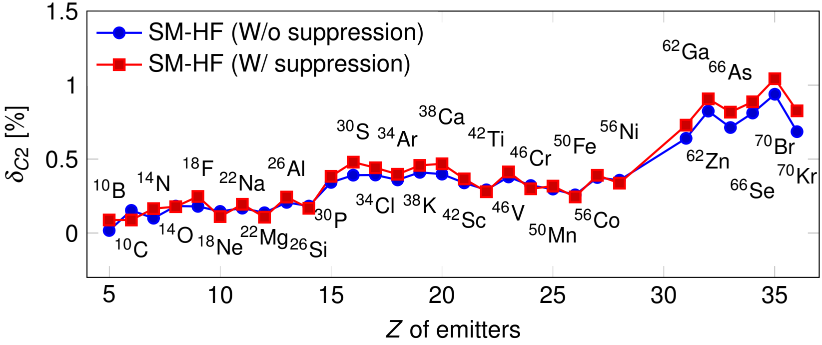
where u_i and s_i are adjustable constant.



- The CIB effect is completely negligible, whereas the CSB contributes 10 to 30 %.

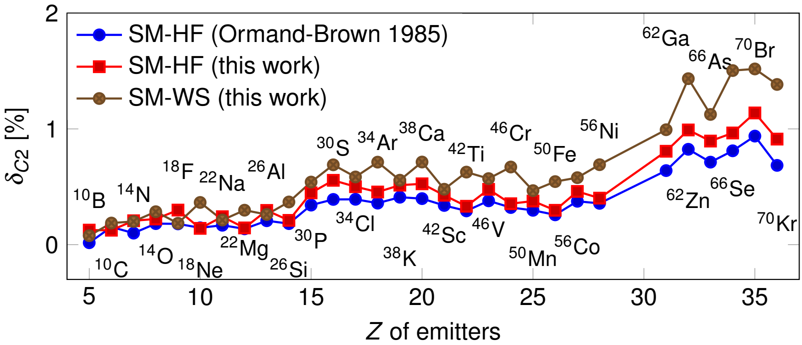
Radial mismatch correction (δ_{C2})

- Suppression of spurious isospin mixing:



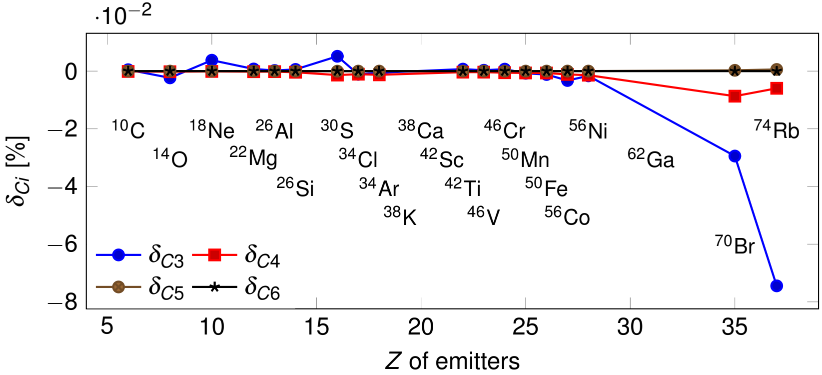
- The suppression leads to a considerable increase for $16 \leq Z \leq 20$ and $Z \geq 33$
- The emitters with $21 \leq Z \leq 28$ are mostly unaffected
- Complicated effect in light nuclei where nuclear isovector is dominated over the Coulomb.

- Our final result is closer to that obtained with WS basis



- Despite our significant improvement, a considerable gap between SM-WS and SM-HF remains. While HF has a solid foundation, it is unsuitable to be used as a basis for shell model. Spurious isospin-mixing is basically unresovable.

- Higher-order contributions

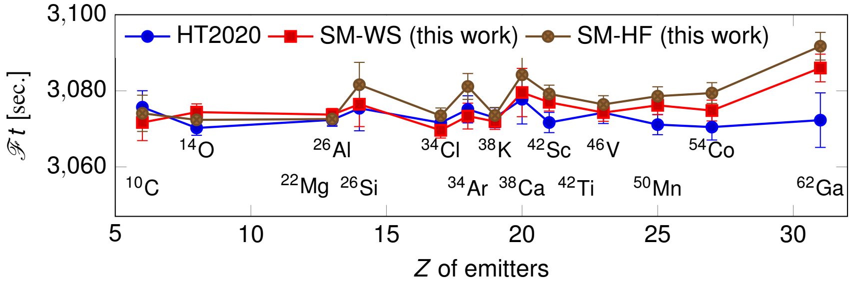


Generally, they are negligibly small as expected. However, δ_{C3} could be significant for ^{74}Rb. Additionally, δ_{C3} is destructive.

Xayavong and Smirnova, PRC109, 014317 (2024)

Standard-Model implications

- Corrected $\mathscr{F}t$ values



- Test of CVC (Constancy of $\mathscr{F}t$)

Calculations	bases	$\overline{\mathscr{F}t}$ [sec.]	χ^2/ν (best 15 cases)
HT2020	Woods-Saxon	3073.148±0.748	0.493
This work	Woods-Saxon	3075.310±0.706	1.869
This work	Hartree-Fock	3078.332±0.706	4.040

Shell model with HF basis poorly agrees with CVC. Significant dependence on model's parameters remains.

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Summary

1) We demonstrate that HF basis is unsuitable for high precision many-body calculations.
2) The model parameters can be fitted in multiple ways. This leads to significant uncertainties to the phenomenological shell-model approach.
3) Experimental tests are recommended for the theoretical approach in highly sensitive processes, such as Gamow-Teller β decays, or Fermi β decays of higher isospin multiplets.