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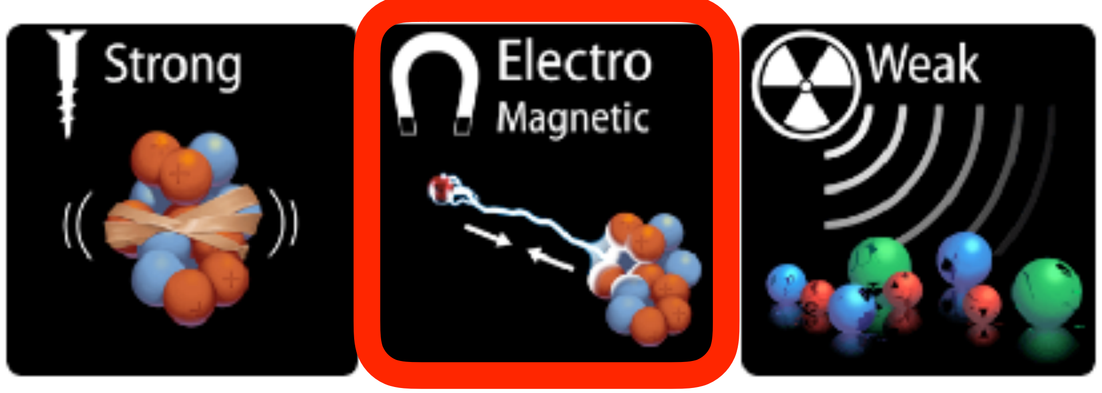
Relativistic theory and ab-initio simulations of electroweak decay spectra in medium-heavy atomic systems

ECT*, 09/04/2019

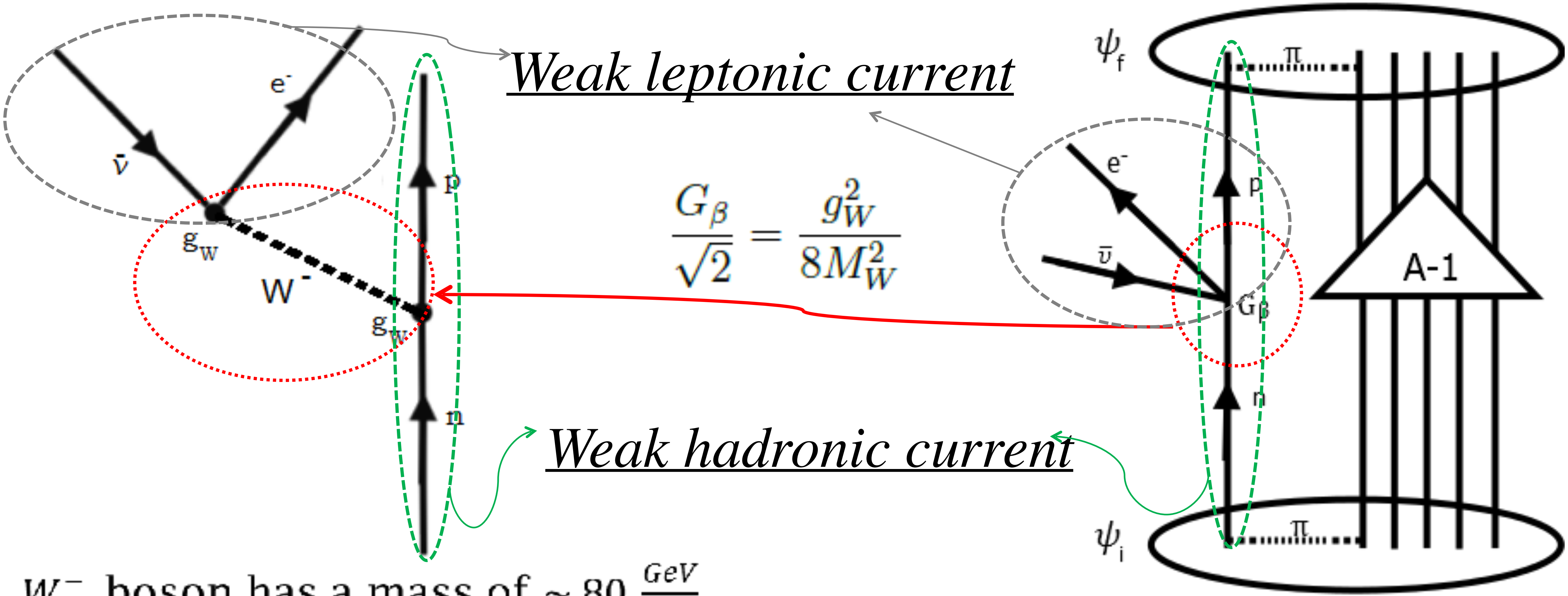
Outline



- Introduction to our relativistic approach to β-decay (β-decay and EC are not only purely nuclear but also atomic processes)
- What is correlation in c.m. and why is important to interpret β-decay lineshapes: a primer on many-body approaches, from semi-empirical to mean-field (HF and DHF)
- Application of our approach to a number of β-decay processes in heavy atoms ($^{36}Cl,^{63}Ni,^{129}I,^{210}Bi,^{241}Pu,$)
- Application to β-decay of Tritium and to EC in ^{163}Ho for the determination of neutrino mass
- Application to astrophysical scenario
- Perspectives, future developments and conclusions

β-decay from a c.m. perspective: tool basket

- **Standard Model of particle physics: weak interaction is caused by emission or absorption of very massive bosons**



Weak leptonic current

$$\frac{G_\beta}{\sqrt{2}} = \frac{g_W^2}{8M_W^2}$$

Weak hadronic current

W^- boson has a mass of $\sim 80\ \frac{GeV}{c^2}$

→ *Uncertainty principle*: W^- can only live $\Delta t \le \frac{\hbar}{M_W \cdot c^2}$ (range of strong interaction)

→ During this time it can travel at most $c\Delta t \le \frac{\hbar}{M_W \cdot c} \sim 10^{-3}\ fm \ll 1\ fm$

Short range=Fermi contact interaction

Validity of the independent particle model to treat the e⁻ -capture and emission

β-decay from a c.m. perspective: tool basket

A typical nuclear β-decay process reads:

$$^{A}_{Z}X_{N} \rightarrow {}^{A}_{Z+1}X'_{N-1} + e^{-} + \bar{\nu}_e$$

Q-value: total energy released by the reaction ($m_\nu = 0$)

$$Q_{\beta-} = m_N(^{A}X) - m_N(^{A}X') \qquad m(^{A}X) = m_N(^{A}X) + Zm_e - \sum_{i=1}^{Z}(B_i)$$

Extra-nuclear factor

$$Q_{\beta-} = \{[m(^{A}X) - Z\cdot m_e] - [m(^{A}X') - (Z+1)\cdot m_e] - m_e\}\cdot c^2 + \boxed{\{\sum_{i=1}^{Z} B_i - \sum_{i=1}^{Z+1} B_i\}}$$

In the traditional theory of β-decay processes, spectra are typically calculated as product of three factors:

$$\frac{dN}{dW} \propto \boxed{pWq^2} F(Z,W)C(W)$$

- **a phase-space factor to deal with the momentum sharing between the β-electron (p) and neutrino (q);**
- **a Fermi function F(Z,W) to take into account the static corrections due to the Coulomb field of the nucleus;**
- **a shape factor C(W) to include the coupling between nuclear and lepton dynamics.**

β-decay from a c.m. perspective: tool basket

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$$ Q_{\beta-} = m_N({}^{A}X) - m_N({}^{A}X') \qquad m({}^{A}X) = m_N({}^{A}X) + Zm_e - \sum_{i=1}^{Z}(B_i) $$

Extra-nuclear factor

$$ Q_{\beta-} = \{[m({}^{A}X) - Z \cdot m_e] - [m({}^{A}X') - (Z+1) \cdot m_e] - m_e\} \cdot c^2 + \boxed{\{\sum_{i=1}^{Z} B_i - \sum_{i=1}^{Z+1} B_i\}} $$

In the traditional theory of β-decay processes, spectra are typically calculated as product of three factors:

$$ \frac{dN}{dW} \propto \boxed{pWq^2}\,\boxed{F(Z,W)}\,C(W) \qquad F(Z,W) = \frac{2\pi\nu}{1 - \exp^{-2\pi\boxed{\nu}}} \qquad \boxed{\nu = \pm Ze^2/\hbar v} $$

- **a phase-space factor to deal with the momentum sharing between the β-electron (p) and neutrino (q);**
- **a Fermi function F(Z,W) to take into account the static corrections due to the Coulomb field of the nucleus;**
- **a shape factor C(W) to include the coupling between nuclear and lepton dynamics.**

β-decay from a c.m. perspective

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$$ Q_{\beta-} = \{[m(^{A}X) - Z \cdot m_e] - [m(^{A}X^{'}) - (Z+1)\cdot m_e] - m_e\} \cdot c^2 + \{\sum_{i=1}^{Z} B_i - \sum_{i=1}^{Z+1} B_i\} $$

In the traditional theory of β-decay processes, spectra are typically calculated as product of three factors:

$$ \frac{dN}{dW} \propto pWq^2 F(Z,W) C(W) \qquad C(W) = (2L'-1)! \sum_{k=1}^{L'} \lambda_k \frac{p^{2(k-1)} q^{2(L'-k)}}{(2k-1)![2(L'-k)+1]!} $$

- **a phase-space factor to deal with the momentum sharing between the β-electron (p) and neutrino (q);**
- **a Fermi function F(Z,W) to take into account the static corrections due to the Coulomb field of the nucleus;**
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β-decay from a c.m. perspective

$$\frac{dN}{dW} \propto pWq^2F(Z,W)C(W)$$

It works well to predict the lineshapes of allowed and forbidden unique transitions, at variance, nuclear structure effects cannot be neglected when dealing with forbidden non-unique transitions, and there is no such a simple relation for C(W)

One can treat first forbidden non-unique transitions as allowed if

$$2\xi = \frac{\alpha Z}{R_{nuc}} >> E_{max}$$

where E_{max} is the maximum escaping energy of the β-electron and α is the fine structure constant

Still a rigours treatment of these transitions from the electronic structure point of view is missing!!!

Our approach to beta-decay helps to solve these issues, related to many-body effects, in the leptonic current term

Standard Model β-decay theory

β-decay rate is calculated by using Fermi's Golden Rule:

$$P_{i\rightarrow f} = 2\pi \int |\langle f|\hat{H}_\beta|i\rangle|^2 \rho(W_f)\delta(W_f - W_i)dW_f$$

Probability P per unit time that a system undergoes a transition from an initial state, *i*, to a number of final states, *f*, under the influence of a perturbation described by the Hamiltonian H_β

Weak Interaction Hamiltonian

$$\mathcal{H}_\beta = \frac{G_\beta}{\sqrt{2}}(\bar{\psi}_{f,p}(\mathbf{r})\gamma^\mu(1 - x\gamma^5)\hat{\psi}_{i,n}(\mathbf{r}))\cdot(\bar{\psi}_{f,e}(\mathbf{r})\gamma_\mu(1 - \gamma^5)\hat{\psi}_{i,\nu}(\mathbf{r})) + h.c.$$

Creates a proton

Destroys a neutron

Creates an electron

Destroys a neutrino (creates an antineutrino)

$\gamma^\mu \rightarrow$ Dirac gamma matrices

$G_\beta = G \cdot c_V \sim 1.13 \cdot 10^{-5} GeV^{-2}$; $x = \frac{c_A}{c_V} \sim 1.27$;

➡ **All the wavefunctions will be written as Dirac spinors**

β-decay theory

Initial nuclear Fock-space state: $|\xi_n, j_n, \mu_n\rangle_A \equiv \hat{a}_n^\dagger |0\rangle_A$

Final nuclear Fock-space: $|\xi_p, j_p, \mu_p\rangle_A \equiv \hat{a}_p^\dagger |0\rangle_A$

Initial lepton Fock-space: $|0;\ 0\rangle_L$

Final lepton Fock-space: $|(n_B, \cancel{\kappa_B, \mu_B} + W_C^f, \kappa_C^f, \mu_C^f); W_\nu, \kappa_\nu, \mu_\nu\rangle_L \equiv (\hat{a}_{C,e}^+ + \hat{a}_{C,e}^+) b_\nu^\dagger |0;0\rangle_L$

$j_{p,n,e}$ nuclear spin

$\mu_{p,n,e}$ projection along the quantization axis

$\xi_{p,n,e}$ quantum number characterizing the nuclear state

initial state: $|i\rangle = |\xi_n, j_n, \mu_n\rangle_A \otimes |0;\ 0\rangle_L$

final state: $|f\rangle \equiv |\xi_p, j_p, \mu_p\rangle_A \otimes |W_C^f, \kappa_C^f, \mu_C^f;\ W_\nu, \kappa_\nu, \mu_\nu\rangle_L$

Field operators entering the Weak Interaction Hamiltonian

$$\hat{\psi}_n(\mathbf{r}) = \sum_{\xi_n, j_n, \mu_n} \langle \mathbf{r} | \xi_n, j_n, \mu_n\rangle\ \hat{a}_n + \text{antineutron creation term}$$

$$\hat{\psi}_e^+(\mathbf{r}) = \cancel{\sum_{n'_B, \kappa'_B, \mu'_B} \langle n'_B, \kappa'_B, \mu'_B | \mathbf{r}\rangle\ \hat{a}_{B,e}^+} + \int dW'_C \sum_{\kappa'_C, \mu'_C} \langle W'_C, \kappa'_C, \mu'_C | \mathbf{r}\rangle\ \hat{a}_{C,e}^+ + \text{positron destruction term}$$

Inclusion of the antisymmetrization

$$\hat{\psi}_\nu(\mathbf{r}) = \int dW_\nu \sum_{\kappa_\nu, \mu_\nu} \left(\langle \mathbf{r} | W_\nu, \kappa_\nu, \mu_\nu\rangle\ \hat{a}_\nu + \langle \mathbf{r} | W_\nu, \kappa_\nu, \mu_\nu\rangle_-\ \hat{b}_\nu^\dagger \right)$$

$$\hat{\psi}_p^+(\mathbf{r}) = \sum_{\xi_p, j_p, \mu_p} \langle \xi_p, j_p, \mu_p | \mathbf{r}\rangle\ \hat{a}_p^+ + \text{antiproton destruction term}$$

→ In the standard approximation, one considers the particles entering the decay as non-interacting single particles

β-decay theory: total decay rate

$$\lambda_t = \frac{\pi G_\beta^2}{(2j_n+1)(2J_B+1)} \sum_{\gamma} \sum_{\mu_n,\mu_p} \sum_{\mu'_B,\mu'_C,\mu_B} \sum_{\mu_\nu} \int |I|^2 \rho(W_f)\delta(Q - T'_C - W_\nu) dW_\nu dW'_C$$

$$\langle f|\mathcal{H}_\beta|i\rangle$$

with electron energy $W_C^f = \sqrt{p^2c^2 + c^4} = c^2 + T_C^f$ and antineutrino energy $W_\nu = c \cdot p_\nu$

μ and γ' runs over magnetic and principal quantum number and where

$$I = \int\int \langle \xi_p, j_p, \mu_p| \; \hat{\psi}_p^+(\mathbf{r}_h)\gamma^0\gamma^\mu(1 - x\gamma^5)\hat{\psi}_n(\mathbf{r}_h) \; |\xi_n, j_n, \mu_n\rangle \cdot$$
$$\langle \bigwedge\nolimits_{B,C} n'_B, \kappa'_B, \mu'_B, W'_C, \kappa'_C, \mu'_C; W_\nu, \kappa_\nu, \mu_\nu| \; \hat{\psi}_e^+(\mathbf{r}_l)\gamma^0\gamma_\mu(1 - \gamma^5)\hat{\psi}_\nu(\mathbf{r}_l) \; |\bigwedge\nolimits_B n_B, \kappa_B, \mu_B; 0\rangle \; \delta(\mathbf{r}_h - \mathbf{r}_l) d\mathbf{r}_h d\mathbf{r}_l$$

expresses the point-like nature of the decay

$$\delta(\mathbf{r}_h - \mathbf{r}_l) = \sum_{L',q} \delta(r_h - r_l) \cdot r_l^{-2} \cdot \boxed{Y_{L',q}(\theta_h, \phi_h)} Y_{L',-q}(\theta_l, \phi_l) \cdot (-)^q$$

Spherical armonics

This notation is useful because it allows to split the matrix element into nuclear and lepton parts

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$$\langle \cancel{\bigwedge_{B,C}} n'_B, \kappa'_B, \mu'_B, W'_C, \kappa'_C, \mu'_C; W_\nu, \kappa_\nu, \mu_\nu|\ \hat{\psi}_e^+(\mathbf{r}_l)\gamma^0\gamma_\mu(1 - \gamma^5)\hat{\psi}_\nu(\mathbf{r}_l)\ |\cancel{\bigwedge_B} n_B, \kappa_B, \mu_B; 0\rangle\ \delta(\mathbf{r}_h - \mathbf{r}_l)d\mathbf{r}_h d\mathbf{r}_l$$

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$$\langle W'_C, \kappa'_C, \mu'_C; W_\nu, \kappa_\nu, \mu_\nu|\ \hat{\psi}_e^+(\mathbf{r}_l)\gamma^0\gamma_\mu(1 - \gamma^5)\hat{\psi}_\nu(\mathbf{r}_l)\ |0;0\rangle\ \delta(\mathbf{r}_h - \mathbf{r}_l)\ d\mathbf{r}_h\ d\mathbf{r}_l =$$

expresses the point-like nature of the decay

$$\delta(\mathbf{r}_h - \mathbf{r}_l) = \sum_{L',q} \delta(r_h - r_l) \cdot r_l^{-2} \cdot \boxed{Y_{L',q}(\theta_h, \phi_h)} Y_{L',-q}(\theta_l, \phi_l) \cdot (-)^q$$

Spherical armonics

This notation is useful because it allows to split the matrix element into nuclear and lepton parts

β-decay theory

To find the eigensolutions of the SM Hamiltonian for the β-decay we make a first major "approximation": we assume that one can factorize this operator as the tensorial product of of two interacting currents:

- hadronic (nuclear);
- leptonic (electron + neutrino)

Explicitly:

$$\langle f|\mathcal{H}_\beta|i\rangle = \frac{G_\beta}{\sqrt{2}} J^{H,\mu}_{i\to f}(\mathbf{r}) J^{L}_{i\to f,\mu}(\mathbf{r})$$

where:

e$^-$ and ν can be considered uncoupled

$$J^{L}_{i\to f,\mu}(\mathbf{r}) = \psi^{+}_{f,e}(\mathbf{r})\gamma_0\gamma_\mu\left(1-\gamma^5\right)\psi_{i,\nu}(\mathbf{r})$$

n and p w.f. can be factorized provided that the nucleus is "hydrogenic", that is composed by a closed shell with only one single nucleon in one open shell embedded in the mean field generated by the closed shell

$$J^{H.\mu}_{i\to f}(\mathbf{r}) = \psi^{+}_{f,p}(\mathbf{r})\gamma_0\gamma^{\mu}\left(1-x\gamma^5\right)\psi_{i,n}(\mathbf{r})$$

β-decay theory in central symmetry

Nuclear matrix element on a real space grid

$$J^{H,\mu}(r_h) = \int d\Omega_h Y_{L',q}(\theta_h,\phi_h)\langle \xi_p, j_p, \mu_p |\ \hat{\psi}_p^+(\mathbf{r}_h)\gamma^0\gamma^\mu(1-x\gamma^5)\hat{\psi}_n(\mathbf{r}_h)\ | \xi_n, j_n, \mu_n\rangle \cdot r_h^2 =$$

$$= \int d\Omega_h Y_{L',q}(\theta_h,\phi_h)\langle 0|\hat{a}_p\ \hat{\psi}_p^+(\mathbf{r}_h)\gamma^0\gamma^\mu(1-x\gamma^5)\hat{\psi}_n(\mathbf{r}_h)\ \hat{a}_n^+|0\rangle \cdot r_h^2$$

inserting the expressions for the field operators

$$J^{H,\mu}(r_h) = \sum_{\xi'_p, j'_p, \mu'_p} \sum_{\xi'_n, j'_n, \mu'_n} \langle 0|\hat{a}_p\ \hat{a}_{p'}^+\hat{a}_{n'}\ \hat{a}_n^+|0\rangle$$

$$\cdot \int d\Omega_h Y_{L',q}(\theta_h,\phi_h)\langle \xi'_p, j'_p, \mu'_p|\mathbf{r}_h\rangle\ \gamma^0\gamma^\mu(1-x\gamma^5)\langle \mathbf{r}_h|\xi'_n, j'_n, \mu'_n\rangle \cdot$$

and applying anti-commutation rules for creation/destruction Fock-space operators

$$\{\hat{a}_p, \hat{a}_n^\dagger\} = \{\hat{a}_p, \hat{a}_n\} = 0$$

$$\{\hat{a}_p, \hat{a}_{p'}^\dagger\} = \delta_{\xi_p,\xi'_p}\ \delta_{j_p,j'_p}\ \delta_{\mu_p,\mu'_p}$$

$$\{\hat{a}_n, \hat{a}_{n'}^\dagger\} = \delta_{\xi_n,\xi'_n}\ \delta_{j_n,j'_n}\ \delta_{\mu_n,\mu'_n}$$

Selection rules

one gets

$$\boxed{J^{H,\mu}(r_h) = \int d\Omega_h Y_{L',q}(\theta_h,\phi_h)\langle \xi_p, j_p, \mu_p|\mathbf{r}_h\rangle\ \gamma^0\gamma^\mu(1-x\gamma^5)\langle \mathbf{r}_h|\xi_n, j_n, \mu_n\rangle \cdot r_h^2}$$

β-decay theory: total decay rate

Lepton matrix element on a real space grid

$$J^L_\mu(r_h) = \int dr_l \int d\Omega_l Y_{L',-q}(\theta_l,\phi_l)\langle \bigwedge\nolimits_{B,C} n'_B, \kappa'_B, \mu'_B, W'_C, \kappa'_C, \mu'_C; W_\nu, \kappa_\nu, \mu_\nu |$$

$$\hat{\psi}^+_e(\mathbf{r}_l)\gamma^0\gamma_\mu(1-\gamma^5)\hat{\psi}_\nu(\mathbf{r}_l) \; |\bigwedge\nolimits_B n_B, \kappa_B, \mu_B; 0\rangle \; \delta(r_h - r_l) =$$

$$= \int dr_l \int d\Omega_l Y_{L',-q}(\theta_l,\phi_l)\langle 0;0|\hat{a}'_{1,e}\ldots\,\hat{a}'_{N,e}\hat{a}'_{C,e}\hat{b}_\nu \; \hat{\psi}^+_e(\mathbf{r}_l)\gamma^0\gamma_\mu(1-\gamma^5)\hat{\psi}_\nu(\mathbf{r}_l)\hat{a}^+_{1,e}\ldots\,\hat{a}^+_{N,e}|0;0\rangle\delta(r_h - r_l$$

inserting the expressions for the field operators

$$J^L_\mu(r_h) = \sum_{n'_B,\kappa'_B,\mu'_B} \int dW'_\nu \sum_{\kappa'_\nu,\mu'_\nu} \langle 0;0|\hat{a}'_{1,e}\ldots\,\hat{a}'_{N,e}\hat{a}'_{C,e}\hat{b}_\nu\hat{a}'^+_{B',e}\hat{b}^+_{\nu'}\hat{a}^+_{1,e}\ldots\,\hat{a}^+_{N,e}|0;0\rangle$$

$$\int dr_l \int d\Omega_l Y_{L',-q}(\theta_l,\phi_l)\langle n'_B, \kappa'_B, \mu'_B|\mathbf{r}_l\rangle\gamma^0\gamma_\mu(1-\gamma^5)\langle\mathbf{r}_l|W'_\nu, \kappa'_\nu, \mu'_\nu\rangle\delta(r_h - r_l) +$$

$$+ \int dW'_C \sum_{\kappa'_C,\mu'_C} \int dW'_\nu \sum_{\kappa'_\nu,\mu'_\nu} \langle 0;0|\hat{a}'_{1,e}\ldots\,\hat{a}'_{N,e}\hat{a}'_{C,e}\hat{b}_\nu\hat{a}'^+_{C',e}\hat{b}^+_{\nu'}\hat{a}^+_{1,e}\ldots\,\hat{a}^+_{N,e}|0;0\rangle$$

$$\int dr_l \int d\Omega_l Y_{L',-q}(\theta_l,\phi_l)\langle W'_C, \kappa'_C, \mu'_C|\mathbf{r}_l\rangle\gamma^0\gamma_\mu(1-\gamma^5)\langle\mathbf{r}_l|W'_\nu, \kappa'_\nu, \mu'_\nu\rangle\delta(r_h - r_l)$$

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Lepton matrix element on a real space grid

and applying anti-commutation rules for creation/destruction Fock-space operators

$$\{\hat{a}'_{B,e}, \hat{a}'^{+}_{B',e}\} = \delta_{n_B,n'_B}\ \delta_{\kappa_B,\kappa'_B}\ \delta_{\mu_B,\mu'_B}$$

$$\{\hat{a}'_{C,e}, \hat{a}'^{+}_{C',e}\} = \delta(W_C - W'_C)\ \delta_{\kappa_C,\kappa'_C}\ \delta_{\mu_C,\mu'_C}$$

$$\{\hat{b}_{\nu}, \hat{b}^{+}_{\nu'}\} = \delta(W_\nu - W'_\nu)\ \delta_{\kappa_\nu,\kappa'_\nu}\ \delta_{\mu_\nu,\mu'_\nu}$$

$$\{\hat{a}_{B/C,e}, \hat{b}_{\nu}\} = \{\hat{a}^{+}_{B/C,e}, \hat{b}_{\nu}\} = \{\hat{a}_{C,e}, \hat{a}^{+}_{B,e}\} = 0$$

one gets

$$J^L_\mu(r_h) = \sum_{j=1}^{N} \prod_{B\neq j} (-)^j \boxed{\langle 0;0|\hat{a}'_{B,e}\hat{a}'_{C,e}\hat{a}^{+}_{1,e}...\hat{a}^{+}_{N,e}|0;0\rangle}$$

Inclusion of post-collisional effects: Fano's and Exchange interactions

$$\int dr_l \int d\Omega_l Y_{L',-q}(\theta_l,\phi_l)\langle n'_B,\kappa'_B,\mu'_B|\mathbf{r}_l\rangle\gamma^0\gamma_\mu(1-\gamma^5)\langle\mathbf{r}_l|W_\nu,\kappa_\nu,\mu_\nu\rangle\delta(r_h-r_l)\ +$$

$$+\boxed{\langle 0;0|\hat{a}'_{1,e}...\ \hat{a}'_{N,e}\hat{a}^{+}_{1,e}...\hat{a}^{+}_{N,e}|0;0\rangle}$$

Standard beta-decay

$$\int dr_l \int d\Omega_l Y_{L',-q}(\theta_l,\phi_l)\langle W'_C,\kappa'_C,\mu'_C|\mathbf{r}_l\rangle\gamma^0\gamma_\mu(1-\gamma^5)\langle\mathbf{r}_l|W_\nu,\kappa_\nu,\mu_\nu\rangle\delta(r_h-r_l)$$

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and applying anti-commutation rules for creation/destruction Fock-space operators

$$\{\hat{a}'_{B,e}, \hat{a}'^{+}_{B',e}\} = \delta_{n_B,n'_B}\ \delta_{\kappa_B,\kappa'_B}\ \delta_{\mu_B,\mu'_B}$$

$$\{\hat{a}'_{C,e}, \hat{a}'^{+}_{C',e}\} = \delta(W_C - W'_C)\ \delta_{\kappa_C,\kappa'_C}\ \delta_{\mu_C,\mu'_C}$$

$$\{\hat{b}_{\nu}, \hat{b}^{+}_{\nu'}\} = \delta(W_\nu - W'_\nu)\ \delta_{\kappa_\nu,\kappa'_\nu}\ \delta_{\mu_\nu,\mu'_\nu}$$

$$\{\hat{a}_{B/C,e}, \hat{b}_{\nu}\} = \{\hat{a}^{+}_{B/C,e}, \hat{b}_{\nu}\} = \{\hat{a}_{C,e}, \hat{a}^{+}_{B,e}\} = 0$$

one gets

$$J^L_\mu(r_h) = \sum_{j=1}^{N} \prod_{B\neq j} (-)^j \langle 0;0|\hat{a}'_{B,e}\hat{a}'_{C,e}\hat{a}^{+}_{1,e}\ldots\hat{a}^{+}_{N,e}|0;0\rangle$$

$$\underbrace{\int dr_l \int d\Omega_l Y_{L',-q}(\theta_l,\phi_l)\langle n'_B,\kappa'_B,\mu'_B|\mathbf{r}_l\rangle\gamma^0\gamma_\mu(1-\gamma^5)\langle\mathbf{r}_l|W_\nu,\kappa_\nu,\mu_\nu\rangle\delta(r_h-r_l)}_{Q_{L',q,B;\mu}(r_h)} +$$

$$+ \langle 0;0|\hat{a}'_{1,e}\ldots\ \hat{a}'_{N,e}\hat{a}^{+}_{1,e}\ldots\hat{a}^{+}_{N,e}|0;0\rangle$$

$$\underbrace{\int dr_l \int d\Omega_l Y_{L',-q}(\theta_l,\phi_l)\langle W'_C,\kappa'_C,\mu'_C|\mathbf{r}_l\rangle\gamma^0\gamma_\mu(1-\gamma^5)\langle\mathbf{r}_l|W_\nu,\kappa_\nu,\mu_\nu\rangle\delta(r_h-r_l)}_{Q_{L',q,C;\mu}(r_h)}$$

$$J^L_\mu(r_h) = \begin{vmatrix} \langle\psi'_1|\phi_1\rangle & \langle\psi'_1|\phi_2\rangle & \cdots & \langle\psi'_1|\phi_N\rangle & Q_{L',q,1;\mu}(r_h) \\ \langle\psi'_2|\phi_1\rangle & \langle\psi'_2|\phi_2\rangle & \cdots & \langle\psi'_2|\phi_N\rangle & Q_{L',q,2;\mu}(r_h) \\ \vdots & & \ddots & & \vdots \\ \langle\psi'_N|\phi_1\rangle & \langle\psi'_N|\phi_2\rangle & \cdots & \langle\psi'_N|\phi_N\rangle & Q_{L',q,N;\mu}(r_h) \\ \langle\psi'_C|\phi_1\rangle & \langle\psi'_C|\phi_2\rangle & \cdots & \langle\psi'_C|\phi_N\rangle & Q_{L',q,C;\mu}(r_h) \end{vmatrix}$$

by combining the leptonic and the hadronic currents

$$J^{H,\mu}(r_h) = \int d\Omega_h Y_{L',q}(\theta_h,\phi_h)\langle\xi_p, j_p, \mu_p|\mathbf{r}_h\rangle \ \gamma^0\gamma^\mu(1-x\gamma^5)\langle\mathbf{r}_h|\xi_n, j_n, \mu_n\rangle \cdot r_h^2$$

Differential decay rate (electron energy spectrum)

$$\frac{d\lambda}{dW^t_e} = \frac{\pi G^2_\beta}{(2j_n+1)(2J_B+1)} \sum_{\gamma'} \sum_{\mu_n,\mu_p} \sum_{\mu'_B,\mu_B} \sum_{\kappa'_C,\mu'_C} \sum_{\kappa_\nu,\mu_\nu}$$

$$\left| \textstyle\sum_{L',q}(-)^q \begin{vmatrix} \langle\psi'_1|\phi_1\rangle & \langle\psi'_1|\phi_2\rangle & \cdots & \langle\psi'_1|\phi_N\rangle & M_{L',q,1}(W_\nu = Q - W^t_e) \\ \langle\psi'_2|\phi_1\rangle & \langle\psi'_2|\phi_2\rangle & \cdots & \langle\psi'_2|\phi_N\rangle & M_{L',q,2}(W_\nu = Q - W^t_e) \\ \vdots & & \ddots & & \vdots \\ \langle\psi'_N|\phi_1\rangle & \langle\psi'_N|\phi_2\rangle & \cdots & \langle\psi'_N|\phi_N\rangle & M_{L',q,N}(W_\nu = Q - W^t_e) \\ \langle\psi'_C|\phi_1\rangle & \langle\psi'_C|\phi_2\rangle & \cdots & \langle\psi'_C|\phi_N\rangle & M_{L',q,C}(W_\nu = Q - W^t_e) \end{vmatrix} \right|^2$$

It gives the number of electrons per unit energy and per unit time

Differential decay rate (electron energy spectrum)

$$\frac{d\lambda}{dW_e^t} = \frac{\pi G_\beta^2}{(2j_n+1)(2J_B+1)} \sum_{\gamma'} \sum_{\mu_n,\mu_p} \sum_{\mu'_B,\mu_B} \sum_{\kappa'_C,\mu'_C} \sum_{\kappa_\nu,\mu_\nu}$$

$$\left| \sum_{L',q} (-)^q \begin{vmatrix} \langle\psi'_1|\phi_1\rangle & \langle\psi'_1|\phi_2\rangle & \cdots & \langle\psi'_1|\phi_N\rangle & M_{L',q,1}(W_\nu = Q - W_e^t) \\ \langle\psi'_2|\phi_1\rangle & \langle\psi'_2|\phi_2\rangle & \cdots & \langle\psi'_2|\phi_N\rangle & M_{L',q,2}(W_\nu = Q - W_e^t) \\ \vdots & & \ddots & & \vdots \\ \langle\psi'_N|\phi_1\rangle & \langle\psi'_N|\phi_2\rangle & \cdots & \langle\psi'_N|\phi_N\rangle & M_{L',q,N}(W_\nu = Q - W_e^t) \\ \langle\psi'_C|\phi_1\rangle & \langle\psi'_C|\phi_2\rangle & \cdots & \langle\psi'_C|\phi_N\rangle & M_{L',q,C}(W_\nu = Q - W_e^t) \end{vmatrix} \right|^2$$

The final orbital was ψ'_i depend on γ' that identifies the possible final (shake-up, shake-off, excited) states

$$\begin{aligned} M_{L',q,B} = \int \Bigg[\int d\Omega_h Y_{L',q}(\theta_h,\phi_h)\langle \xi_p, j_p, \mu_p|\mathbf{r}_h\rangle\ \gamma^0\gamma^\mu(1-x\gamma^5)\langle \mathbf{r}_h|\xi_n, j_n, \mu_n\rangle \cdot r_h^2 \cdot \\ \int dr_l \int d\Omega_l Y_{L',-q}(\theta_l,\phi_l)\langle n'_B, \kappa'_B, \mu'_B|\mathbf{r}_l\rangle\gamma^0\gamma_\mu(1-\gamma^5)\langle \mathbf{r}_l|W_\nu, \kappa_\nu, \mu_\nu\rangle\delta(r_h - r_l)\Bigg] dr_h; \end{aligned}$$

$$\begin{aligned} M_{L',q,C} = \int \Bigg[\int d\Omega_h Y_{L',q}(\theta_h,\phi_h)\langle \xi_p, j_p, \mu_p|\mathbf{r}_h\rangle\ \gamma^0\gamma^\mu(1-x\gamma^5)\langle \mathbf{r}_h|\xi_n, j_n, \mu_n\rangle \cdot r_h^2 \cdot \\ \int dr_l \int d\Omega_l Y_{L',-q}(\theta_l,\phi_l)\langle W'_C, \kappa'_C, \mu'_C|\mathbf{r}_l\rangle\gamma^0\gamma_\mu(1-\gamma^5)\langle \mathbf{r}_l|W_\nu, \kappa_\nu, \mu_\nu\rangle\delta(r_h - r_l)\Bigg] dr_h; \end{aligned}$$

Using L' = 0, $\langle\psi'_i|\phi_j\rangle = \delta_{ij}$,e$^-$ wfs at nuclear radius, and γ_0 one recovers standard beta-decay

Calculation of the leptonic and hadronic wfs: DHF

The time independent Dirac Hamiltonian of a many particles system In the case of two different types of interactions, e.g. represented by scalar (g_S) and vector (g_V) potentials, the Dirac equation reads

$$\left\{\sum_i \left(c\boldsymbol{\alpha}_i \cdot \mathbf{p}_i + \beta_i mc^2 + V_i\right) + \sum_{i<j} \left[\beta_i \beta_j g_{S,ij} + \left(1 - \boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j\right) g_{V,ij}\right]\right\} \psi\left(\mathbf{r}_1, \cdots \mathbf{r}_N\right) = E\psi\left(\mathbf{r}_1, \cdots \mathbf{r}_N\right)$$

which in second quantization can be written as follows:

$$H = \sum_{s_1 s_2} \int d\mathbf{r}\ \hat{\psi}^+_{s_1}(\mathbf{r}) \left[-ic\boldsymbol{\alpha}_{s_1 s_2} \cdot \boldsymbol{\nabla} + \beta_{s_1 s_2} mc^2 + \delta_{s_1 s_2} V(\mathbf{r})\right] \hat{\psi}_{s_2}(\mathbf{r}) +$$
$$+ \frac{1}{2} \sum_{s_1 s_2 s_1' s_2'} \int d\mathbf{r} d\mathbf{r}'\ \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}^+_{s_1'}(\mathbf{r}') \left[\beta_{s_1 s_2} \beta_{s_1' s_2'} g_S\left(\mathbf{r}, \mathbf{r}'\right) + \left(\delta_{s_1 s_2} \delta_{s_1' s_2'} - \boldsymbol{\alpha}_{s_1 s_2} \cdot \boldsymbol{\alpha}'_{s_1' s_2'}\right) g_V\left(\mathbf{r}, \mathbf{r}'\right)\right] \hat{\psi}_{s_2'}(\mathbf{r}') \hat{\psi}_{s_2}(\mathbf{r})$$

where s_1, s_2, s_1’,s_2’ index the bispinor two-components

To compute the electronic and hadronic current we use the HF approximation

$$\left\langle \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}^+_{s_1'}(\mathbf{r}') \hat{\psi}_{s_2'}(\mathbf{r}') \hat{\psi}_{s_2}(\mathbf{r}) \right\rangle = \left\langle \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}_{s_2}(\mathbf{r}) \right\rangle \left\langle \hat{\psi}^+_{s_1'}(\mathbf{r}') \hat{\psi}_{s_2'}(\mathbf{r}') \right\rangle - \left\langle \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}_{s_2'}(\mathbf{r}') \right\rangle \left\langle \hat{\psi}^+_{s_1'}(\mathbf{r}') \hat{\psi}_{s_2}(\mathbf{r}) \right\rangle$$

Calculation of the leptonic and hadronic wfs: DHF

$$\begin{pmatrix} mc^2 + W_V + W_S + \mathbf{A}_P \cdot \boldsymbol{\sigma} - E & -c\boldsymbol{\sigma} \cdot i\boldsymbol{\nabla} - \boldsymbol{\sigma} \cdot \mathbf{A} + W_{PS} \\ -c\boldsymbol{\sigma} \cdot i\boldsymbol{\nabla} - \boldsymbol{\sigma} \cdot \mathbf{A} + W_{PS} & -mc^2 + W_V + \mathbf{A}_P \cdot \boldsymbol{\sigma} - W_S - E \end{pmatrix} \begin{pmatrix} \psi_L \\ \psi_S \end{pmatrix} = 0$$

where

$$\begin{array}{rccc} W_S & - & \text{scalar} & \text{potential} \\ W_V & - & \text{vectorial} & \text{potential} \\ W_{PS} & - & \text{pseudoscalar} & \text{potential} \\ \mathbf{A}_P & - & \text{pseudo-vectorial} & \text{potential} \end{array}$$

For leptons:

$$W_S = \text{Coulomb interaction}$$

$$W_V = 0$$

$$A_P = 0$$

For hadrons:

$$\begin{array}{lccc} W_V + W_S & - & \text{Wood-Saxon} & \text{potential} \\ W_V - W_S & - & \text{spin-orbit} & \text{potential} \end{array}$$

$\mathbf{A}_P$ − magnetic field **= 0**

Calculation of the leptonic wfs

Dirac equation in a spherical potential

$$H\psi(\mathbf{r}) = (c\boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc^2 + V(r))\psi(\mathbf{r}) = W\psi(\mathbf{r})$$

solutions are of the form: $\psi(\mathbf{r}) = \psi_{\kappa,\mu}(\mathbf{r}) = \begin{pmatrix} f_\kappa(r)\,\chi_{\kappa,\mu}(\Omega) \\ ig_\kappa(r)\,\chi_{-\kappa,\mu}(\Omega) \end{pmatrix}$

where $\chi_{\kappa,\mu}(\Omega) = \sum_{m_s=-\frac{1}{2}}^{\frac{1}{2}} \langle l\mu - m_s; \frac{1}{2}m_s|j\mu\rangle Y_{l,\mu-m_s}(\Omega)\phi_{m_s}$ are the spherical harmonics tensor

and calling $f_\kappa = \frac{u_\kappa}{r}$; $g_\kappa = \frac{v_\kappa}{r}$ u_κ and v_κ are solutions of

$$\begin{cases} \frac{\partial u_\kappa}{\partial r} = -\frac{\kappa}{r}u_\kappa + \frac{1}{c}(W - V(r) + mc^2)v_\kappa(r) = 0 \\ \frac{\partial v_\kappa}{\partial r} = \frac{\kappa}{r}v_\kappa - \frac{1}{c}(W - V(r) - mc^2)u_\kappa(r) = 0 \end{cases}$$

where $V(r) = -\frac{Z_f}{r} + \int \frac{\rho(r')}{r_>} d^3r' - V_{ex}(r)$

and we assume $V_{ex} = \frac{3}{2}\alpha_X\left[\frac{3}{\pi}\rho(r)\right]^{1/3}$ **which is local (TF or LDA)**

To numerically solve the DHF equations we use the collocation methods, which a Runge-Kutta type integration method

Calculation of the hadronic wfs: DHF

By changing the interaction potential, the calculation of the hadronic wavefunctions within the nuclear matrix elements can be performed

Nuclear wfs simulations out of scope (WS model potential)

$$V_C(r) = -V_C \left[1 + \exp\left(\frac{r-R}{a}\right)\right]^{-1} \qquad V_C = V_0 \left(1 \overset{\text{Protons}}{\underset{\text{Neutrons}}{\pm}} \chi \frac{N-Z}{A}\right)$$

$$\tilde{V}_{SO}(r) = \tilde{V}_{SO} \left[1 + \exp\left(\frac{r-R_{SO}}{a_{SO}}\right)\right]^{-1} \qquad \tilde{V}_{SO} = \lambda V_C$$

$R = R_0 A^{1/3}$ **and** $R_{SO} = R_{0,SO} A^{1/3}$ **= nuclear radius**

a **and** a_{SO} **= diffuseness**

$V_0, \chi, \lambda, a = a_{SO}, R_0, R_{0,SO}$ **are parameters to be optimised according to experiments or ab-initio nuclear structure simulations**

$$V_0 = 52.06\ MeV, \chi = 0.639, R_0 = 1.260\ fm, R_{0,SO} = 1.160\ fm, \lambda = 24.1, a = a_{SO} = 0.662\ fm$$

The beta-decay spectrum of $^{63}Ni,^{129}I,^{241}Pu$

Allowed Gamow-Teller

$^{63}_{28}Ni_{35}$ **= even-odd**

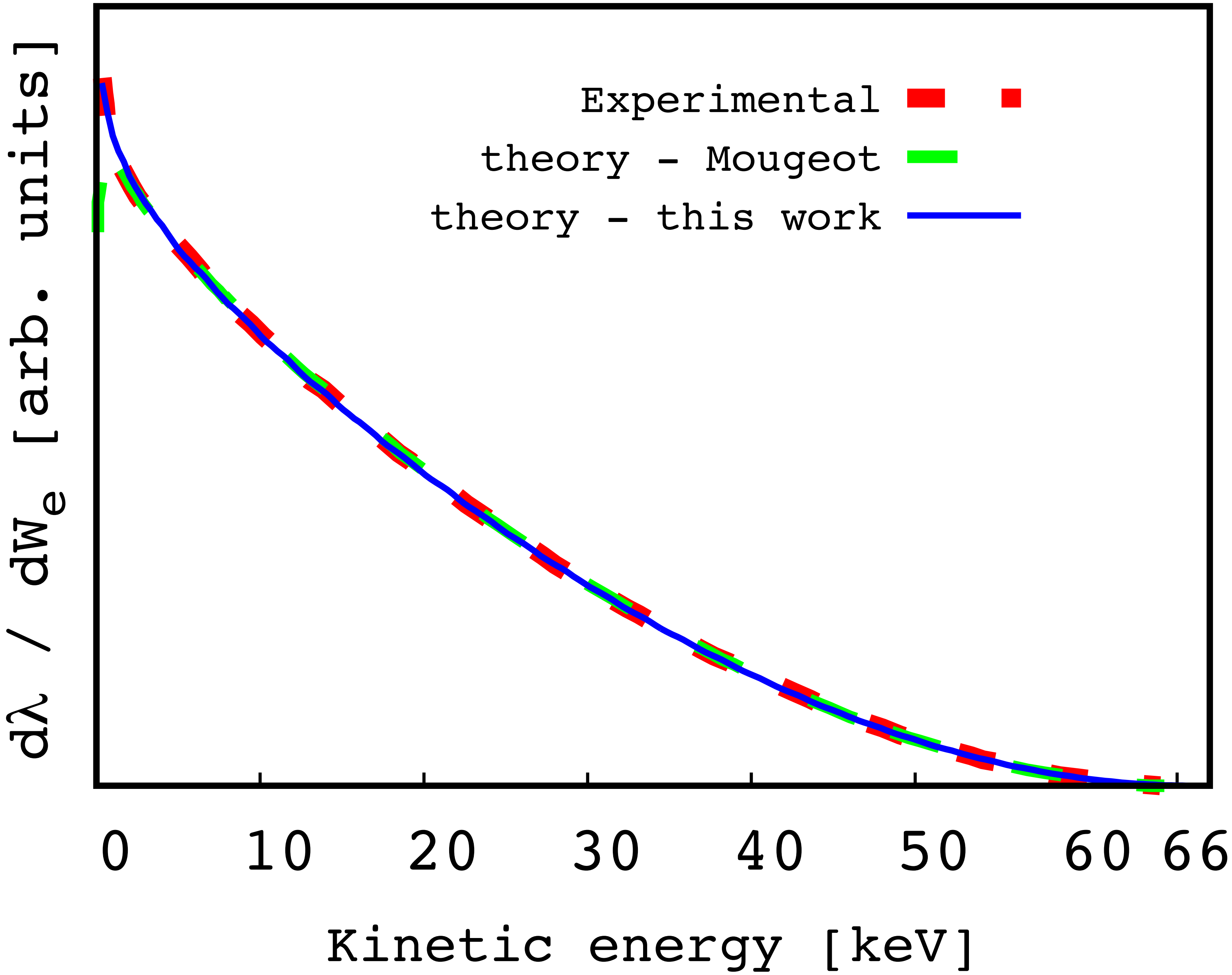
$^{63}_{29}Cu_{34}$ **= odd-even**

100% via β^- half-life = 101.2 y

Q-value = 66.945 keV
(ground state to ground state)

$$^{63}_{28}\mathrm{Ni}_{35} \rightarrow\, ^{63}_{29}\mathrm{Cu}_{34} + e^- + \bar{\nu}_e$$

$$J = 1/2^- \rightarrow J = 3/2^-$$



Mean-field DHF + screening + exchange works just fine as other approaches!!!!

The beta-decay spectrum of $^{63}Ni, ^{129}I, ^{241}Pu$

$$^{129}I \rightarrow \; 17374.6321 \; > \; 5486.6741$$

$$^{241}Pu \rightarrow \; 30566.4823 \; >> \; 763.6509$$

$$^{129}_{53}\mathrm{I}_{76} \rightarrow {}^{129}_{54}\mathrm{Xe}^{*}_{75} + e^{-} + \bar{\nu}_e$$

$$J = 7/2^{+} \rightarrow J = 3/2^{+}$$

Second forbidden

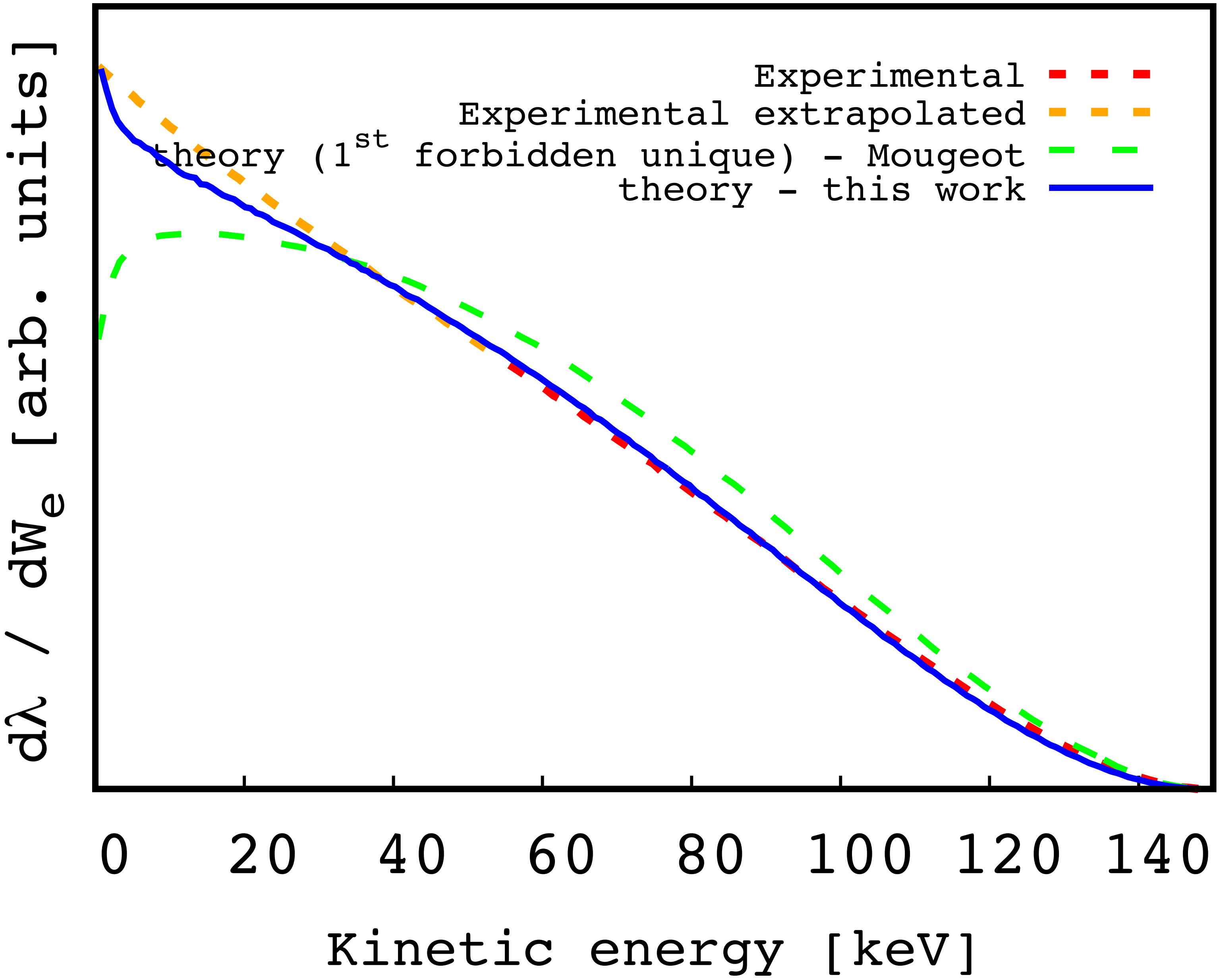
$^{129}_{53}I_{76}$ **= odd-even**

$^{129}_{54}\mathrm{Xe}_{75}$ **= even-odd**

β^{-} **half-life = 1.57X10^{7} y (10.05)**

Q-value = 149.4 keV (ground state to excited state)

γ **= 39.578 keV**



Mean-field DHF + screening + exchange works just better than other approaches!!!!

The beta-decay spectrum of $^{63}Ni, ^{129}I, ^{241}Pu$

$^{129}I \rightarrow \;\; 17374.6321 \;\; > \;\; 5486.6741$

$^{241}Pu \rightarrow \;\; 30566.4823 \;\; >> \;\; 763.6509$

$^{241}_{94}\mathrm{Pu}_{147} \rightarrow {}^{241}_{95}\mathrm{Am}_{146} + e^- + \bar{\nu}_e$

$J = 5/2^+ \rightarrow J = 5/2^-$

First forbidden

$^{241}_{94}\mathrm{Pu}_{147}$ **= even-odd**

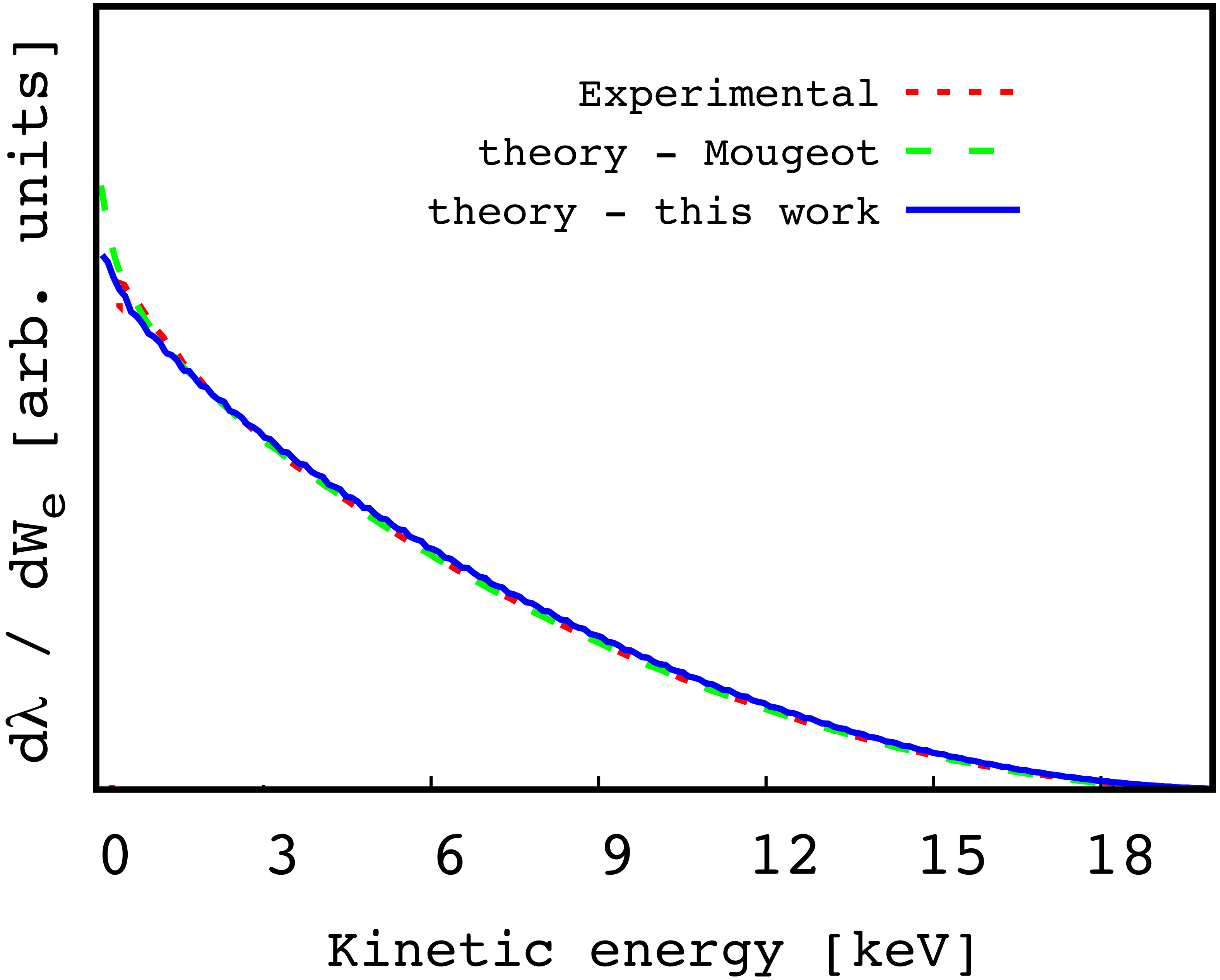
$^{241}_{95}\mathrm{Am}_{146}$ **= odd-even**

β^- **half-life = 14.329 y (6.85)**

Q-value = 20.78 keV
(ground state to excited state)

γ **= 39.578 keV**

Mean-field DHF + screening + exchange works just fine as other approaches!!!!



The beta-decay spectrum of $^{36}_{17}\mathrm{Cl}_{19}$

$$^{36}_{17}\mathrm{Cl}_{19} \rightarrow {}^{36}_{18}\mathrm{Ar}_{18} + e^{-} + \bar{\nu}_e$$

$$J = 2^{+} \rightarrow J = 0^{+}$$

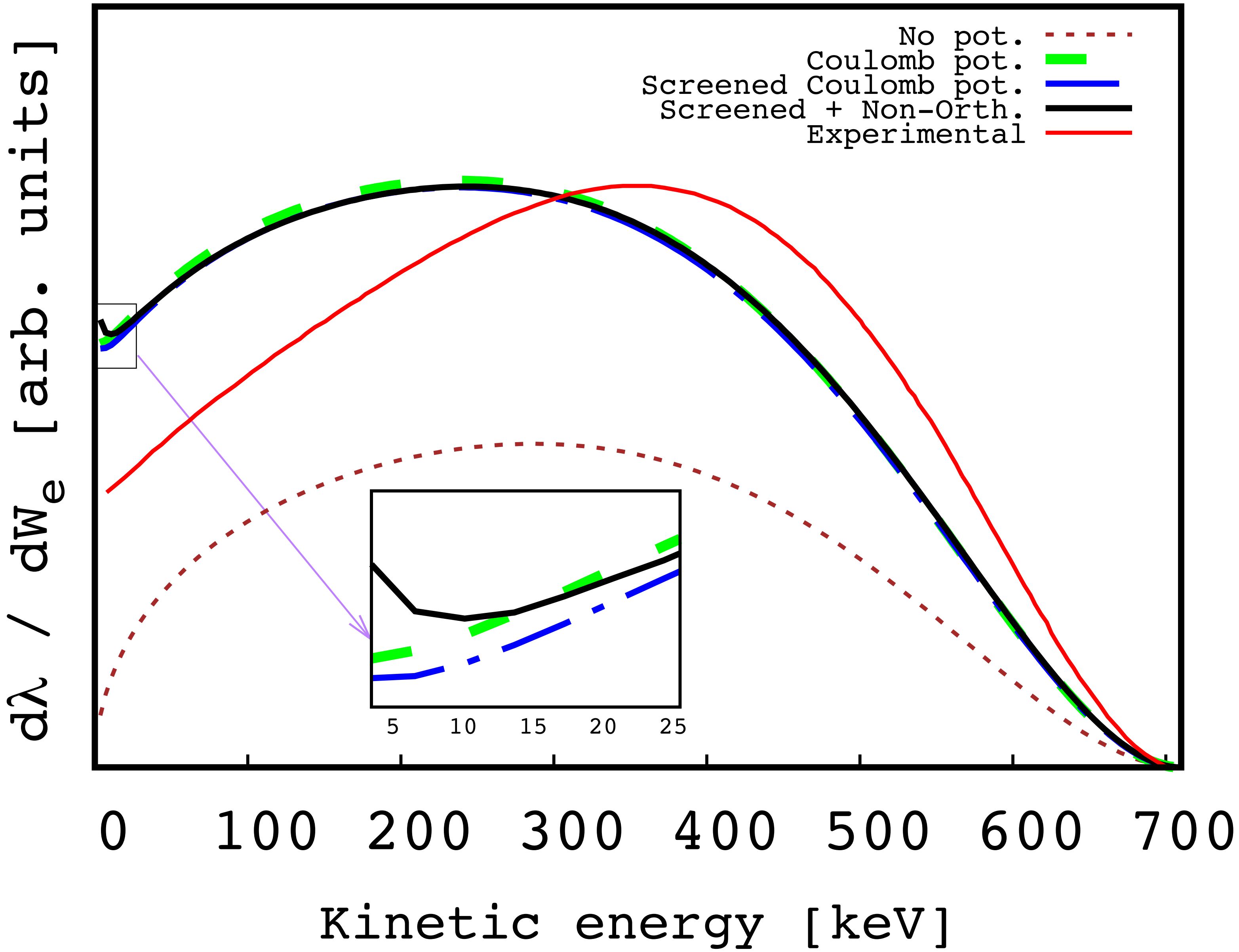
Second forbidden non-unique

$^{36}_{17}\mathrm{Cl}_{19}$ **= odd-odd**

$^{36}_{18}\mathrm{Ar}_{18}$ **= even-even**

β^{-} **half-life = 3.01X10^{5} y**

Q-value = 709.547 keV
(ground state to excited state)



Mean-field DHF + screening (self-consistent DHF) + exchange (discrete-continuum interaction) does not work fine as standard approaches !!!!

Shake-up and shake-off modifies the decay by only 5%

The beta-decay spectrum of $^{210}_{83}\mathrm{Bi}_{127}$

$^{210}_{83}\mathrm{Bi}_{127} \rightarrow {}^{210}_{84}\mathrm{Po}_{126} + e^{-} + \bar{\nu}_e$

$J = 1^{-} \rightarrow J = 0^{+}$

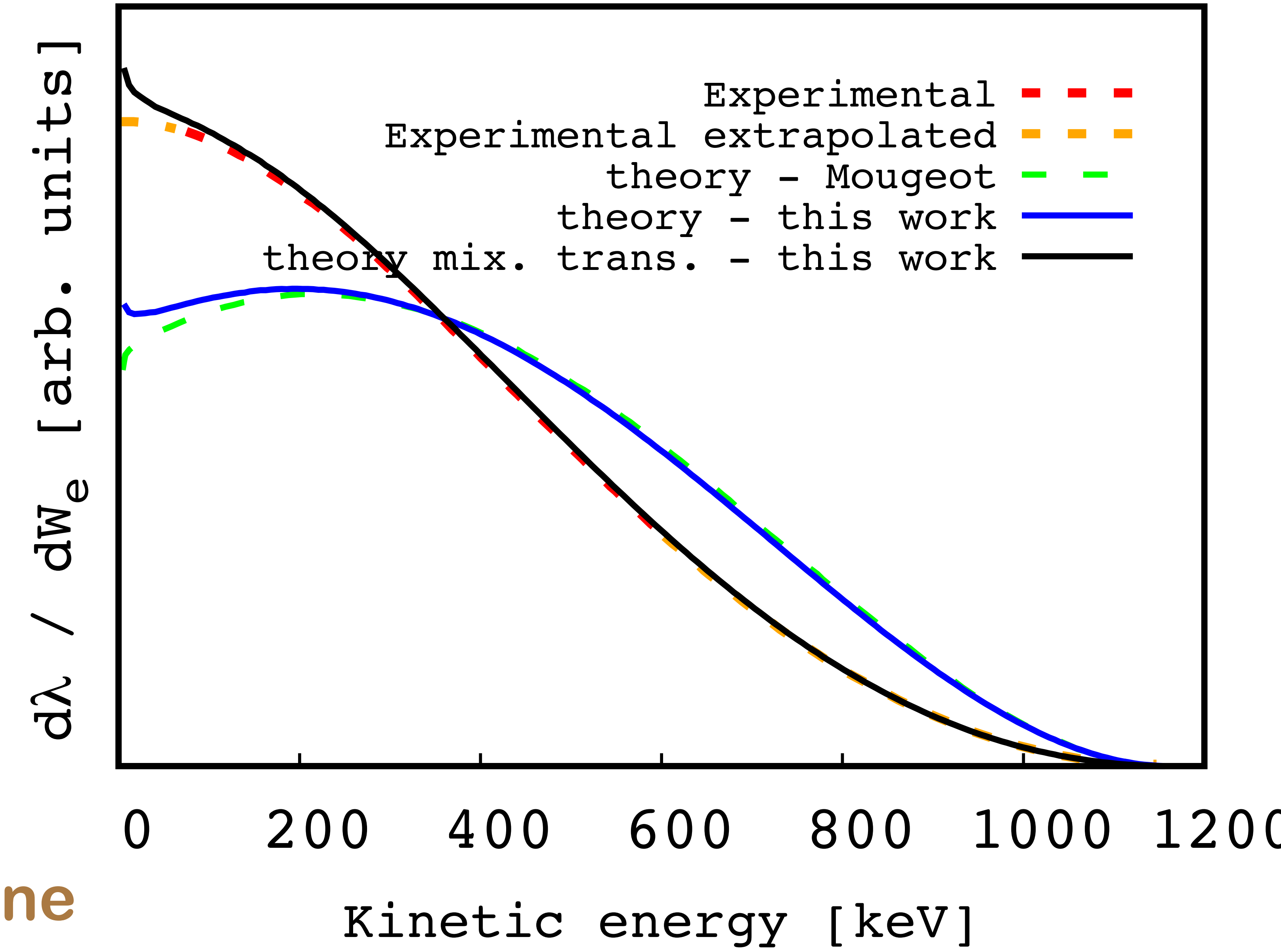
First forbidden non-unique

$^{210}_{83}\mathrm{Bi}_{127}$ **= odd-odd**

$^{210}_{84}\mathrm{Po}_{126}$ **= even-even**

β^{-} **half-life = 5.012 d**

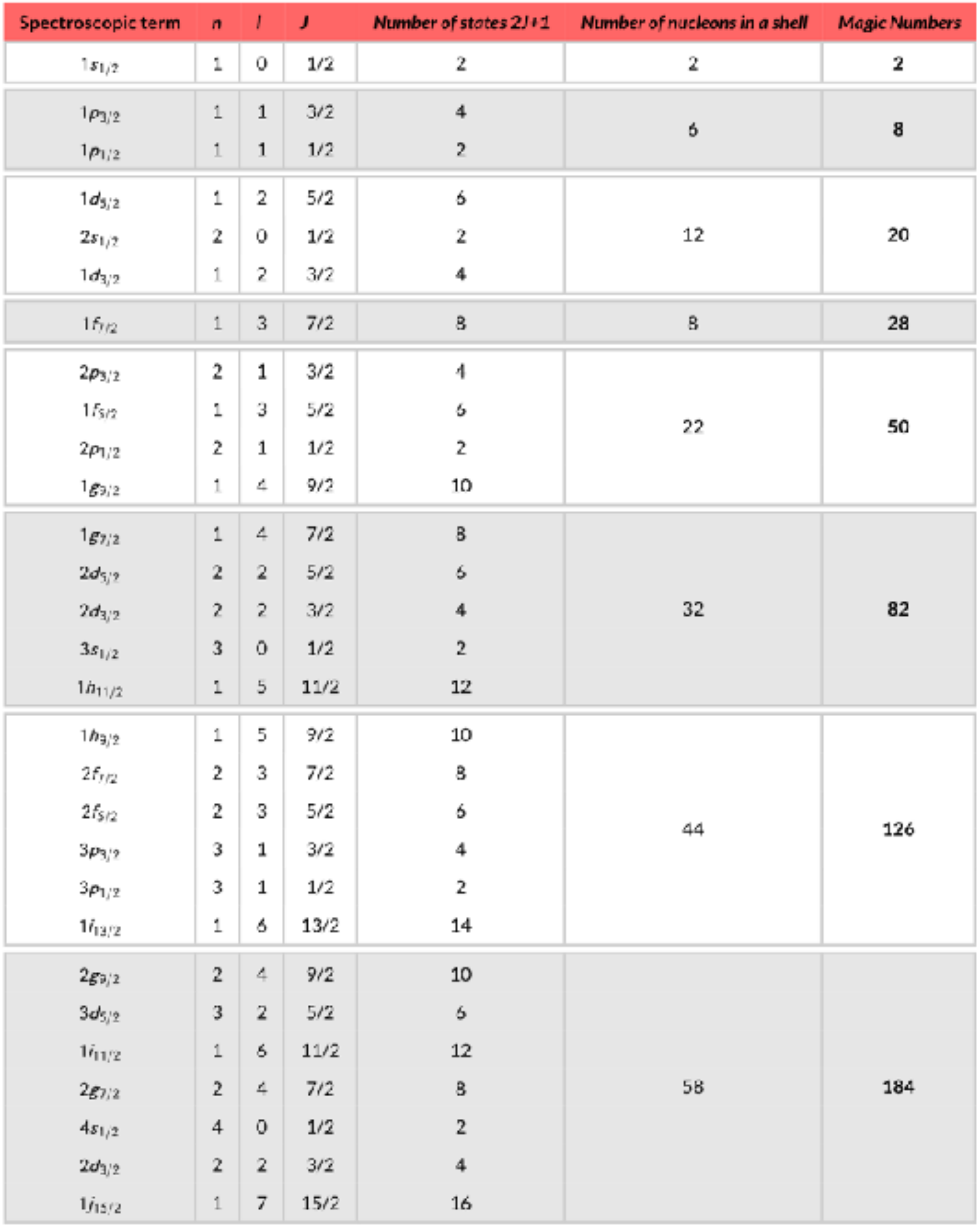
Q-value = 1162.2 keV (ground state to excited state)



Mean-field DHF + screening + exchange does not work fine as standard approaches !!!!

Shake-up and shake-off modifies the decay by only 5%

Final-state nuclear many-body affects on beta-decay spectra of odd-odd nuclei?



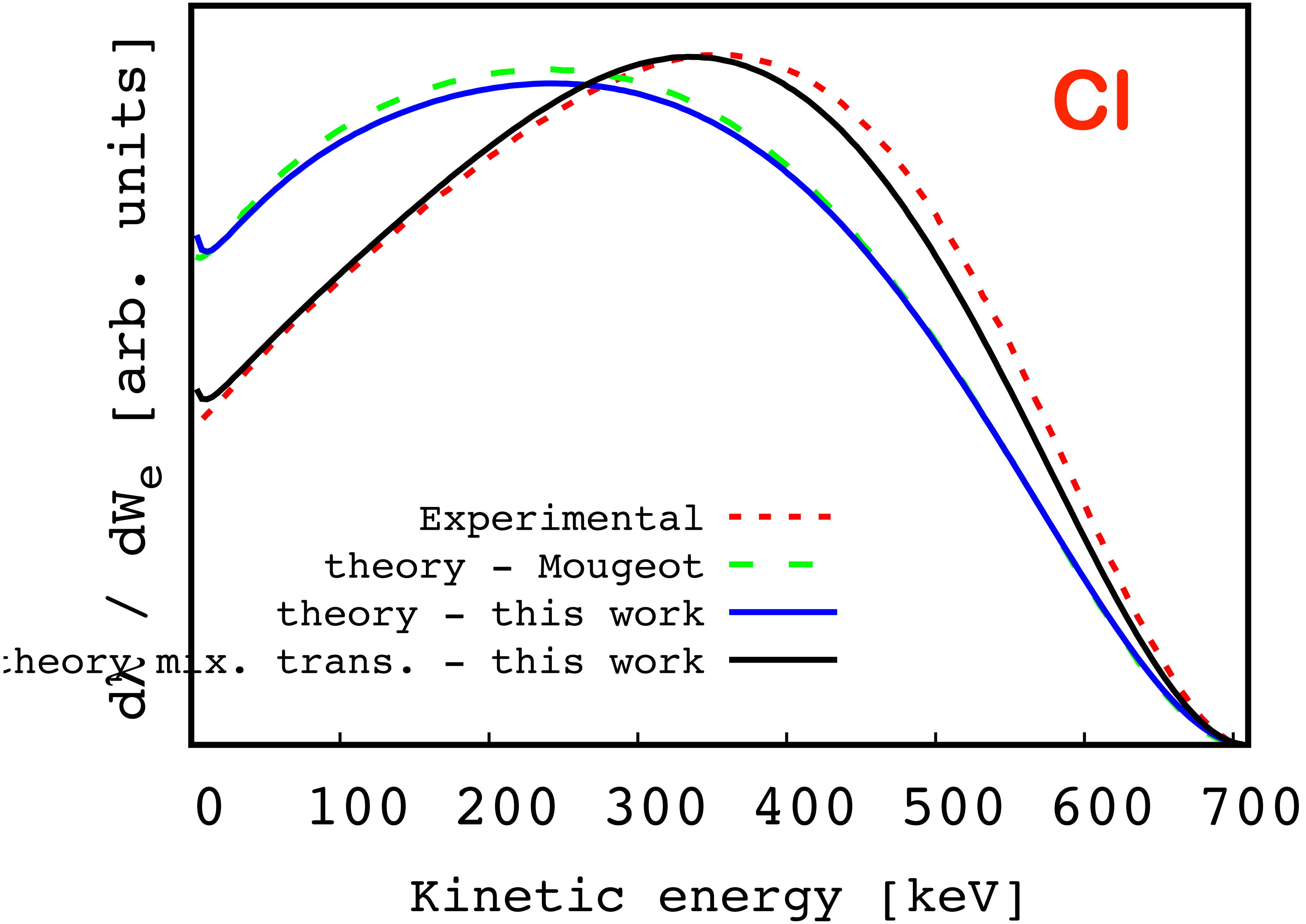
Spectroscopic term	n	l	J	Number of states 2J+1	Number of nucleons in a shell	Magic Numbers
$1s_{1/2}$	1	0	1/2	2	2	2
$1p_{3/2}$	1	1	3/2	4	6	8
$1p_{1/2}$	1	1	1/2	2		
$1d_{5/2}$	1	2	5/2	6	12	20
$2s_{1/2}$	2	0	1/2	2		
$1d_{3/2}$	1	2	3/2	4		
$1f_{7/2}$	1	3	7/2	8	8	28
$2p_{3/2}$	2	1	3/2	4	22	50
$1f_{5/2}$	1	3	5/2	6		
$2p_{1/2}$	2	1	1/2	2		
$1g_{9/2}$	1	4	9/2	10		
$1g_{7/2}$	1	4	7/2	8	32	82
$2d_{5/2}$	2	2	5/2	6		
$2d_{3/2}$	2	2	3/2	4		
$3s_{1/2}$	3	0	1/2	2		
$1h_{11/2}$	1	5	11/2	12		
$1h_{9/2}$	1	5	9/2	10	44	126
$2f_{7/2}$	2	3	7/2	8		
$2f_{5/2}$	2	3	5/2	6		
$3p_{3/2}$	3	1	3/2	4		
$3p_{1/2}$	3	1	1/2	2		
$1i_{13/2}$	1	6	13/2	14		
$2g_{9/2}$	2	4	9/2	10	58	184
$3d_{5/2}$	3	2	5/2	6		
$1i_{11/2}$	1	6	11/2	12		
$2g_{7/2}$	2	4	7/2	8		
$4s_{1/2}$	4	0	1/2	2		
$2d_{3/2}$	2	2	3/2	4		
$1j_{15/2}$	1	7	15/2	16		

The experimentally determined final state of the $^{36}_{18}\mathrm{Ar}_{18}$ daughter nucleus is 0+. Within the nuclear shell model two protons and two neutrons all occupy the $1d_{3/2}$ single-particle state. By coupling the $1d_{3/2}$ proton to a $1d_{3/2}$ “core” to construct a 0+ final symmetry state, and by calculating the hadronic matrix element for this transition only, we obtain the lineshape reported as a blue curve in the previous figure. We could not yet find a good agreement between simulations and experimental data.

Adding “nuclear many-body effects” by mixing transitions to the $1d_{3/2}$ orbital, possibly the highest populated orbital according to the nuclear shell model, with the $2s_{1/2}$ level, which is energetically close, we find good agreement with experiments

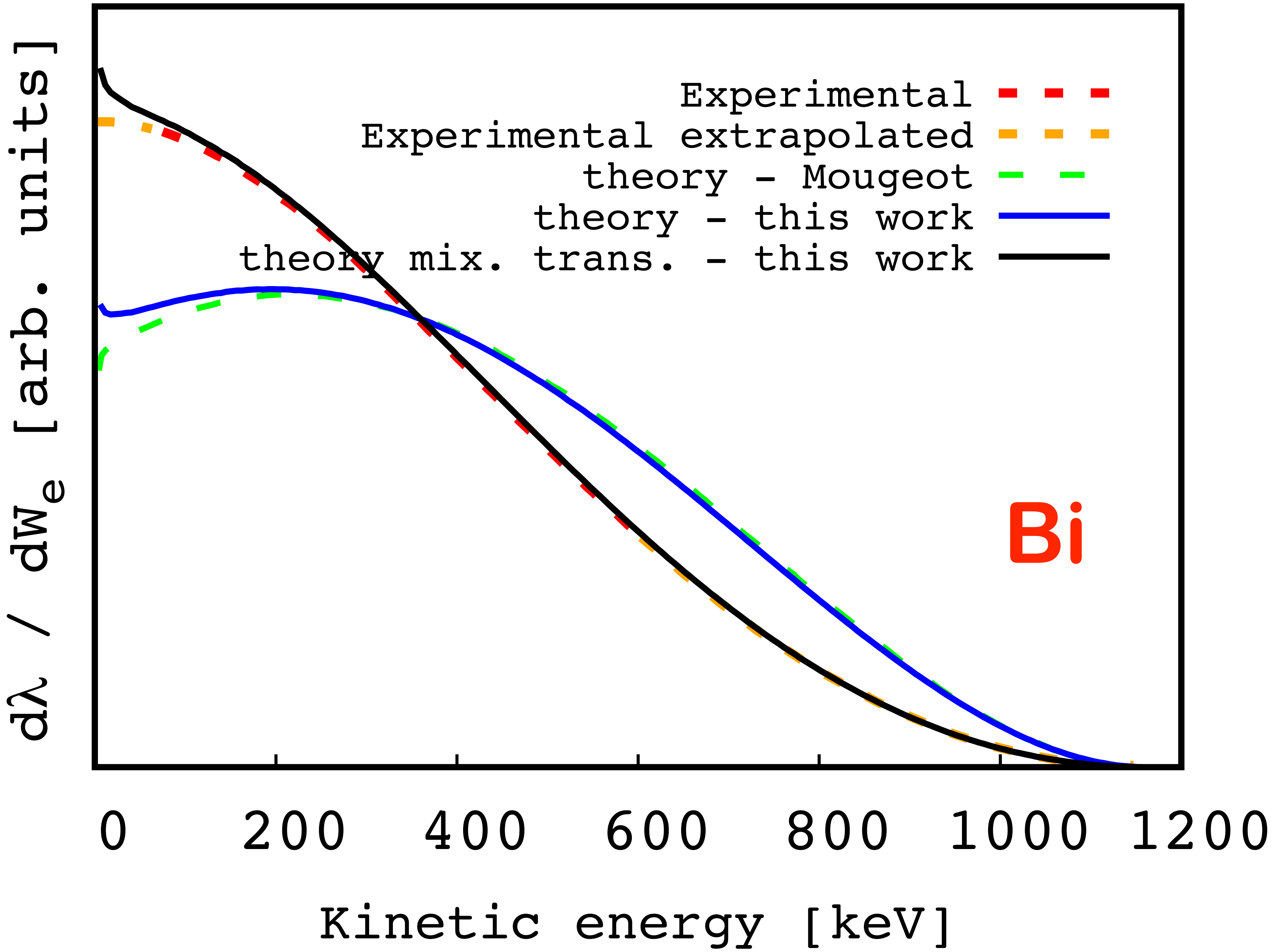
Final-state nuclear many-body affects on beta-decay spectra of odd-odd nuclei?

$$1 \times J^{H,\mu}_{1d_{3/2}\rightarrow 1d_{3/2}} - 2.55 \times J^{H,\mu}_{1d_{3/2}\rightarrow 2s_{1/2}}$$

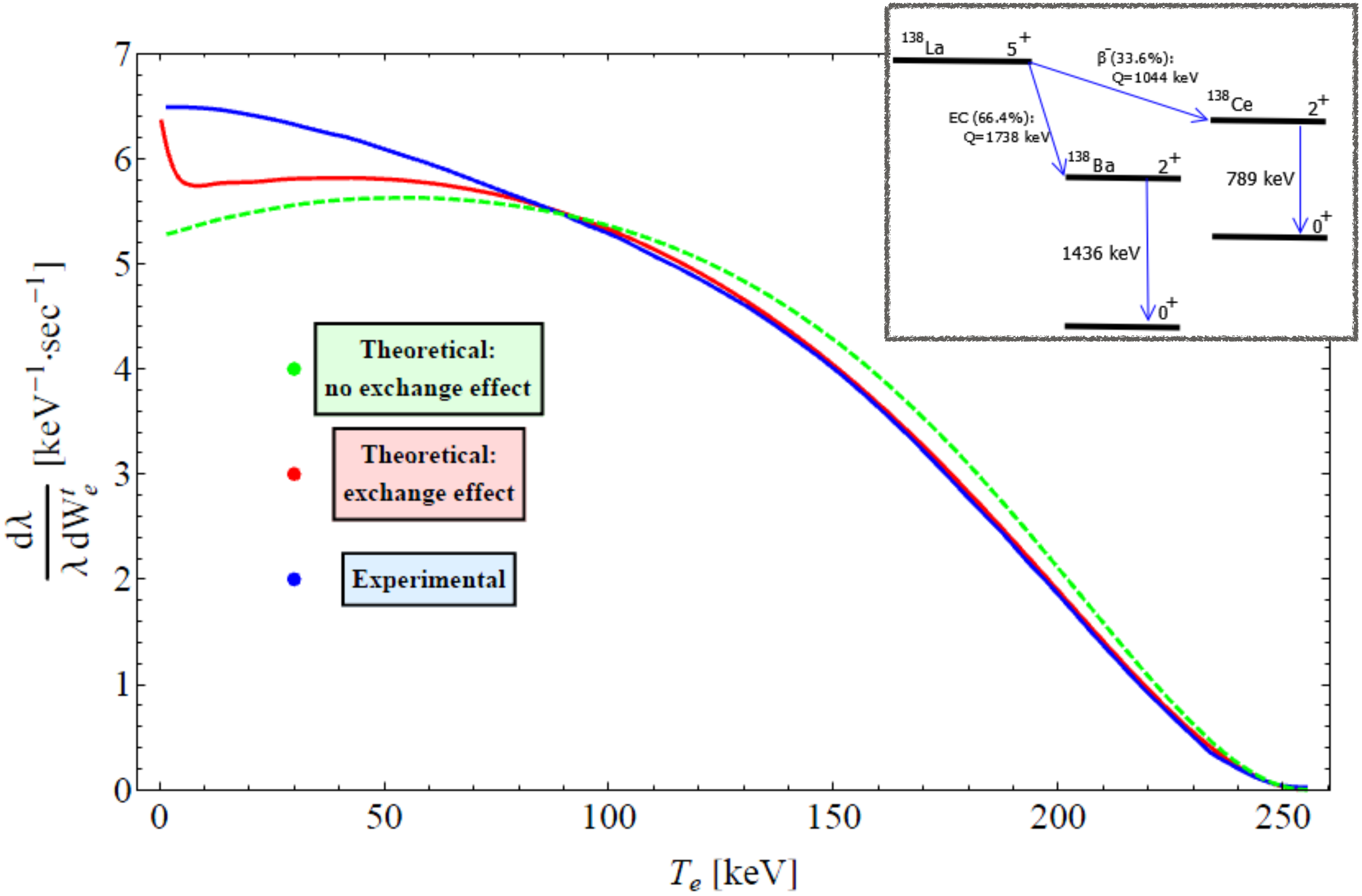


Nuclear many-body affects on beta-decay spectra of odd-odd nuclei?

$$1 \times J^{H,\mu}_{2g_{9/2} \rightarrow 1h_{9/2}} - 0.92 \times J^{H,\mu}_{2g_{9/2} \rightarrow 1h_{11/2}}$$



β-decay theory: higher order approximations - results



Electron capture of Lantanum

$$^{138}_{57}\mathrm{La}_{81} + e^{-} \rightarrow {}^{138}_{56}\mathrm{Ba}_{82} + \nu_e$$

$$J = 5^{+} \rightarrow J = 2^{+}$$

Just take the hermitian conjugate in the previous expression of the field operators

Second forbidden unique

half-life = 1.03X 10^{11} y

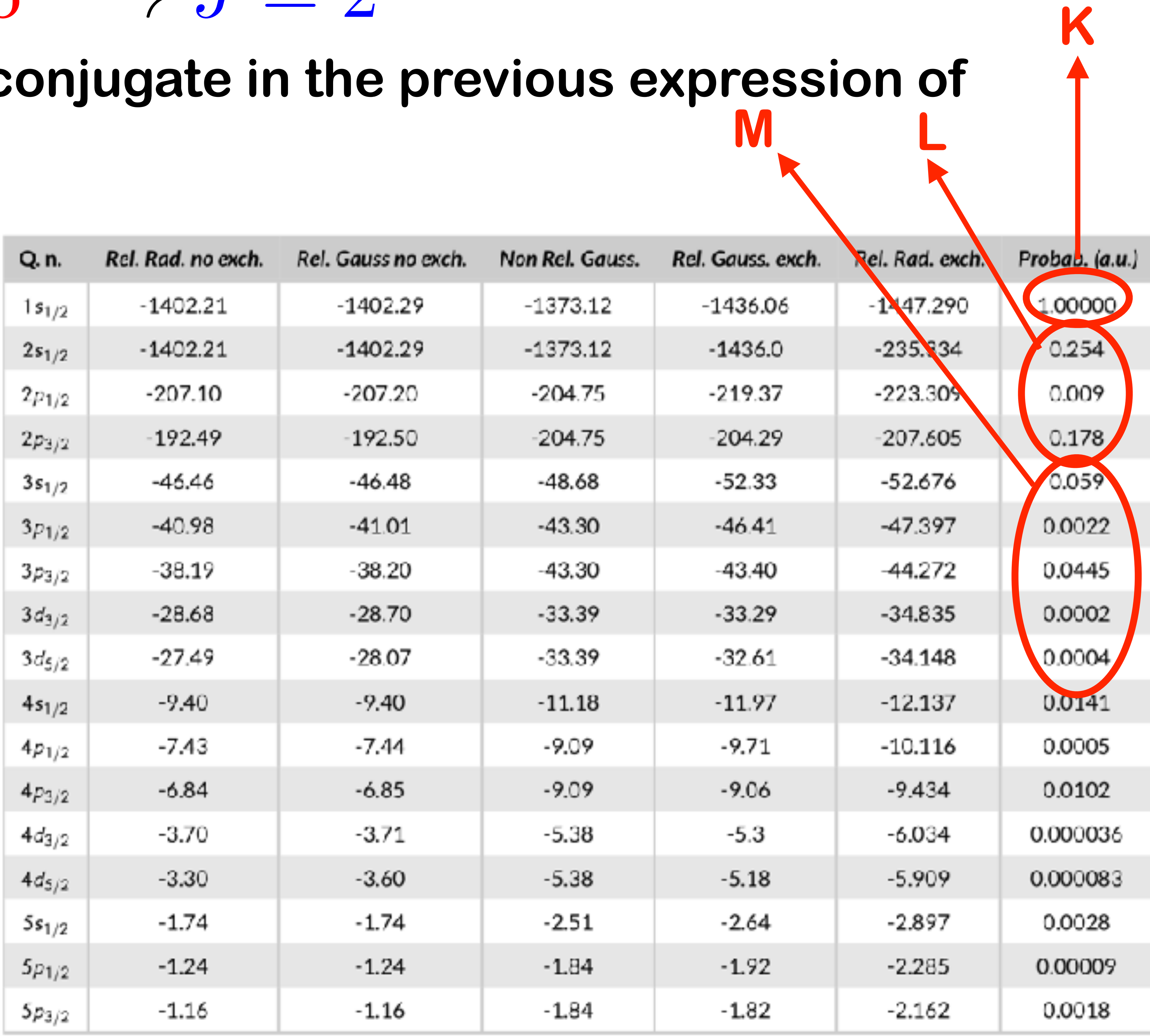
Q-value = 1742 keV (ground state to excited state)

L/K=0.44 (0.391)

M/K=0.106 (0.102)

M/L=0.241 (0.261)

Most likely capture occurs by capturing $1s_{1/2}$ and $2s_{1/2}$ electrons



Q. n.	Rel. Rad. no exch.	Rel. Gauss no exch.	Non Rel. Gauss.	Rel. Gauss. exch.	Rel. Rad. exch.	Probab. (a.u.)
$1s_{1/2}$	-1402.21	-1402.29	-1373.12	-1436.06	-1447.290	1.00000
$2s_{1/2}$	-1402.21	-1402.29	-1373.12	-1436.0	-235.334	0.254
$2p_{1/2}$	-207.10	-207.20	-204.75	-219.37	-223.309	0.009
$2p_{3/2}$	-192.49	-192.50	-204.75	-204.29	-207.605	0.178
$3s_{1/2}$	-46.46	-46.48	-48.68	-52.33	-52.676	0.059
$3p_{1/2}$	-40.98	-41.01	-43.30	-46.41	-47.397	0.0022
$3p_{3/2}$	-38.19	-38.20	-43.30	-43.40	-44.272	0.0445
$3d_{3/2}$	-28.68	-28.70	-33.39	-33.29	-34.835	0.0002
$3d_{5/2}$	-27.49	-28.07	-33.39	-32.61	-34.148	0.0004
$4s_{1/2}$	-9.40	-9.40	-11.18	-11.97	-12.137	0.0141
$4p_{1/2}$	-7.43	-7.44	-9.09	-9.71	-10.116	0.0005
$4p_{3/2}$	-6.84	-6.85	-9.09	-9.06	-9.434	0.0102
$4d_{3/2}$	-3.70	-3.71	-5.38	-5.3	-6.034	0.000036
$4d_{5/2}$	-3.30	-3.60	-5.38	-5.18	-5.909	0.000083
$5s_{1/2}$	-1.74	-1.74	-2.51	-2.64	-2.897	0.0028
$5p_{1/2}$	-1.24	-1.24	-1.84	-1.92	-2.285	0.00009
$5p_{3/2}$	-1.16	-1.16	-1.84	-1.82	-2.162	0.0018

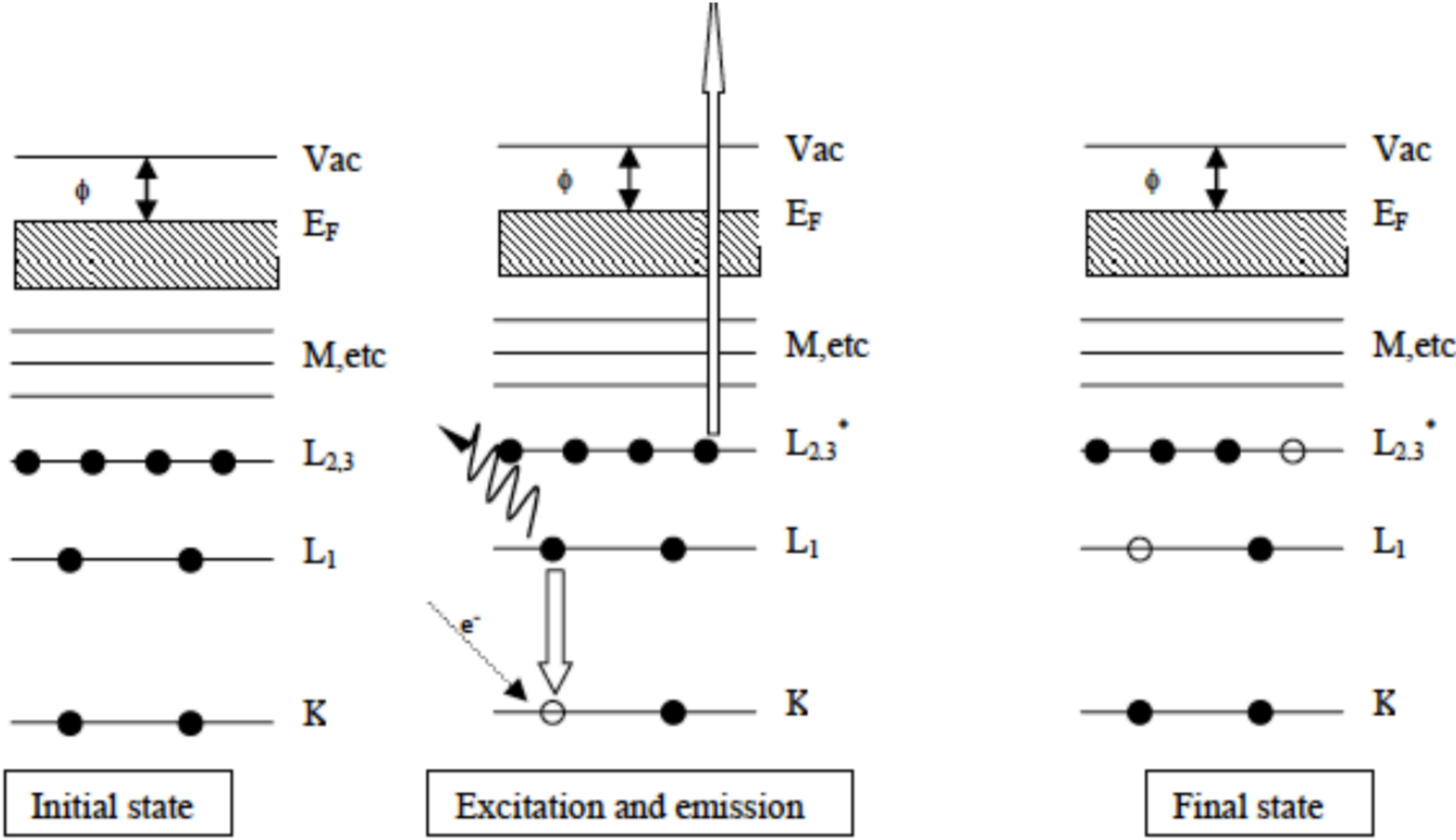
Electron capture of Lantanum

- To reproduce the experimental line shape one has to include all the decay processes following the e-capture

- In particular, one has to include K- and L- shell Auger decays that compete with γ-ray emission. The daughter system undergoes most likely (49.1%) Auger decay from the L-shell and less likely (4.16%) the Auger decay proceeds from the K-shell, even though the K-shell capture is more likely

- Indeed, one may guess that the system, before the Auger non-radiative process takes place, undergoes a radiative transition which afterwards favours the Auger decay from the L-shell with respect to the K-shell.

Autoionization, Auger, shake-up and shake-off



General considerations on the determination of ν mass

- EC and β-decay are sensitive to a neutrino mass ≠ 0 (≤ 0.1 eV) in the region very close to the end-point
- The ratio between the region modified by a value of the neutrino mass ≠ 0 and the Q-value is higher for lower Q-values
- Instruments have a sensitivity inverse proportional to the Q-value. For the same sensitivity, the possible influence of the neutrino mass on the β-spectrum is more evident in low Q-value processes
- The most promising candidates are ^{163}Ho and ^{3}H because they have a small Q-value
- One- and two core-hole, shake-up, shake-off processes can dramatically affect the end-point of the reaction

Beyond SM?

Determination of the anti-neutrino mass by beta-decay

KATRIN = Karlsruhe Tritium Neutrino Experiment

$${}^{3}_{1}\mathrm{T}_{2} \rightarrow {}^{3}_{2}\mathrm{He}_{1} + e^{-} + \bar{\nu}_{e}$$

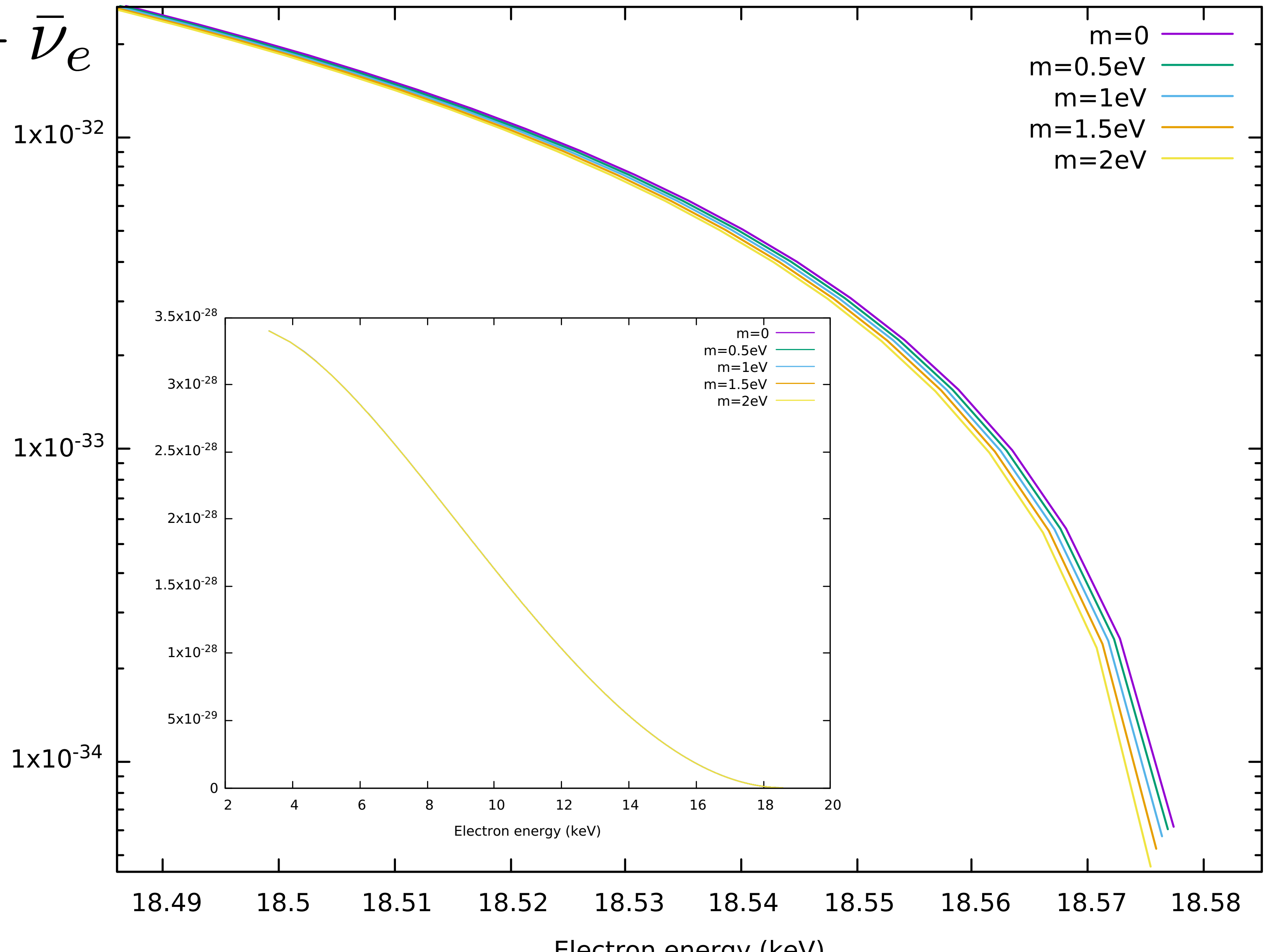
$$J = 1/2^{+} \rightarrow J = 1/2^{+}$$

Allowed transition

half-life = 12.32 y

Q-value = 18.592 keV

Recoil energy is negligible



Beyond SM?

Determination of the neutrino mass by electron capture

ECHo = Electron Capture by Ho - Heidelberg

$$^{163}_{67}\mathrm{Ho}_{96} + e^- \rightarrow \,^{163}_{66}\mathrm{Dy}_{97} + \nu_e$$

$$J = 7/2^- \rightarrow J = 5/2^-$$

Allowed transition

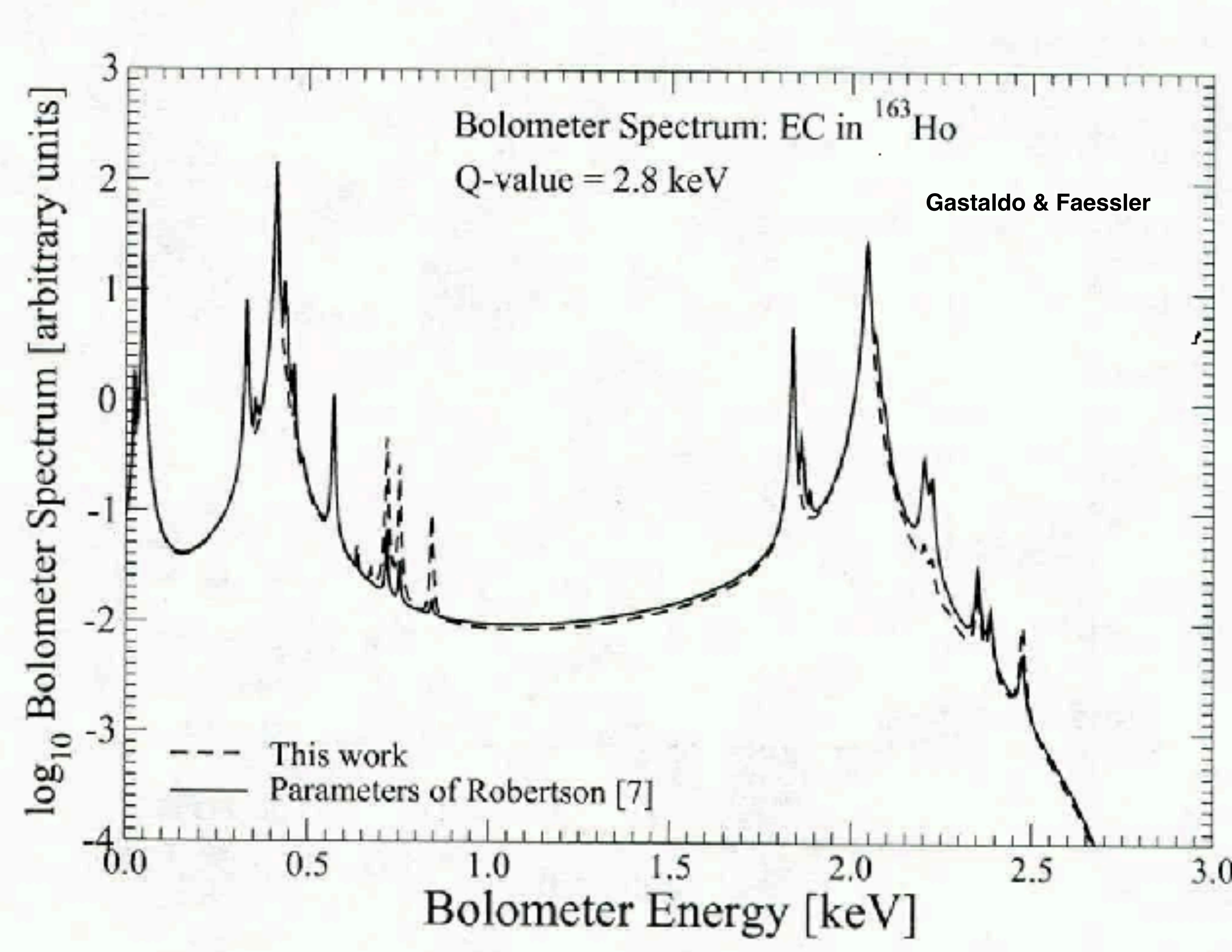
half-life = 4570 y

Q-value = 2,83 keV

Ho Electronic configuration

[Xe]$4f^{11}$ $6s^2$

Recoil energy is negligible



Electronic capture rate:

$$\frac{dN}{dE_c} = A(Q_{EC} - E_c)\sqrt{1 - \frac{m_\nu^2}{(Q_{EC} - E_c)^2}} \sum_H C_H n_H B_H \phi_H(0)^2 \frac{\Gamma_H/2\pi}{(E_C - E_H)^2 + \Gamma_H^2/4}$$

- The calorimeter measure all the energy, so that the e^--rate of Ho coincides with the de-excitation spectrum of Dy
- The sum runs over all the orbitals from which the e^- can be captured
- The line shape is a sum of Lorentzian functions centered in E_H
- The spectrum depends on the energy Ec = [0:2,833] keV and parametrically on the neutrino mass.
- We assume that all the other parameters are constant
- $\phi_H(0)$ is the DHF orbital wf from which the capture occurs, but in the final metastable Dy state

1) Electron at nucleus → $s_{1/2}$ and $p_{1/2}$

2) Electron binding energy < Q-value ≈ 2.8 [keV]

$E(1s_{1/2}, K,Ho) = 55.6$ keV

$E(2s_{1/2}, L1,Ho) = 9.4$ keV

$E(2p_{1/2},L2,Ho) = 8.9$ keV

$E(2p_{3/2},L3,Ho) = 8.1$ keV

$E(3s_{1/2} ,M1,Ho) = 2.0$ keV

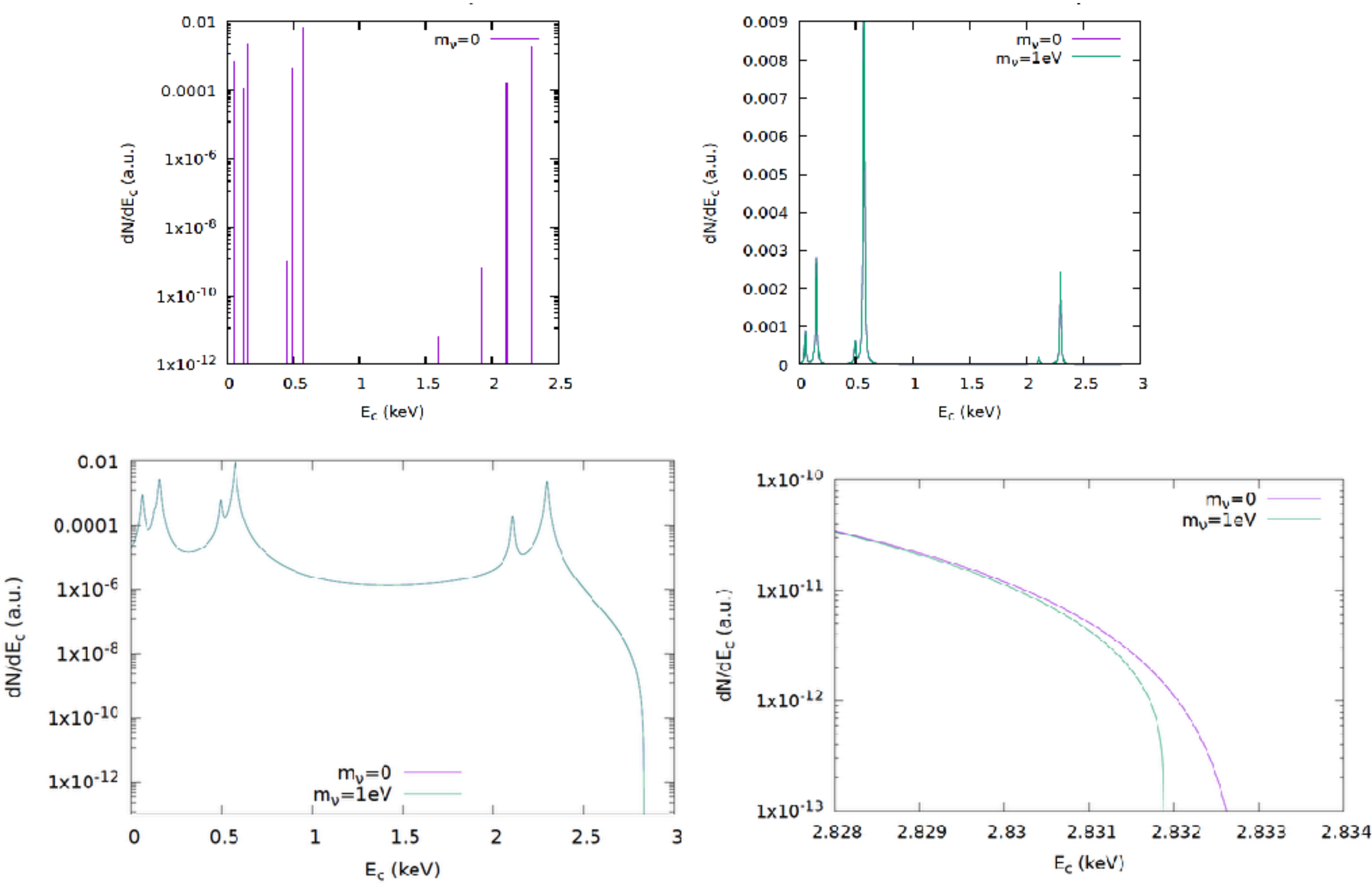
$E(3p_{1/2},M2,Ho) = 1.8$ keV

$E(4s_{1/2} , N1,Ho) = 0.4$ keV

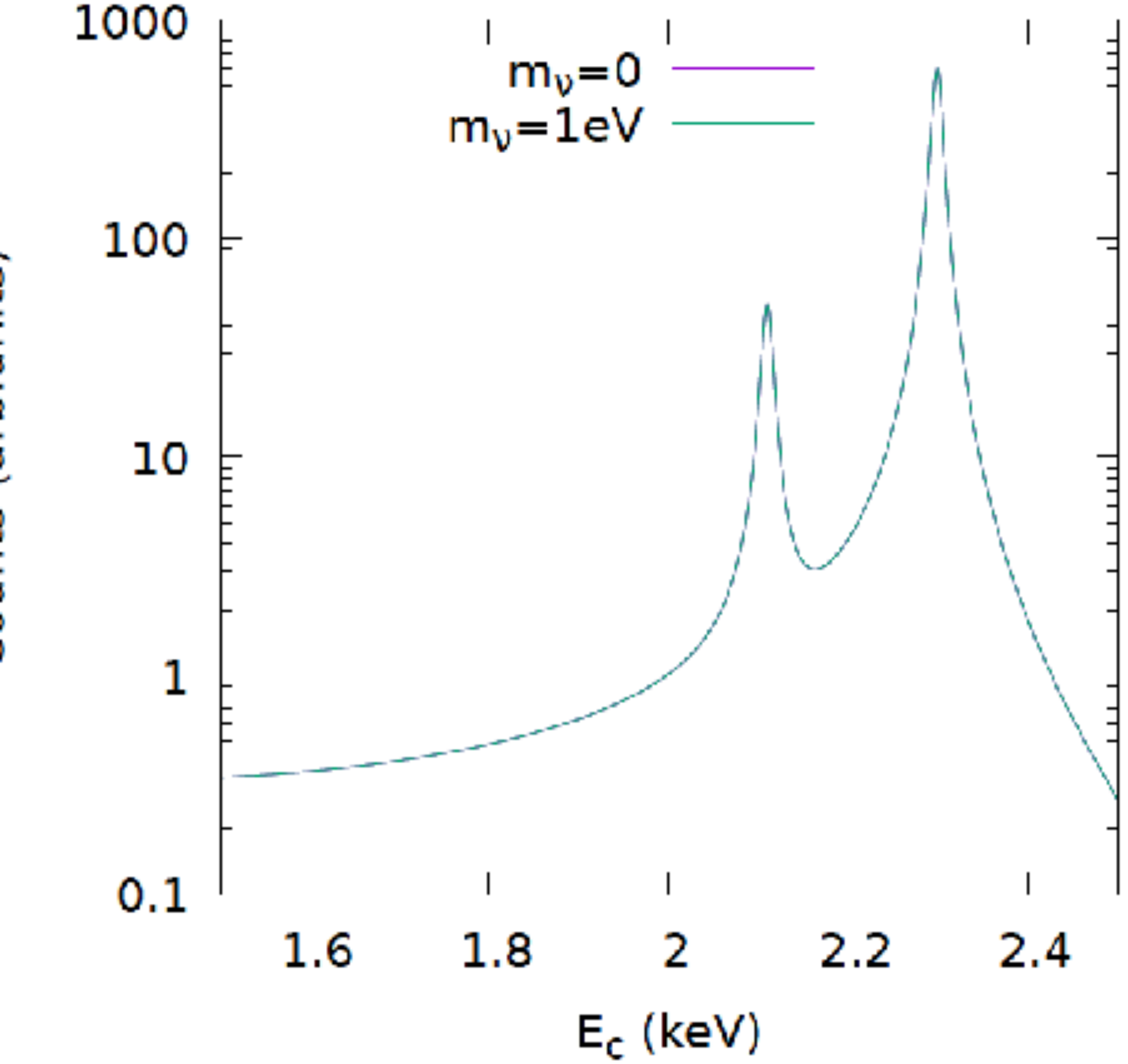
$E(4p_{1/2}, N2,Ho) = 0.3$ keV

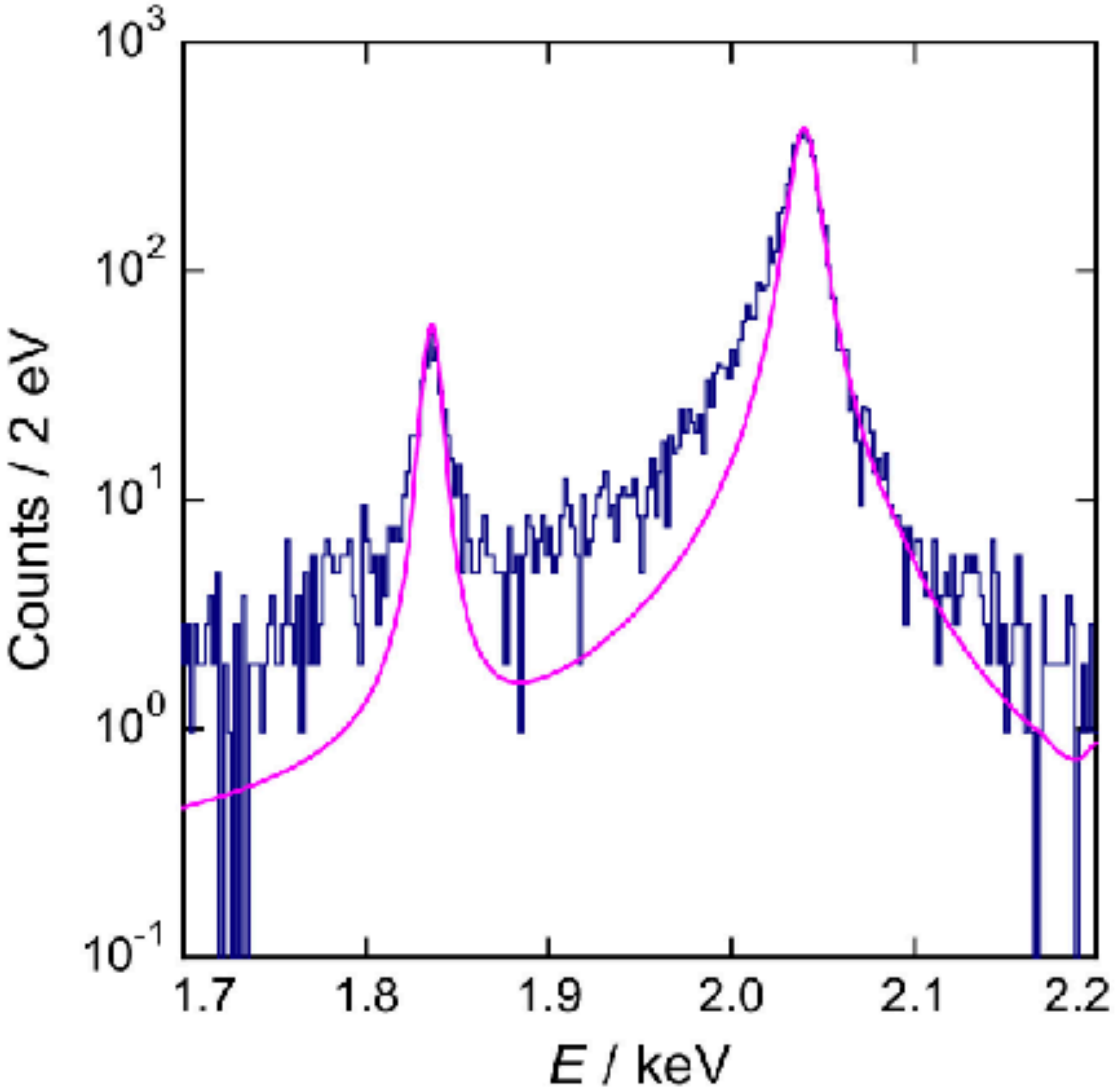
$E(5s_{1/2} ,O1,Ho) = 0.05$ keV

Autoionization only spectral line shape (first-order transitions)



Theory vs. Experiments (first-order transitions)





To determine the neutrino mass we need to assess the contribution to the spectrum in proximity of the end-point: Lorentzian peaks

$$W_f^{\mathrm{rel}} \approx \frac{S_{f=j(p)}}{\Delta E_f^2}$$

$$S_{f=j(p)} = |\psi_j(R)|^2$$

- $W_{j=3s_{1/2}} = \frac{100\%}{(2{,}8-2{,}04)^2} = 17{,}4\ keV^{-2}$
- $W_{j=4s_{1/2}} = \frac{24{,}4\%}{(2{,}8-0{,}41)^2} = 4{,}3\ keV^{-2}$
- $W_{j=3s_{1/2},p=4s_{1/2}} = \frac{100\%}{(2{,}8-2{,}47)^2} = 2{,}6\ keV^{-2}$

EC in Be

The knowledge of β decay and electronic capture rates are of paramount importance for our understanding of stellar nucleosynthesis and isotopic abundances in stellar and interstellar gases

Motivation of this work: provide the missing weak-interaction input data for Li nucleosynthesis calculations

$$W \propto \delta(\vec{r})$$

insensitive to extra-nuclear factors, such as chemical environment, ionization degree, pressure and temperature.

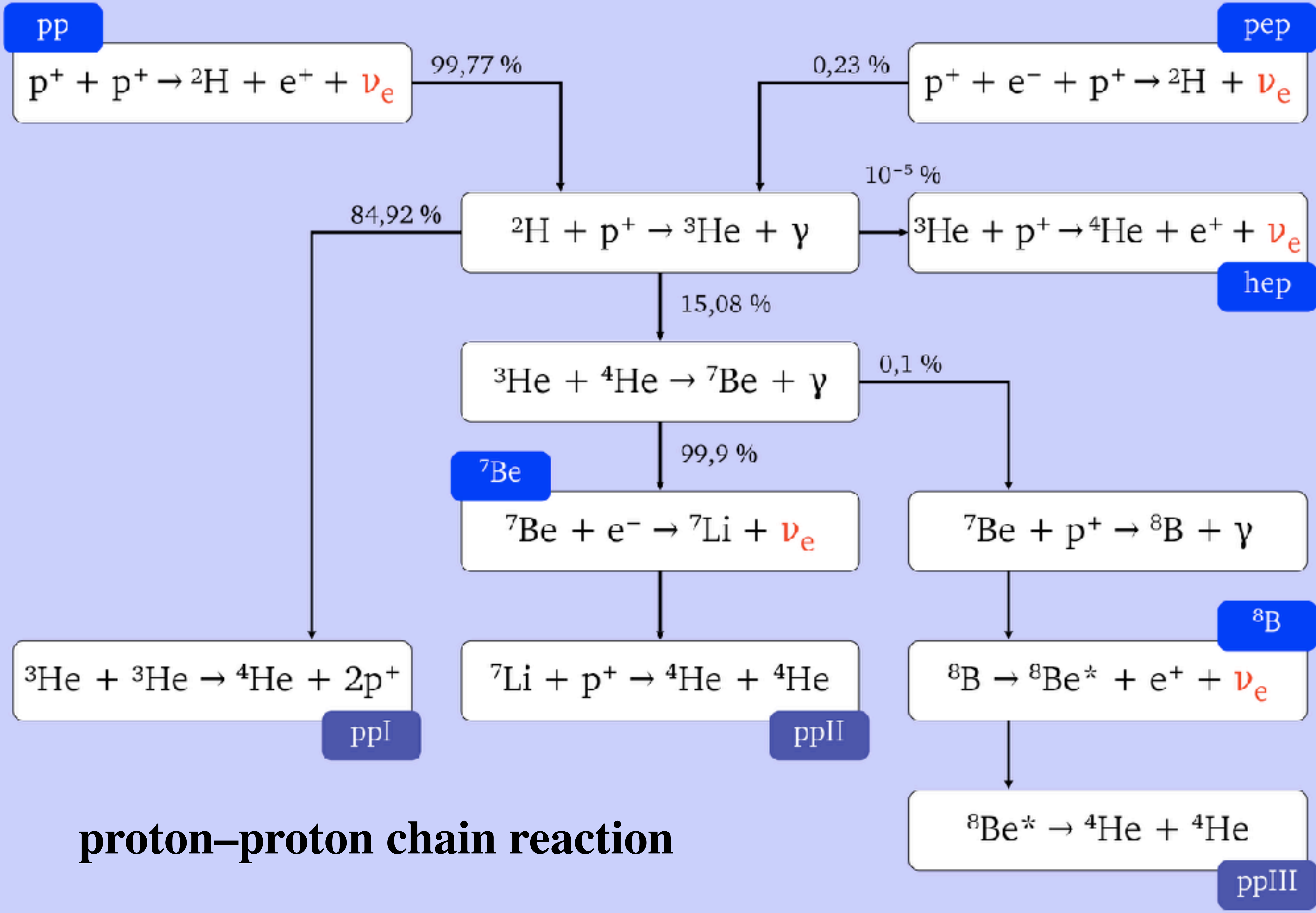
$$^7_4\mathrm{Be} + e^- \rightarrow \ ^7_3\mathrm{L}i + \nu_e$$

At ambient conditions ^{7}Be decays in 53 days into the ground state of ^{7}Li (3/2-) for 89.7% of cases, 10.3% it decays into the first excited state (1/2-)

A small amount of ^{7}Li is produced in stars, but is thought to be burned during MS as fast as produced when convective processes can carry it to temperatures of a few millions K, where it undergoes p-captures.

Galactic Cosmic Rays do not produce much ^{7}Li

Nucleosynthesis and Solar Neutrinos



pp

$p^+ + p^+ \rightarrow {}^2H + e^+ + \nu_e$

99,77 %

0,23 %

pep

$p^+ + e^- + p^+ \rightarrow {}^2H + \nu_e$

84,92 %

$^2H + p^+ \rightarrow {}^3He + \gamma$

10^{-5} %

$^3He + p^+ \rightarrow {}^4He + e^+ + \nu_e$

hep

15,08 %

$^3He + {}^4He \rightarrow {}^7Be + \gamma$

0,1 %

99,9 %

7Be

$^7Be + e^- \rightarrow {}^7Li + \nu_e$

$^7Be + p^+ \rightarrow {}^8B + \gamma$

8B

$^3He + {}^3He \rightarrow {}^4He + 2p^+$

ppI

$^7Li + p^+ \rightarrow {}^4He + {}^4He$

ppII

$^8B \rightarrow {}^8Be^* + e^+ + \nu_e$

$^8Be^* \rightarrow {}^4He + {}^4He$

ppIII

proton–proton chain reaction

How do we actually calculate e-capture rates?

The e-capture rate for ^{7}Be is proportional to the electronic density at the nucleus!!!

Factors affecting this density, such as T, ϱ, the level of ionization and the presence of other charged particles, screening the interaction, can appreciably modify the decay rate

How to calculate $\rho_e(0)$?

State-of-the-art techniques are based on the the Debye-Hückel (DH) models of screening, valid only for solar conditions and when electrons are not degenerate (but in RBG they could).

Does DH approximation really stand???

Our model system of stellar plasma is a Fermi gas in the presence of neutralising particles, such as proton, helium, etc…

Condition of the stellar material at high T

DEGENERACY CONDITIONS: CLASSICAL vs. QUANTUM

- The separation between identical particles is << λ_{DB}
- The density is >> N_q where N_q is the number of available quantum states

Solar core: T=15.6 X 10^6 K → ^{7}Be atoms are all ionized

(12000 K = 1 eV)!!!

De Broglie wavelength in the core of the Sun

$$l << \lambda_{DB} = h/p \simeq h/(3m_e kT)^{1/2} = 2.731 \times 10^{-11}\ m$$

Electronic density

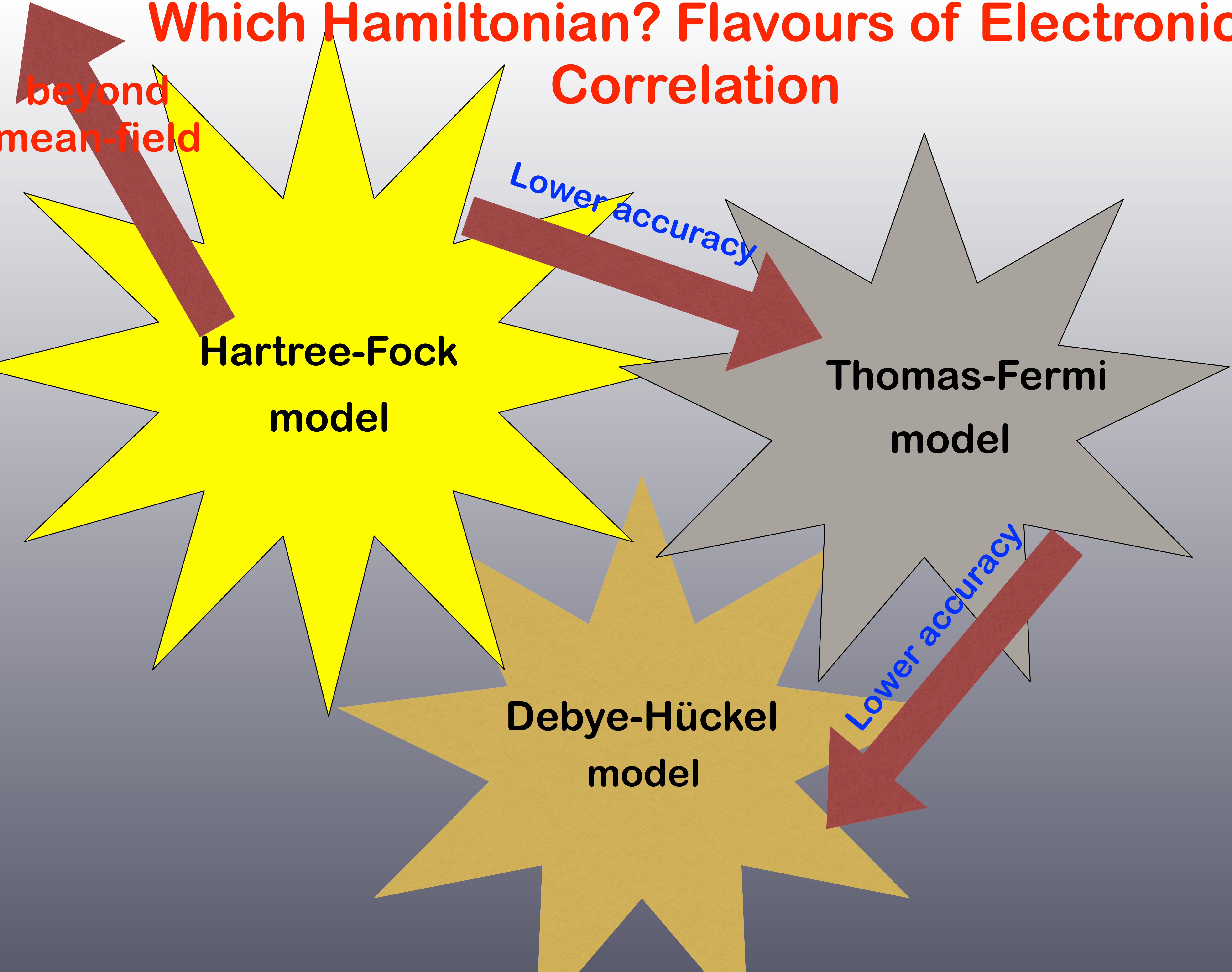
$$\rho_e >> n_{QNR} = (2\pi m_e kT/h^2)^{3/2} = 6.65 \times 10^{31}\ m^{-3}$$

$T \propto 1/R$ and thus $n_{QNR} \propto T^{(3/2)} \propto R^{-3/2}$, which cannot keep the pace with $\rho_e \propto R^{-3}$. To have degeneracy $T << h^2 \rho^{2/3}/(2\pi mk) = 9.12 \times 10^6$ K

In the solar core the temperature is marginally too high for degeneracy of electrons, but decreasing R can set it in...

Cold? Fermi gas can be degenerate even at millions of K.

Which Hamiltonian? Flavours of Electronic Correlation



beyond mean-field

Hartree-Fock model

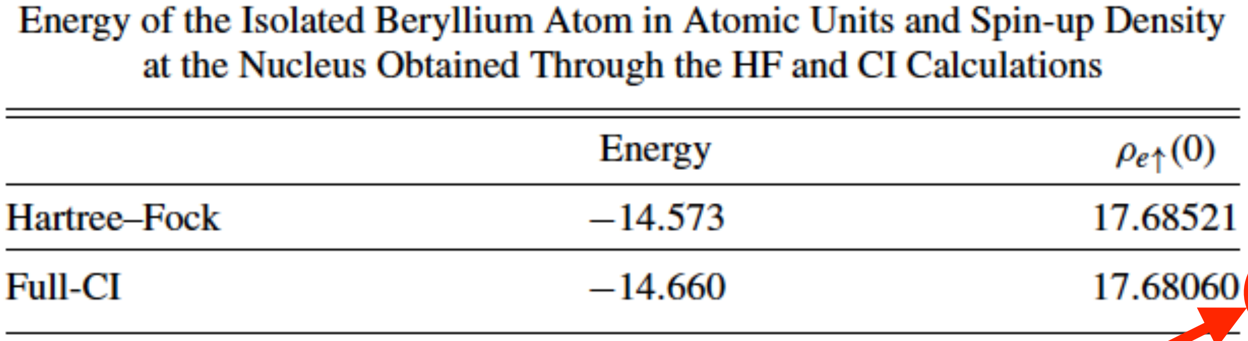
Lower accuracy

Thomas-Fermi model

Lower accuracy

Debye-Hückel model

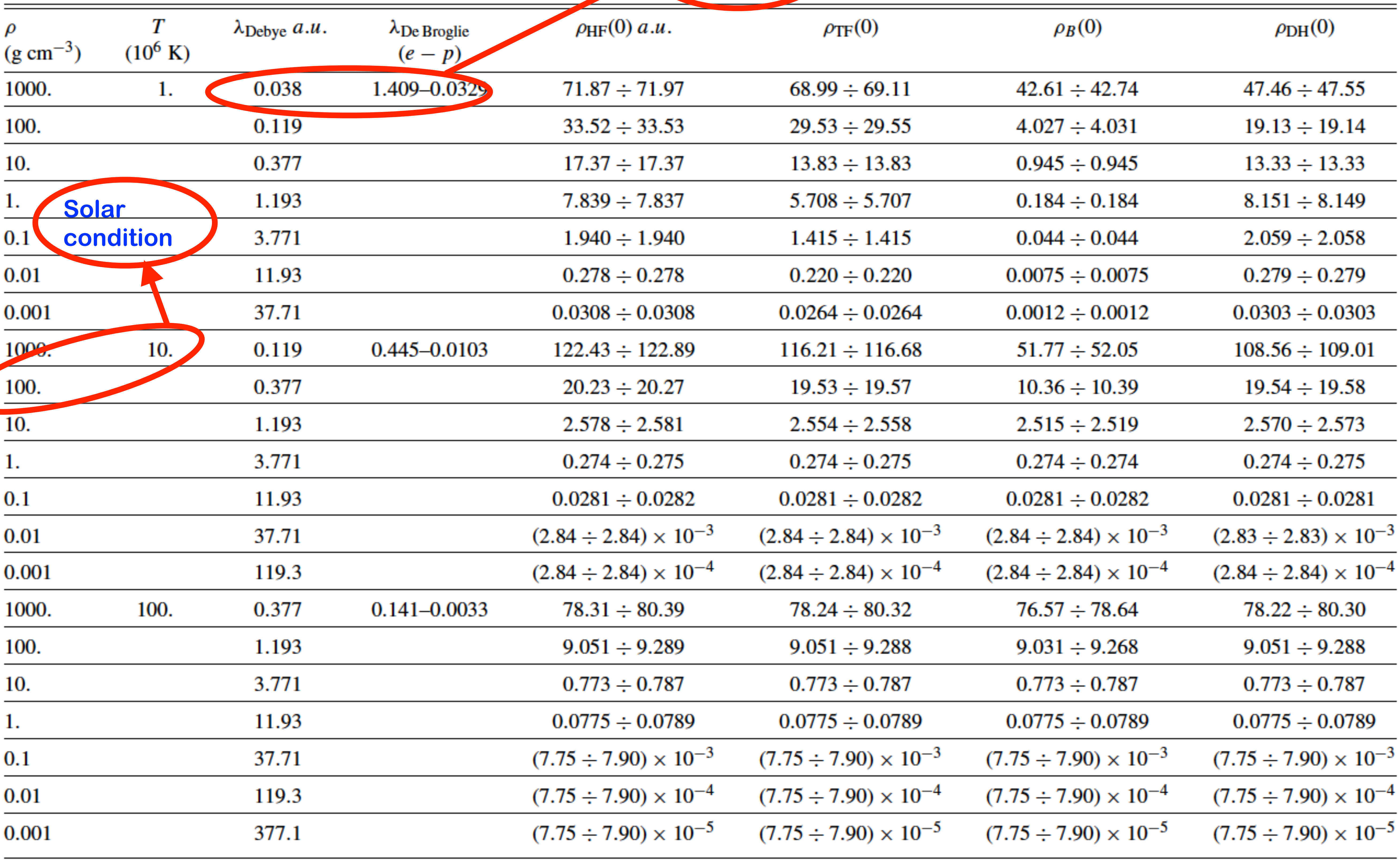
Some data...



Energy of the Isolated Beryllium Atom in Atomic Units and Spin-up Density at the Nucleus Obtained Through the HF and CI Calculations

	Energy	$\rho_{e\uparrow}(0)$
Hartree–Fock	−14.573	17.68521
Full-CI	−14.660	17.68060

Degenerate condition

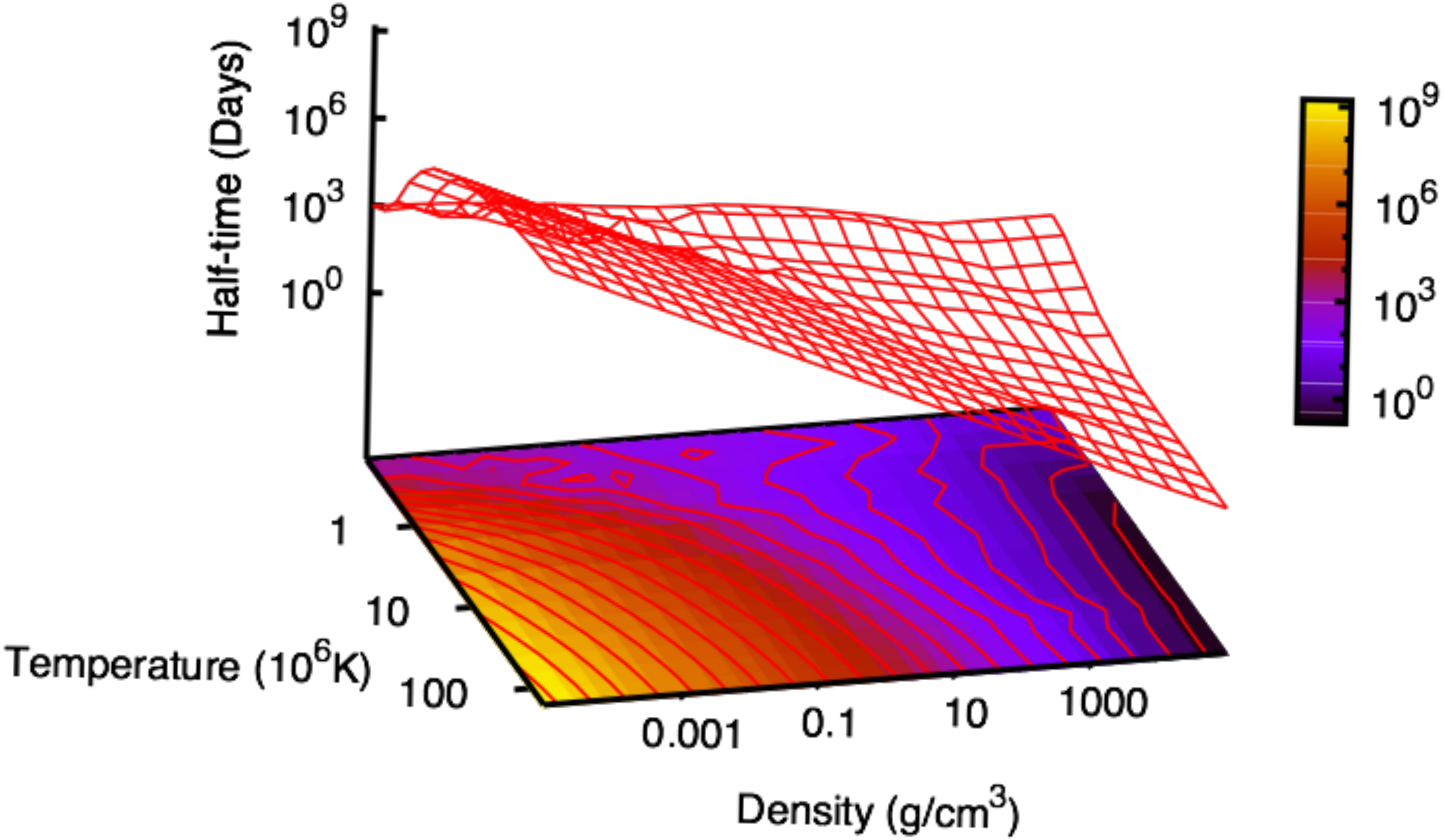


ρ (g cm^{-3})	T (10^6 K)	λ_{Debye} $a.u.$	$\lambda_{\text{De Broglie}}$ $(e-p)$	$\rho_{\text{HF}}(0)$ $a.u.$	$\rho_{\text{TF}}(0)$	$\rho_B(0)$	$\rho_{\text{DH}}(0)$
1000.	1.	0.038	1.409–0.0329	71.87 ÷ 71.97	68.99 ÷ 69.11	42.61 ÷ 42.74	47.46 ÷ 47.55
100.		0.119		33.52 ÷ 33.53	29.53 ÷ 29.55	4.027 ÷ 4.031	19.13 ÷ 19.14
10.		0.377		17.37 ÷ 17.37	13.83 ÷ 13.83	0.945 ÷ 0.945	13.33 ÷ 13.33
1.		1.193		7.839 ÷ 7.837	5.708 ÷ 5.707	0.184 ÷ 0.184	8.151 ÷ 8.149
0.1		3.771		1.940 ÷ 1.940	1.415 ÷ 1.415	0.044 ÷ 0.044	2.059 ÷ 2.058
0.01		11.93		0.278 ÷ 0.278	0.220 ÷ 0.220	0.0075 ÷ 0.0075	0.279 ÷ 0.279
0.001		37.71		0.0308 ÷ 0.0308	0.0264 ÷ 0.0264	0.0012 ÷ 0.0012	0.0303 ÷ 0.0303
1000.	10.	0.119	0.445–0.0103	122.43 ÷ 122.89	116.21 ÷ 116.68	51.77 ÷ 52.05	108.56 ÷ 109.01
100.		0.377		20.23 ÷ 20.27	19.53 ÷ 19.57	10.36 ÷ 10.39	19.54 ÷ 19.58
10.		1.193		2.578 ÷ 2.581	2.554 ÷ 2.558	2.515 ÷ 2.519	2.570 ÷ 2.573
1.		3.771		0.274 ÷ 0.275	0.274 ÷ 0.275	0.274 ÷ 0.274	0.274 ÷ 0.275
0.1		11.93		0.0281 ÷ 0.0282	0.0281 ÷ 0.0282	0.0281 ÷ 0.0282	0.0281 ÷ 0.0281
0.01		37.71		(2.84 ÷ 2.84) × 10^{-3}	(2.84 ÷ 2.84) × 10^{-3}	(2.84 ÷ 2.84) × 10^{-3}	(2.83 ÷ 2.83) × 10^{-3}
0.001		119.3		(2.84 ÷ 2.84) × 10^{-4}	(2.84 ÷ 2.84) × 10^{-4}	(2.84 ÷ 2.84) × 10^{-4}	(2.84 ÷ 2.84) × 10^{-4}
1000.	100.	0.377	0.141–0.0033	78.31 ÷ 80.39	78.24 ÷ 80.32	76.57 ÷ 78.64	78.22 ÷ 80.30
100.		1.193		9.051 ÷ 9.289	9.051 ÷ 9.288	9.031 ÷ 9.268	9.051 ÷ 9.288
10.		3.771		0.773 ÷ 0.787	0.773 ÷ 0.787	0.773 ÷ 0.787	0.773 ÷ 0.787
1.		11.93		0.0775 ÷ 0.0789	0.0775 ÷ 0.0789	0.0775 ÷ 0.0789	0.0775 ÷ 0.0789
0.1		37.71		(7.75 ÷ 7.90) × 10^{-3}	(7.75 ÷ 7.90) × 10^{-3}	(7.75 ÷ 7.90) × 10^{-3}	(7.75 ÷ 7.90) × 10^{-3}
0.01		119.3		(7.75 ÷ 7.90) × 10^{-4}	(7.75 ÷ 7.90) × 10^{-4}	(7.75 ÷ 7.90) × 10^{-4}	(7.75 ÷ 7.90) × 10^{-4}
0.001		377.1		(7.75 ÷ 7.90) × 10^{-5}	(7.75 ÷ 7.90) × 10^{-5}	(7.75 ÷ 7.90) × 10^{-5}	(7.75 ÷ 7.90) × 10^{-5}

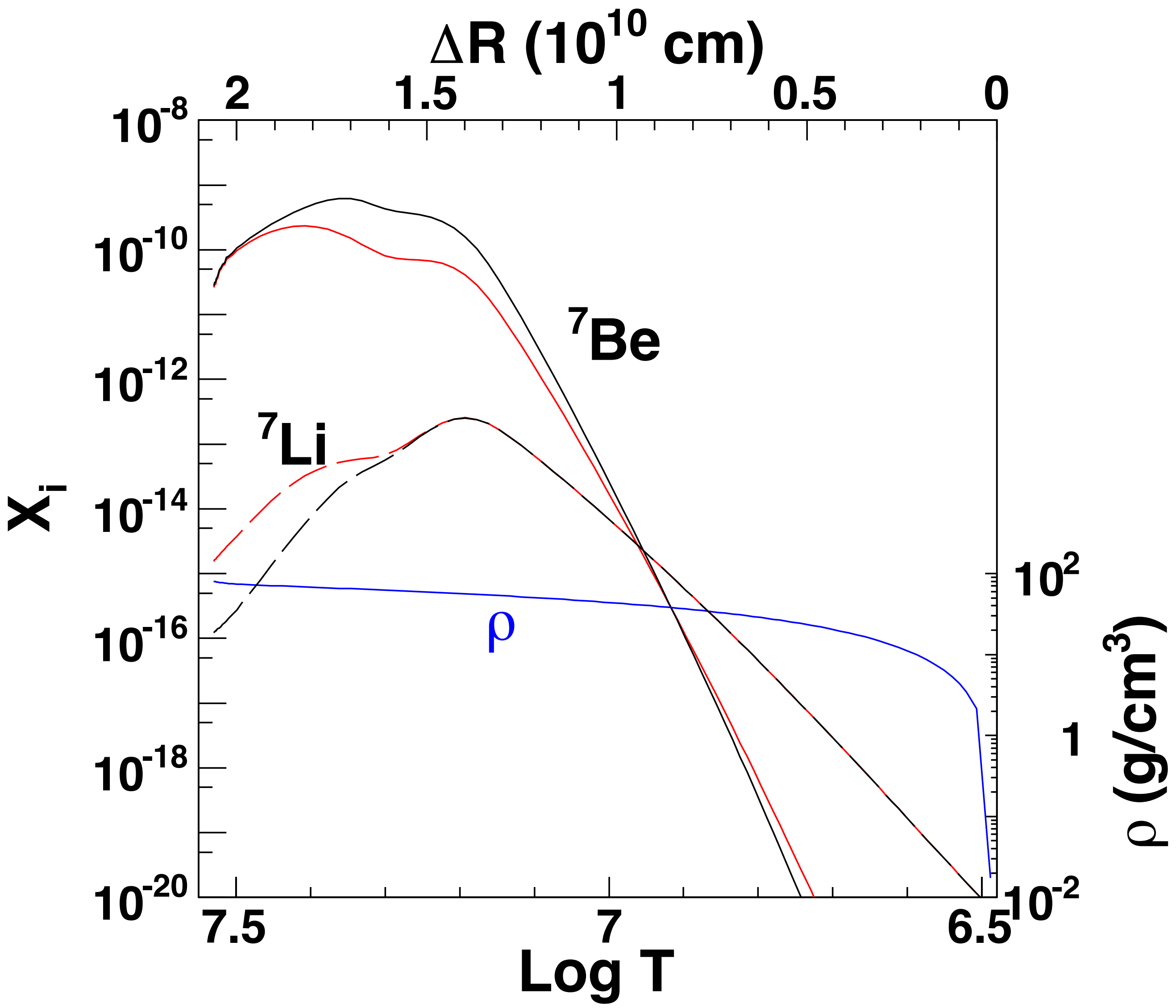
Solar condition

A pictorial view of ^{7}Be half-life…

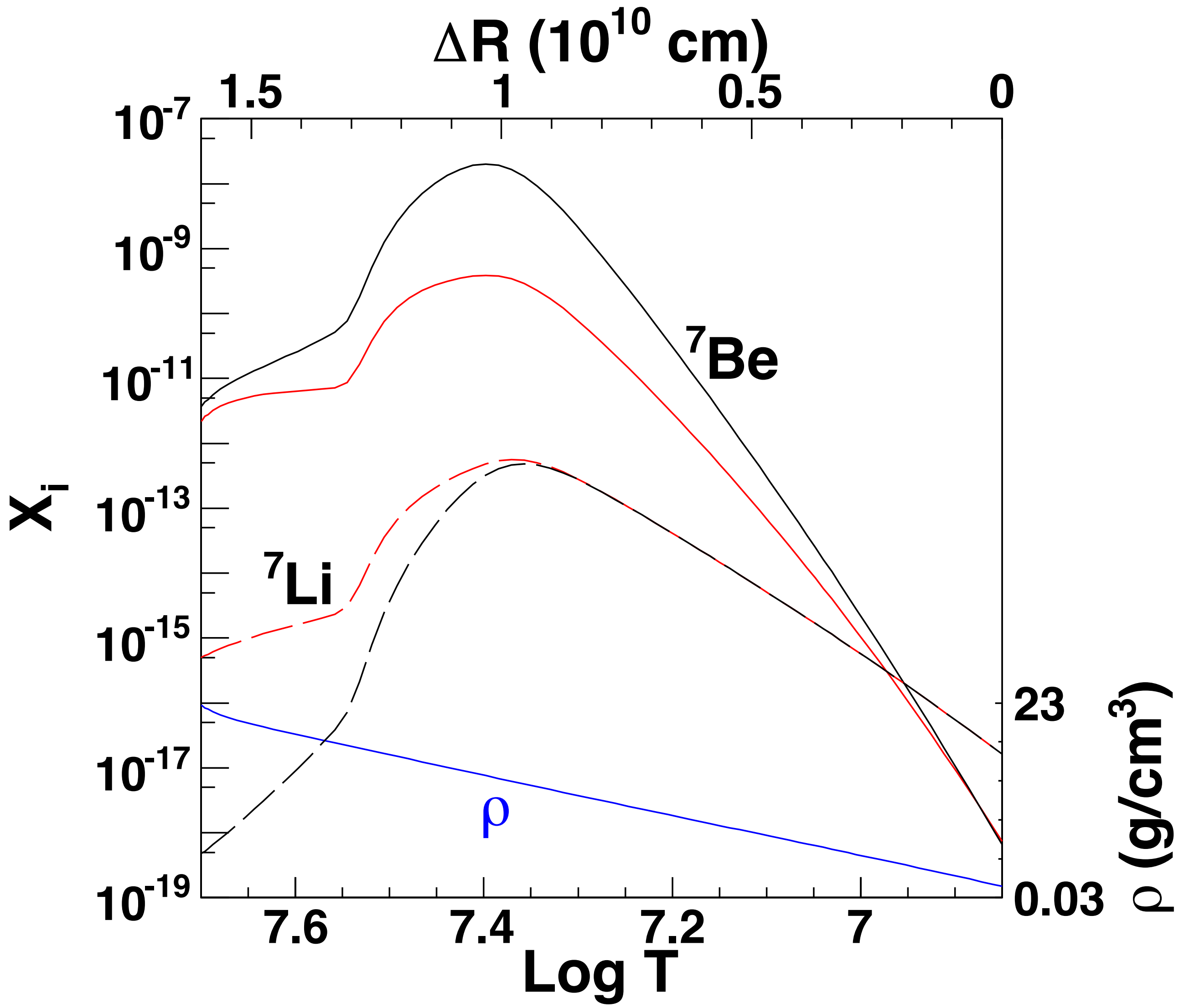
half-life (days)= 941.86881/$\varrho(0)$



Astrophysical consequences of the new rate



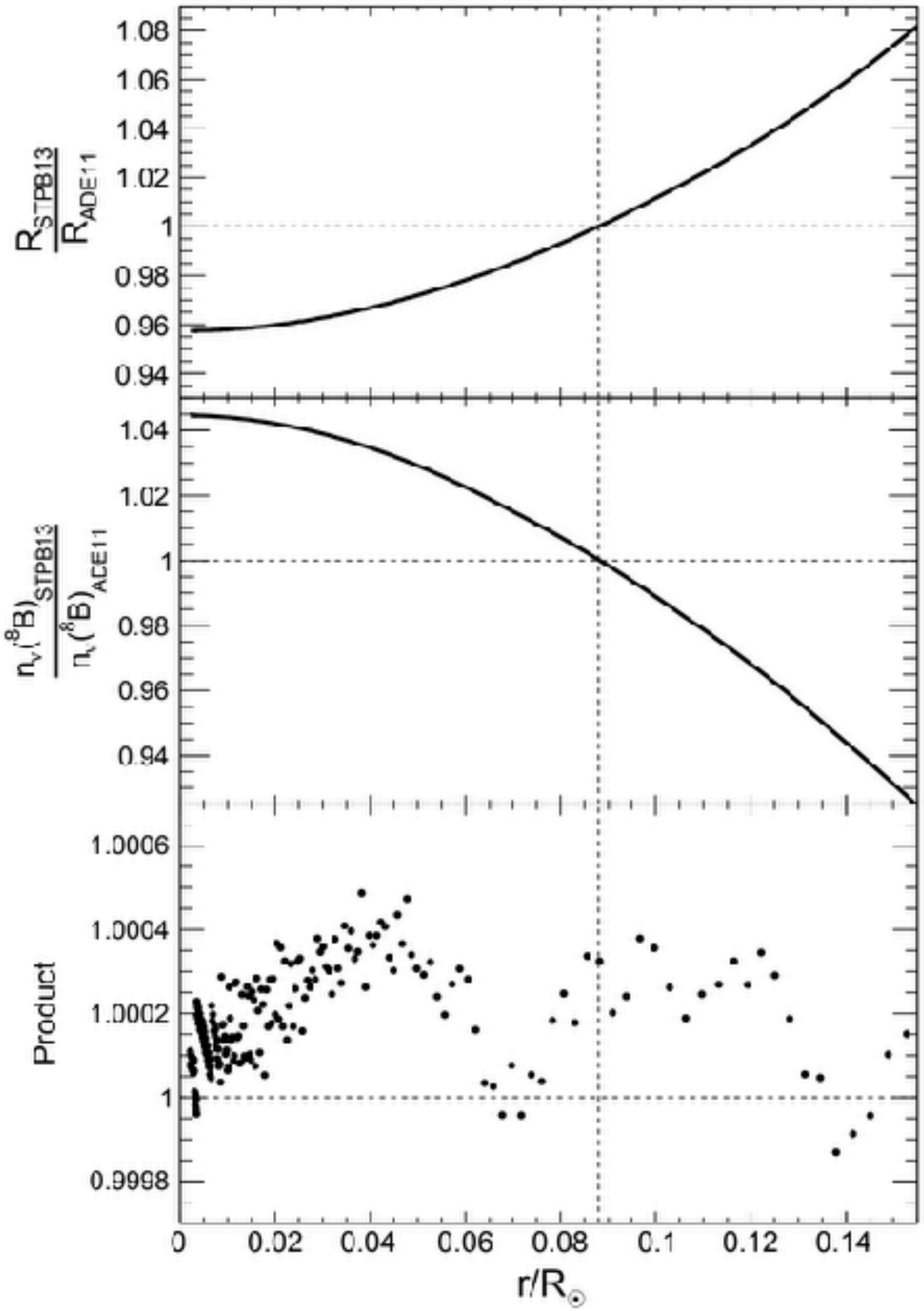
typical RGB conditions



AGB stages

Equilibrium abundances of ^{7}Be and ^{7}Li in the layers above the H-burning shell using our ^{7}Be life-time (red line) and the solar extrapolated rate (black line), in a 2 M⊙ evolved star of solar metallicity. The matter density is also shown (blue line), and is referred to the scale on the right axis.

Being the relative rates very sensitive to the solar core temperature, one can infer from neutrino fluxes important information about the physics of the solar interior.



Top panel: ratio between the STPB13's e^--capture and ADE11's rates in the production region of ^{8}B neutrinos, both computed on the solar structure resulting from the ADE11 SSM, with PLJ14 composition.

Middle panel: ratio between the neutrinos fraction in STPB13 SSM and ADE11, both computed with a PLJ14 composition.

Bottom panel:

$$\frac{n_\nu(^8\mathrm{B})_{STPB13} \cdot R_{STPB13}}{(n_\nu(^8\mathrm{B})_{ADE11} \cdot R_{ADE11})}$$

S. Palmerini
(UniPG)

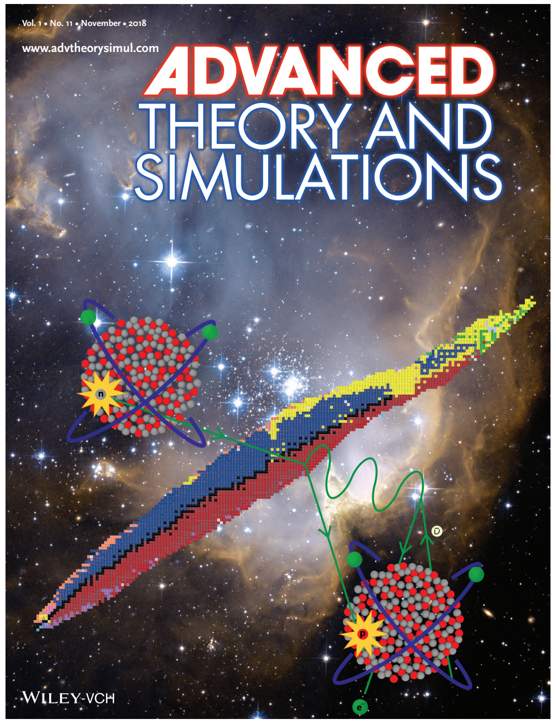
I am deep in debt to ....

S. Simonucci
(Unicam)

M. Busso
(UniPG)

T. Morresi
(ECT* and UNITN)

Conclusions



- A new method for calculating β- and e^--capture decay spectra in medium to heavy nuclei, which extend the standard approach in several ways

- This method can be applied to any nuclear beta decay and include relativistic, many-body screening and post-collisional effects

- Our approach works better than state-of-the-art

Outlook

- Inclusion of shake-up and shake-off effects into the calculation of the spectrum;

- Application of the DHF equations to calculate accurately Auger spectra in molecules containing high A atoms = extension to multi-centric systems (almost done);

- Extension of this approach to include rigorously the nuclear current over nuclear volume to see the influence on β-spectrum lineshape


That's all Folks!