

QRPA calculations of stellar weak decay rates

P. Sarriguren

Instituto de Estructura de la Materia
CSIC, Madrid, Spain



E. Moya de Guerra,
R. Alvarez-Rodriguez, O. Moreno
Universidad Complutense Madrid



International School of Nuclear Physics. 36th Course. Nuclei in the Laboratory and
in the Cosmos. Erice-Sicily. September 16-24, 2014

Weak-decay rates

Problem :

- Weak-decay rates determine late stages of stellar evolution.
- Experimental extrapolations or theoretical predictions:
Reproduce exp information on $T_{1/2}$ and BGT under terrestrial conditions.

Theoretical approach :

- Deformed HF+BCS+QRPA formalism with Skyrme forces and residual interactions in both ph and pp channels.

Results : Weak-decay rates at various (ρ, T) in stellar scenarios

- pf-shell nuclei. Main constituents of stellar core in presupernova formations: Sc, Ti, V, Mn, Fe, Co, Ni, Zn isotopes.
BGT measured in laboratory (Charge exchange reactions) and compared with benchmark Shell Model calculations.
- Neutron-deficient waiting-point isotopes (Ni-Sn) at (ρ, T) typical of rp-process.
- Neutron rich Zr-Mo isotopes: r process.

Weak decay rates

$$\lambda = \ln 2 (T_{1/2})^{-1} = \frac{\ln 2}{D} \sum_{if} P_i(T) \mathbf{B}_{if} \Phi_{if}(\rho, T)$$

Initial states thermally populated

$$P_i(T) = \frac{2J_i + 1}{G} e^{-E_i/(kT)}, \quad G = \sum_i (2J_i + 1) e^{-E_i/(kT)}$$

$$P_{i=g.s.}(T=0) = 1$$

Nuclear structure

$$B_{if}(GT) = \left(\frac{g_A}{g_V} \right)_{\text{eff}}^2 \left\langle f \left\| \sum_k \sigma^k t_{\pm}^k \right\| i \right\rangle^2$$

Phase space factors :

$$\beta^+, EC : \Phi_{if} = \Phi_{if}^{EC} + \Phi_{if}^{\beta^+}$$

$$\beta^- : \Phi_{if} = \Phi_{if}^{\beta^-}$$

$\lambda(\rho, T)$ are different from laboratory (P_i, cEC)

Phase space factors

$$\Phi_{if}^{\beta^-} = \int_1^{Q_{if}} \omega \sqrt{\omega^2 - 1} (Q_{if} - \omega)^2 F(Z+1, \omega) [1 - S_e(\omega)] [1 - S_v(Q_{if} - \omega)] d\omega$$

$$\Phi_{if}^{\beta^+} = \int_1^{Q_{if}} \omega \sqrt{\omega^2 - 1} (Q_{if} - \omega)^2 F(-Z+1, \omega) [1 - S_p(\omega)] [1 - S_v(Q_{if} - \omega)] d\omega$$

$$\Phi_{if}^{cEC} = \int_{\omega_\ell}^{\infty} \omega \sqrt{\omega^2 - 1} (Q_{if} + \omega)^2 F(Z, \omega) S_e(\omega) [1 - S_v(Q_{if} + \omega)] d\omega$$

$$\Phi^{oEC} = \frac{\pi}{2} \left[q_K^2 g_K^2 B_K + q_L^2 g_L^2 B_{L_1} + \dots \right]$$

q Neutrino energy
g Radial components of the e-wf at r=0
B Exchange and overlap corrections

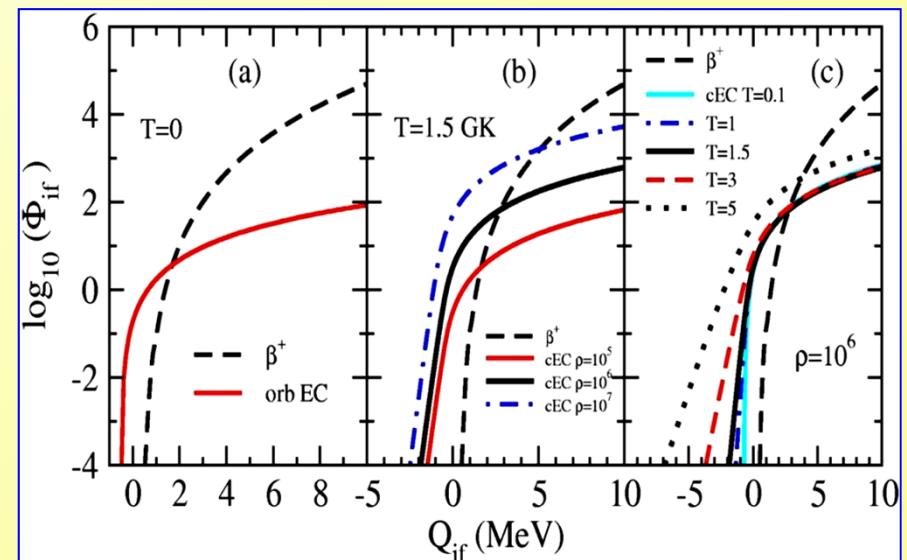
Distribution functions

$$S_p = S_v = 0$$

S_e : Fermi-Dirac distribution

$$S_e = \frac{1}{\exp[(\omega - \mu_e)/(kT)] + 1}$$

$$Q_{if} = \frac{1}{m_e c^2} (M_p - M_d + E_i - E_f)$$



Hartree-Fock method

$$H = \sum_{k=1}^A T(k) + \sum_{k < l=1}^A W(k, l)$$

How to extract a single-particle potential $U(k)$
out of the sum of two-body interactions $W(k, l)$

$$H = \sum_{k=1}^A [T(k) + U(k)] + \left[\sum_{k < l=1}^A W(k, l) - \sum_{k=1}^A U(k) \right] = H_0 + V_{res}$$

Hartree-Fock: Selfconsistent method to derive the single-particle potential
Variational principle: Search for the best Slater det. minimizing the energy
Assume that the resulting residual interaction is small

Skyrme effective interactions

Two-body interaction: zero-range limit of a finite range force

- leading term: delta-function with strength t_0 and spin exchange x_0
- leading finite range corrections t_1, x_1, t_2, x_2 (finite range = momentum dependence)
- short-range spin-orbit interaction with strength W_0

Short-range density-dependent two-body force t_3, x_3, α

$$\begin{aligned} V_{ij} = & t_0 (1 + x_0 P_\sigma) \delta(\vec{r}_i - \vec{r}_j) + \frac{1}{2} t_1 (1 + x_1 P_\sigma) \delta(\vec{r}_i - \vec{r}_j) (k^2 + k'^2) \\ & + t_2 (1 + x_2 P_\sigma) \vec{k}' \cdot \delta(\vec{r}_i - \vec{r}_j) \vec{k} + i W_0 (\vec{\sigma}_i + \vec{\sigma}_j) \cdot \vec{k}' \times \delta(\vec{r}_i - \vec{r}_j) \vec{k} \\ & + \frac{1}{6} t_3 (1 + x_3 P_\sigma) \delta(\vec{r}_i - \vec{r}_j) \rho^\alpha \left(\frac{\vec{r}_i + \vec{r}_j}{2} \right) \end{aligned}$$

Parameters (10) fitted using nuclear matter properties and ground state properties of a selected set of nuclei (binding energies, charge radii,...)

Sk3, SG2, SLy4

Skyrme Hartree-Fock

Schroedinger equation

$$\left[-\vec{\nabla} \cdot \frac{\hbar^2}{2m^*(\vec{r})} \vec{\nabla} + U_q(\vec{r}) + \vec{W}(\vec{r}) \cdot (-i) (\vec{\nabla} \times \vec{\sigma}) \right] \phi_i = e_i \phi_i$$

$$m^*(\vec{r}), \quad U_q(\vec{r}), \quad \vec{W}(\vec{r})$$

Algebraic combinations of the densities

$[\rho, \tau, J]$

$$\rho_{st}(\vec{r}) = \sum_i \left| \phi_i(\vec{r}, s, t) \right|^2, \quad \tau_{st}(\vec{r}) = \sum_i \left| \vec{\nabla} \phi_i(\vec{r}, s, t) \right|^2, \quad \vec{J}_{st}(\vec{r}) = \sum_{i,s'} \phi_i^*(\vec{r}, s', t) (-i \vec{\nabla} \times \vec{\sigma}) \phi_i(\vec{r}, s, t)$$

$$\frac{\hbar^2}{2m_q^*(\vec{r})} = \frac{\hbar^2}{2m} + \frac{1}{8} [t_1(2+x_1) + t_2(2+x_2)] \rho(\vec{r}) - \frac{1}{8} [t_1(1+2x_1) + t_2(1+2x_2)] \rho_q(\vec{r})$$

$$\begin{aligned} U_q(\vec{r}) = & \frac{1}{2} t_0 [(2+x_0) \rho - (1+2x_0) \rho_q] + \frac{1}{24} t_3 \left\{ (2+x_3)(2+\alpha) \rho^{\alpha+1} - (2x_3+1) [2\rho^\alpha \rho_q + \alpha \rho^{\alpha-1} (\rho_p^2 + \rho_n^2)] \right\} \\ & + \frac{1}{8} [t_1(2+x_1) + t_2(2+x_2)] \tau + \frac{1}{8} [t_2(1+2x_2) - t_1(1+2x_1)] \tau_q + \frac{1}{16} [-3t_1(2+x_1) + t_2(2+x_2)] \nabla^2 \rho \\ & + \frac{1}{16} [3t_1(1+2x_1) + t_2(1+2x_2)] \nabla^2 \rho_q + \frac{1}{8} (t_1 - t_2) \vec{J}_q - \frac{1}{8} (t_1 x_1 + t_2 x_2) \vec{J} + \delta_{q,p} V_{coul}(\vec{r}) \end{aligned}$$

$$\vec{W}_q(\vec{r}) = \frac{1}{2} W_0 (\vec{\nabla} \rho + \vec{\nabla} \rho_q)$$

Axially symmetric deformed nuclei

$$\Phi_i^{\Omega_i \pi_i} (\vec{R}, \sigma, q) = \chi_{q_i}(q) \left[\Phi_i^+(r, z) e^{i\Lambda^- \varphi} \chi_{+1/2}(\sigma) + \Phi_i^-(r, z) e^{i\Lambda^+ \varphi} \chi_{-1/2}(\sigma) \right]$$

Expansion into eigenfunctions of deformed harmonic oscillator

$$V(r, z) = \frac{1}{2} M \omega_\perp^2 r^2 + \frac{1}{2} M \omega_z^2 z^2$$

$$\left\{ \begin{array}{l} \phi_\alpha(\vec{R}, \sigma) = \psi_{n_r}^\Lambda(r) \psi_{n_z}^\Lambda(z) \frac{e^{i\Lambda\phi}}{\sqrt{2\pi}} \chi_\Sigma(\sigma) \\ \psi_{n_r}^\Lambda(r) = N_{n_r}^\Lambda \beta_\perp \sqrt{2} \eta^{\Lambda/2} e^{-\eta/2} L_{n_r}^\Lambda(\eta) \\ \psi_{n_z}^\Lambda(z) = N_{n_z}^\Lambda \beta_z^{1/2} e^{-\xi^2/2} H_{n_z}^\Lambda(\xi) \end{array} \right.$$

Optimal basis to minimize truncation effects

N= 12 major shells

$$\beta_o = \left[M (\omega_\perp^2 \omega_z)^{1/3} \right]^{1/2} = (\beta_\perp^2 \beta_z)^{1/3}$$

$$q = \frac{\omega_\perp}{\omega_z} = \left(\frac{\beta_\perp}{\beta_z} \right)^2$$

$$\Phi_i(\vec{R}, \sigma, q) = \chi_{q_i} \sum_{\alpha} C_{\alpha}^i \phi_{\alpha}(\vec{R}, \sigma), \quad \alpha = \{n_r, n_z, \Lambda, \Sigma\}$$

Pairing correlations in BCS approximation

BCS ground state

$$|\varphi_{BCS}\rangle = \prod_{i>0} (u_i + v_i a_i^+ a_i^-) |0\rangle$$

$$H = \sum_{k>0} \epsilon_k (a_k^+ a_k^- + a_{\bar{k}}^+ a_{\bar{k}}^-) - G \sum_{kk'>0} a_k^+ a_{\bar{k}}^+ a_{\bar{k}'}^- a_{k'}^-$$

Variational equation constrained by the expectation value of particle number

BCS eqs.

Number eq.

$$2 \sum_i v_i^2 = N$$

Gap eq.

$$\Delta = G \sum_{k>0} u_k v_k$$

$$v_i^2 = \frac{1}{2} \left[1 - \frac{e_i - \lambda}{E_i} \right]; \quad E_i = \sqrt{(e_i - \lambda)^2 + \Delta^2}$$

Fixed gaps taken from phenomenology

$$\Delta_n = \frac{1}{8} [B(N-2, Z) - 4B(N-1, Z) + 6B(N, Z) - 4B(N+1, Z) + B(N+2, Z)]$$

Residual interactions

Particle-hole residual interaction consistent with the HF mean field

$$V_{ph} = \frac{1}{16} \sum_{sts't'} \left[1 + (-1)^{s-s'} \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right] \left[1 + (-1)^{t-t'} \vec{\tau}_1 \cdot \vec{\tau}_2 \right] \frac{\delta^2 E}{\delta \rho_{st}(\vec{r}_1) \delta \rho_{s't'}(\vec{r}_2)} \delta(\vec{r}_1 - \vec{r}_2)$$

$$\begin{aligned} V_{ph}^{\sigma\tau} &= \frac{1}{16} \sum_{sts't'} (-1)^{s-s'} (-1)^{t-t'} \vec{\sigma}_1 \cdot \vec{\sigma}_2 \vec{\tau}_1 \cdot \vec{\tau}_2 \frac{\delta^2 E}{\delta \rho_{st}(\vec{r}_1) \delta \rho_{s't'}(\vec{r}_2)} \delta(\vec{r}_1 - \vec{r}_2) \\ &= \frac{1}{16} \left[-4t_0 - 2t_1 k_F^2 + 2t_2 k_F^2 - \frac{2}{3} t_3 \rho^\alpha \right] \vec{\sigma}_1 \cdot \vec{\sigma}_2 \vec{\tau}_1 \cdot \vec{\tau}_2 \delta(\vec{r}_1 - \vec{r}_2) \end{aligned}$$

Average over nuclear volume \rightarrow Separable forces

$$\left\{ \begin{array}{l} V_{GT}^{ph} = 2\chi_{GT}^{ph} \sum_{K=0,\pm 1} (-1)^K \beta_K^+ \beta_{-K}^- , \quad \beta_K^+ = \sigma_K t^+ = \sum_{\pi\nu} \langle \nu | \sigma_K | \pi \rangle a_\nu^+ a_\pi^- \\ \chi_{GT}^{ph} = -\frac{3}{8\pi R^3} \left\{ t_0 + \frac{1}{2} k_F^2 (t_1 - t_2) + \frac{1}{6} t_3 \rho^\alpha \right\} \\ V_{GT}^{pp} = -2\kappa_{GT}^{pp} \sum_{K=0,\pm 1} (-1)^K P_K^+ P_K^- , \quad P_K^+ = \sum_{\pi\nu} \langle \nu | (\sigma_K)^+ | \pi \rangle a_\nu^+ a_\pi^+ \end{array} \right.$$

pnQRPA with separable forces

Phonon operator

$$\Gamma_{\omega_K}^+ = \sum_{\gamma_K} \left[X_{\gamma_K}^{\omega_K} A_{\gamma_K}^+ - Y_{\gamma_K}^{\omega_K} A_{\gamma_K}^- \right], \quad A_{\gamma_K}^+ = \alpha_n^+ \alpha_{\bar{p}}^+$$

$$\Gamma_{\omega_K} |0\rangle = 0, \quad \Gamma_{\omega_K}^+ |0\rangle = |\omega_K\rangle$$

pnQRPA equations

Transition amplitudes

$$\langle \omega_K | \sigma_K t^\pm | 0 \rangle = \mp M_\pm^{\omega_K}$$

$$M_-^{\omega_K} = \sum_{\pi\nu} (q_{\pi\nu} X_{\pi\nu}^{\omega_K} + \tilde{q}_{\pi\nu} Y_{\pi\nu}^{\omega_K})$$

$$M_+^{\omega_K} = \sum_{\pi\nu} (\tilde{q}_{\pi\nu} X_{\pi\nu}^{\omega_K} + q_{\pi\nu} Y_{\pi\nu}^{\omega_K})$$

$$\tilde{q}_{\pi\nu} = u_\nu v_\pi \Sigma_K^{\pi\nu}, \quad q_{\pi\nu} = v_\nu u_\pi \Sigma_K^{\pi\nu}, \quad \Sigma_K^{\pi\nu} = \langle \nu | \sigma_K | \pi \rangle$$

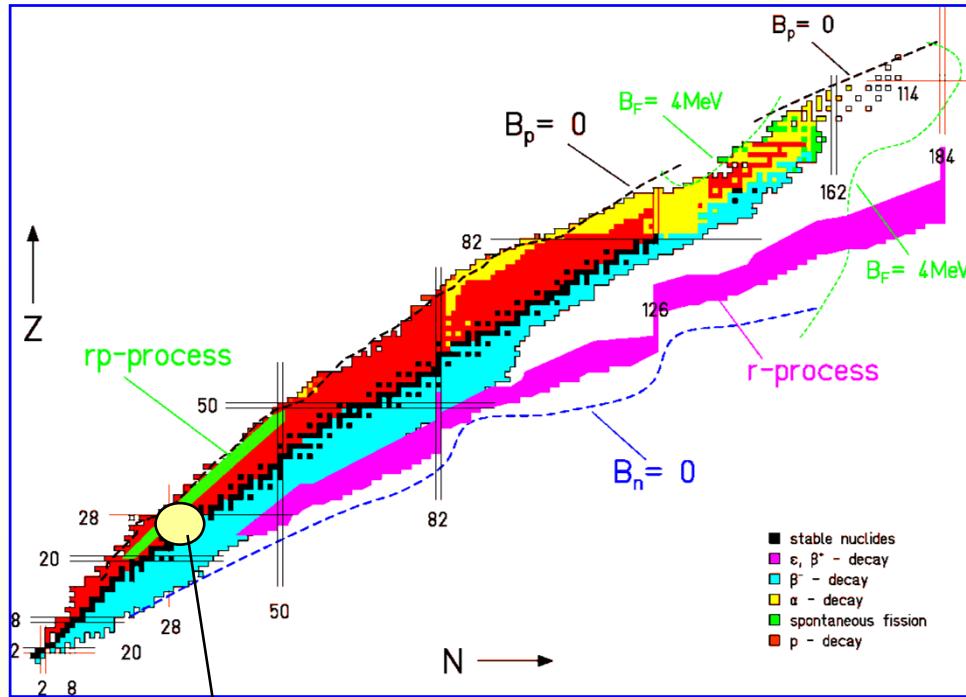
Single-particle states from deformed Skyrme Hartree-Fock
 u, v: Occupation amplitudes from BCS pairing

B(GT) in the lab. system

$$I_i K_i (0^+ 0) \rightarrow I_f K_f (1^+ K)$$

$$B_\omega(GT^\pm) = \delta(\omega_0 - \omega) \langle \omega_0 | \sigma_0 t^\pm | 0 \rangle^2 + 2\delta(\omega_1 - \omega) \langle \omega_1 | \sigma_1 t^\pm | 0 \rangle^2$$

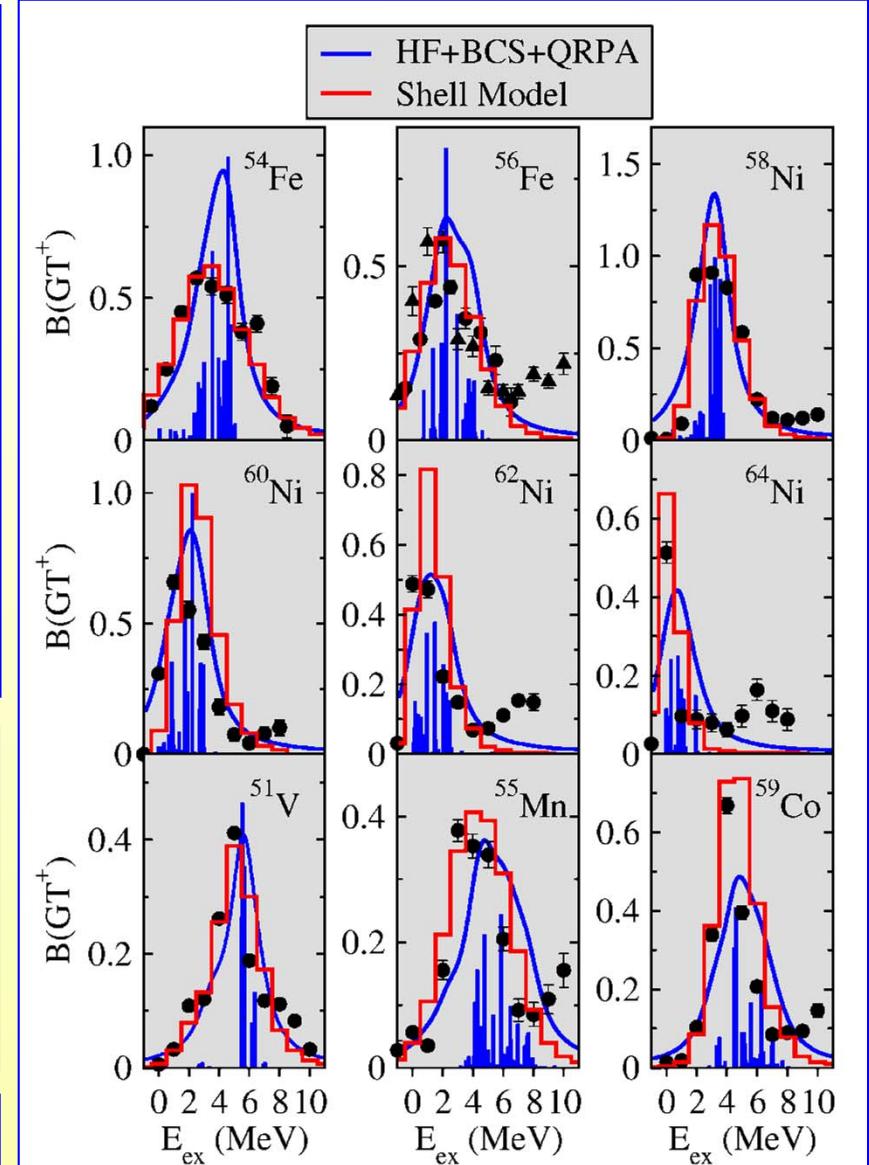
Stable nuclei in Fe-Ni mass region: Theory vs experiment



Main constituents of stellar core in presupernovae. Comparison with :

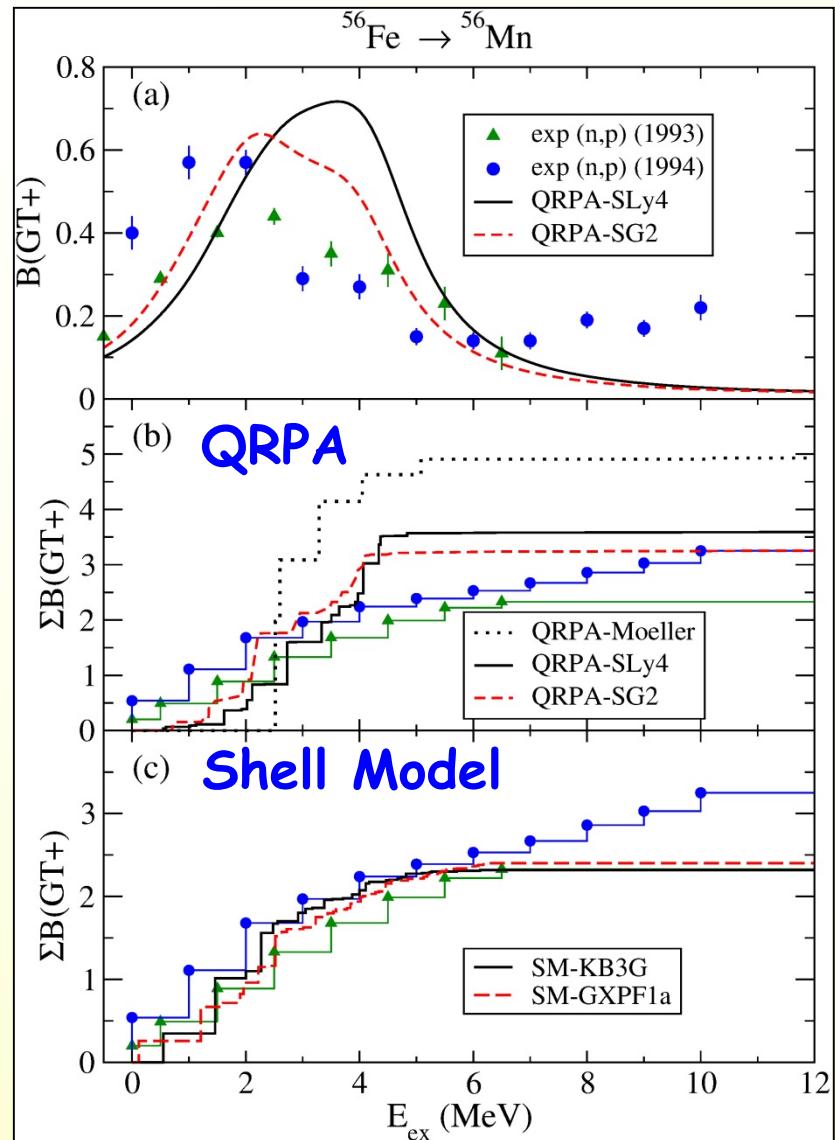
- exp. (n,p) , (p,n)
- SM calculations

GT properties: Test of QRPA



SM: NPA 653, 439 (1999)
QRPA: NPA 716, 230 (2003)

Weak decay rates in pf-shell nuclei



Calculations for several isotopes:

Sc, Ti, V, Fe, Mn, Ni, Co, Zn

exp: charge exchange reactions
(n, p)

$$B_{if}(GT) \propto \langle f | \sigma t | i \rangle^2$$

Accumulated GT strength

A.L. Cole PRC 86, 015809 (2012)
P.S. PRC87, 045801 (2013)

Weak decay rates in pf-shell nuclei

$$\lambda(\rho, T) \propto \sum_{if} P_i(T) B_{if} \Phi_{if}(\rho, T)$$

Electron Capture from e^- plasma

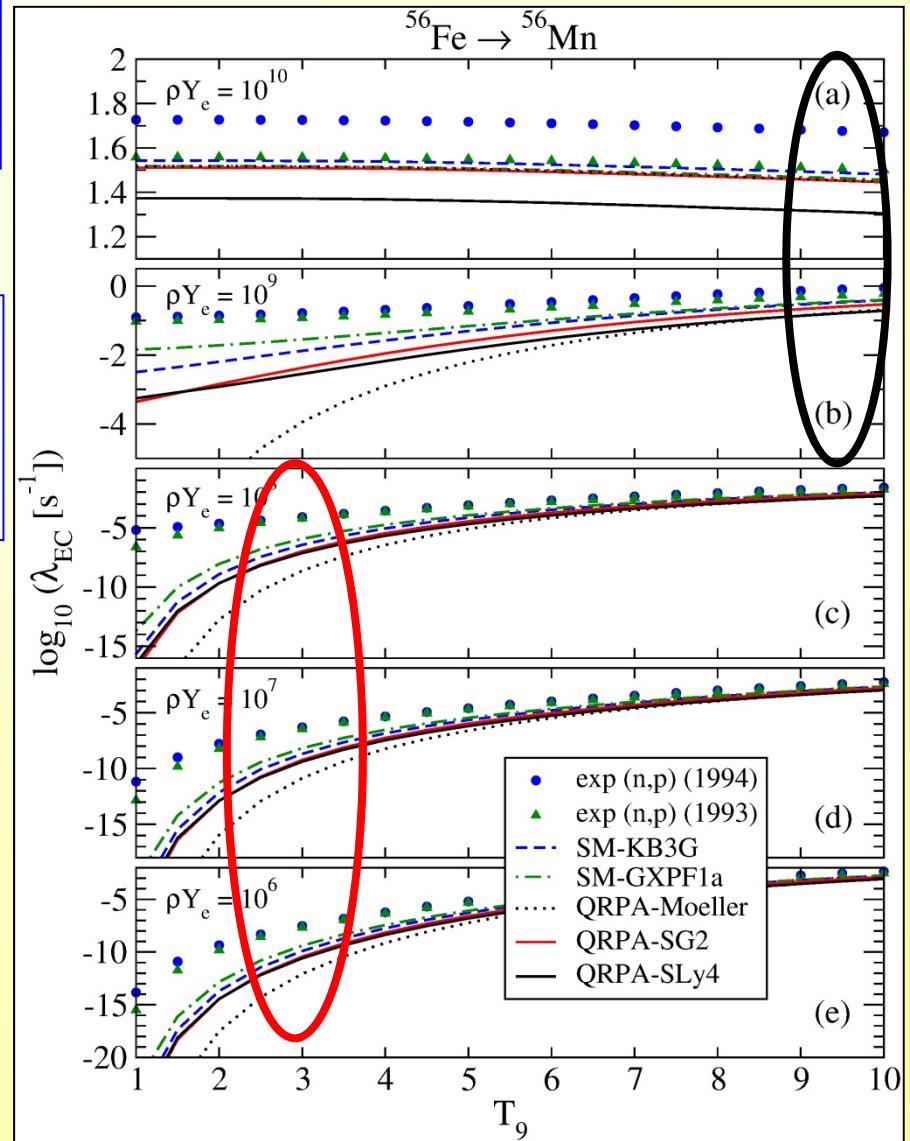
$$\Phi_{if}^{cEC} = \int_{\omega_\ell}^{\infty} \omega \sqrt{\omega^2 - 1} (Q_{if} + \omega)^2 F(Z, \omega) \times S_e(\omega) [1 - S_v(Q_{if} + \omega)] d\omega$$

$$S_e = \frac{1}{\exp[(\omega - \mu_e)/(kT)] + 1}$$

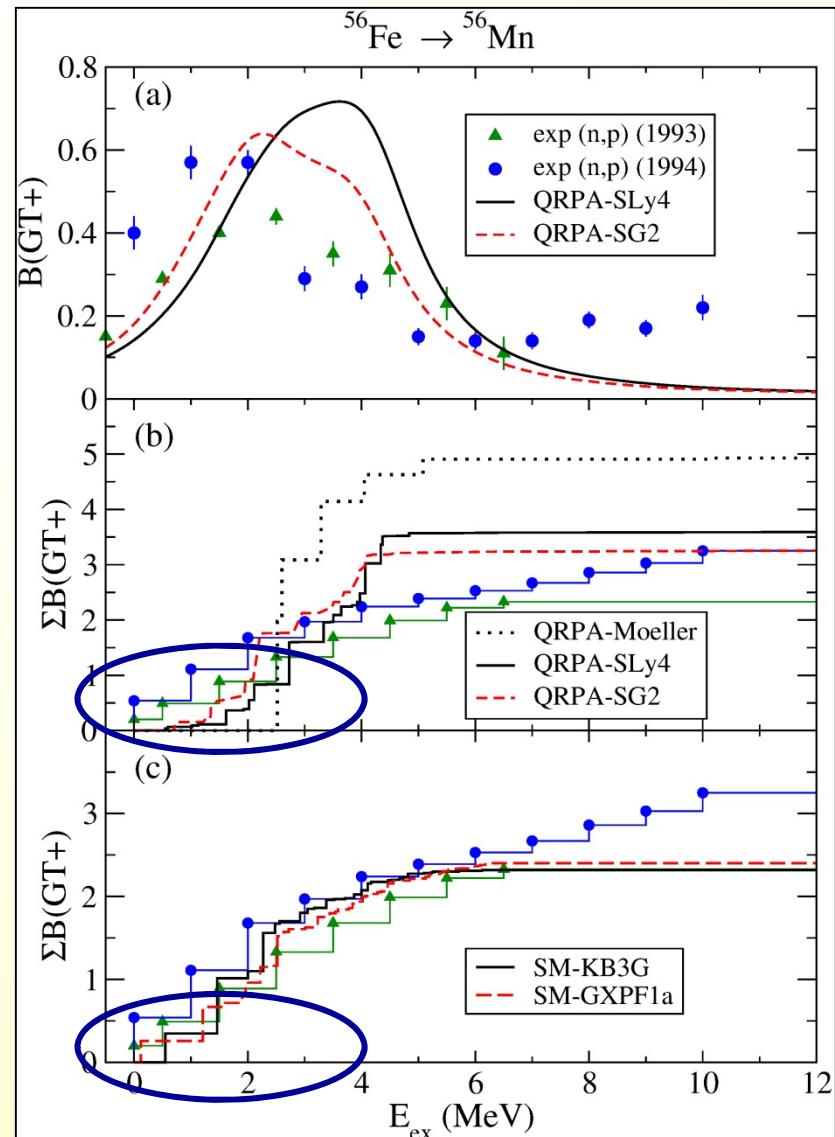
$$Q_{if} = \frac{1}{m_e c^2} (M_p - M_d + E_i - E_f)$$

Si burning

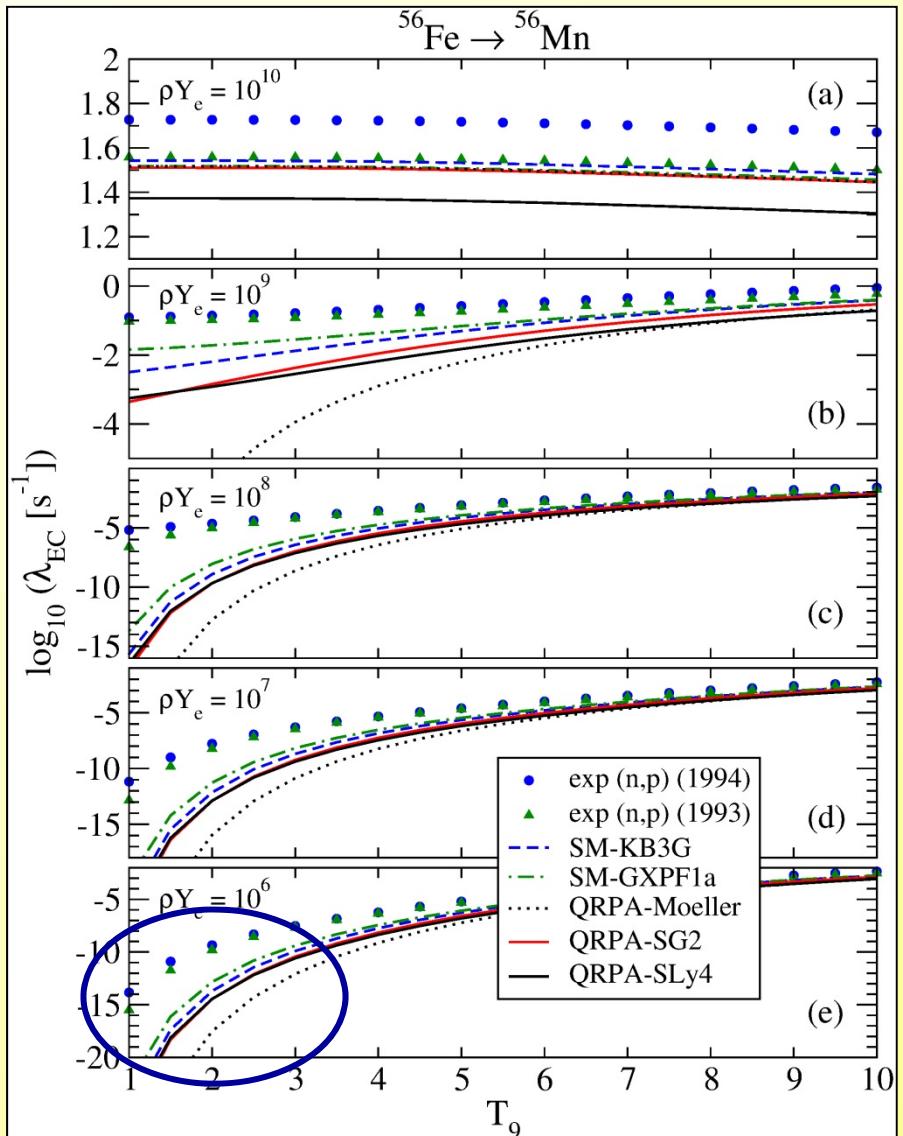
Ia Supernova



Weak decay rates in pf-shell nuclei

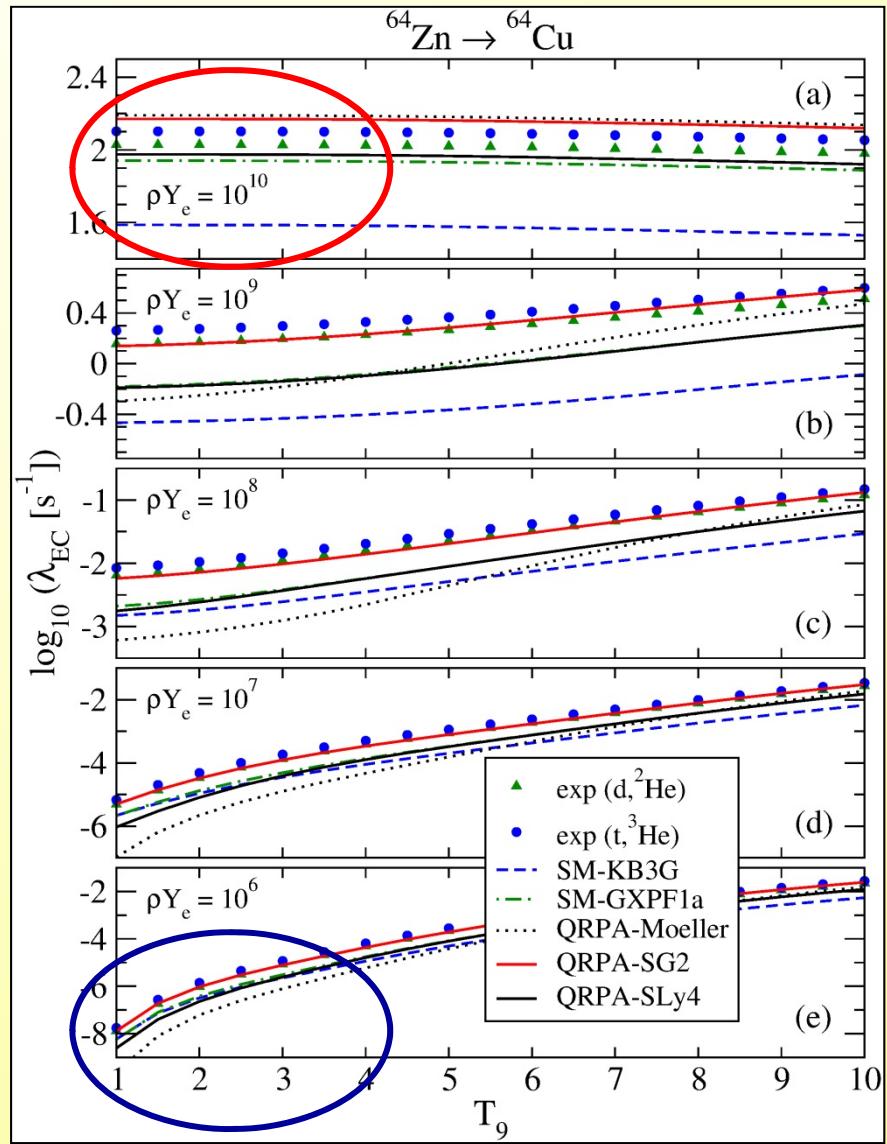
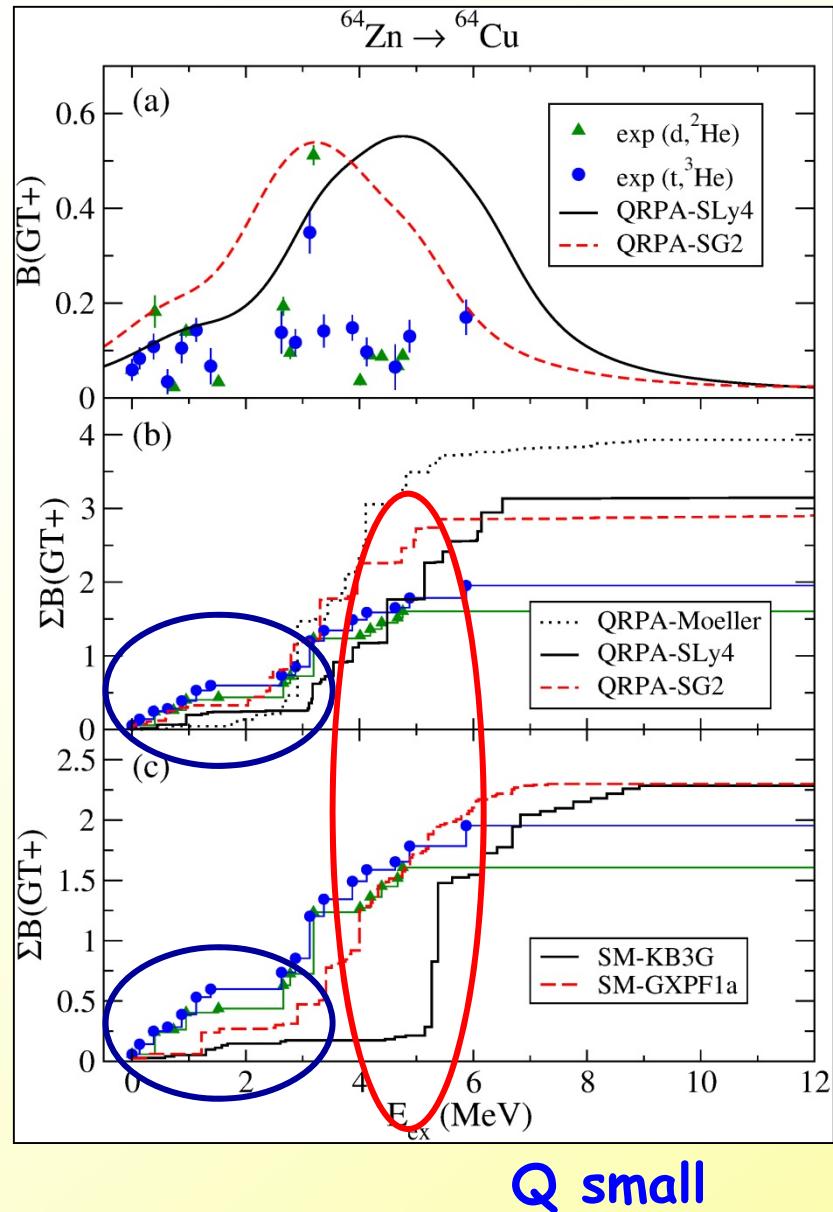


(Q<0) large: sensitive low-lying exc.



P.S. PRC87, 045801 (2013)

Weak decay rates in pf-shell nuclei



Exotic Nuclei : Nuclear Astrophysics

X-ray bursts: Source of intense X-ray emissions generated by thermonuclear runaway in the H-rich environment of an accreting n-star, fed from a binary red giant companion.

Nucleosynthesis mechanism: rp capture process

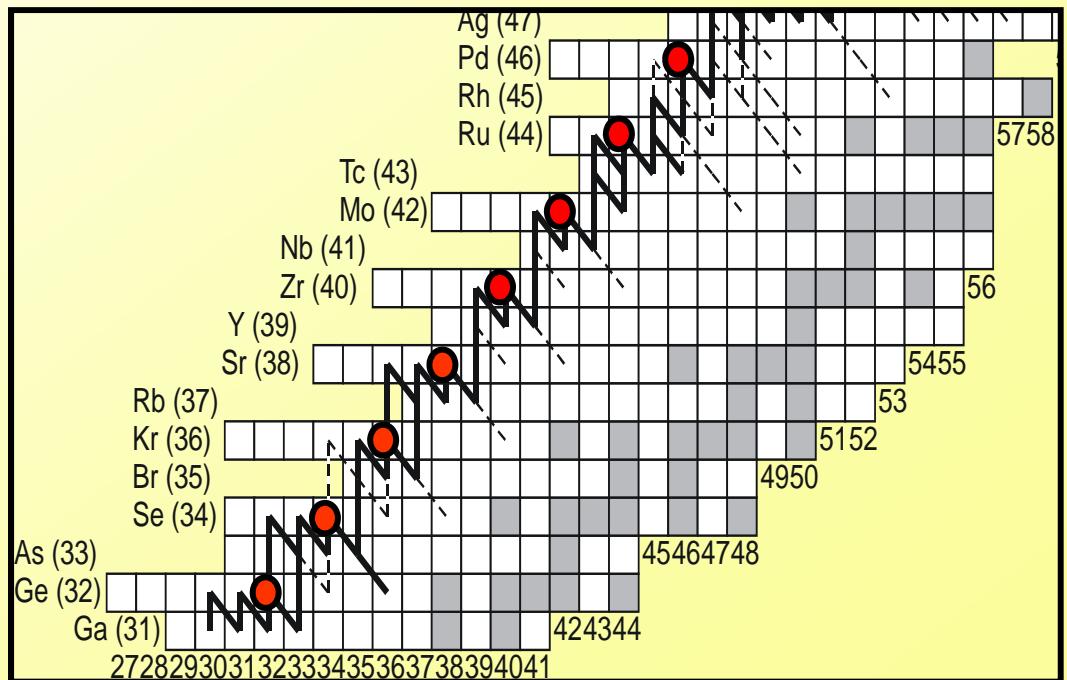
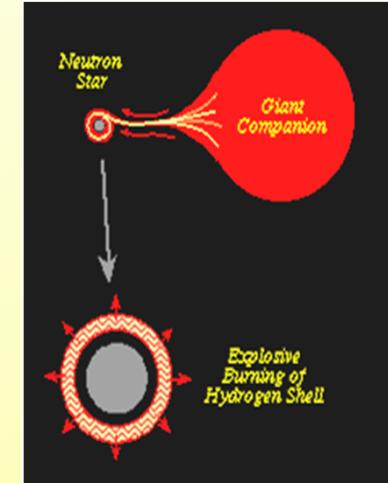
rp-process: Proton capture reaction rates are orders of magnitude faster than the competing β^+ -decays.

Waiting point nuclei: When the dominant p-capture is inhibited, the reaction flow waits for a slow beta-decay to proceed further.

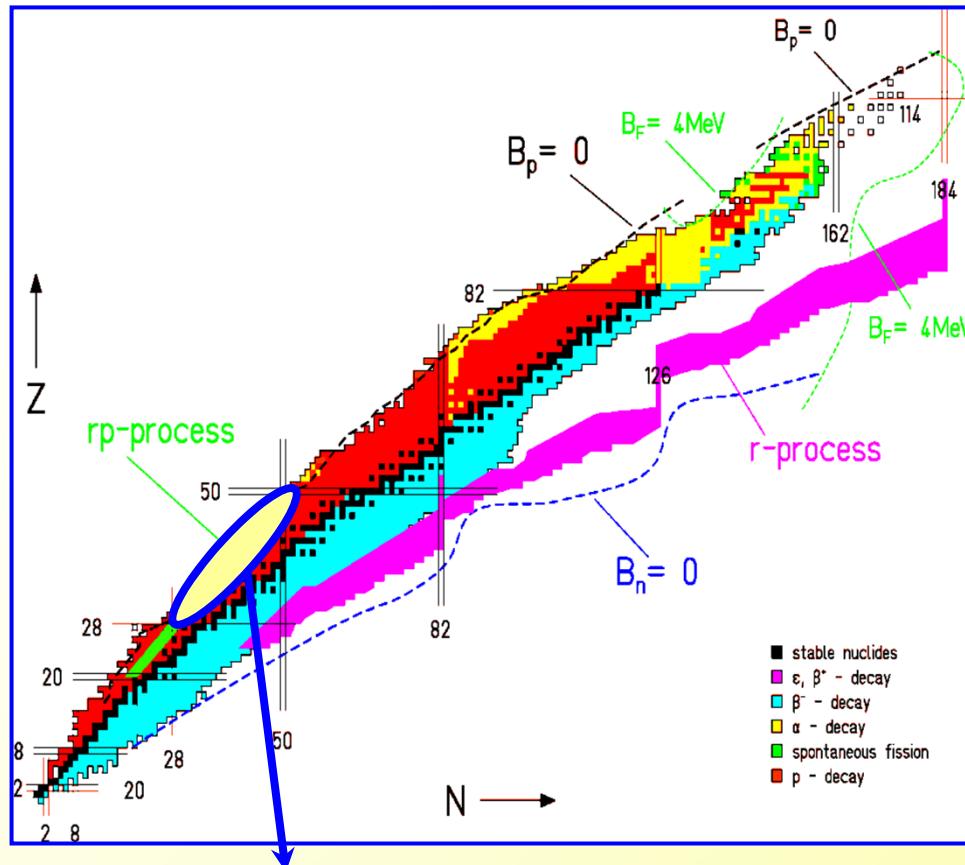
Time scale

Isotope abundances

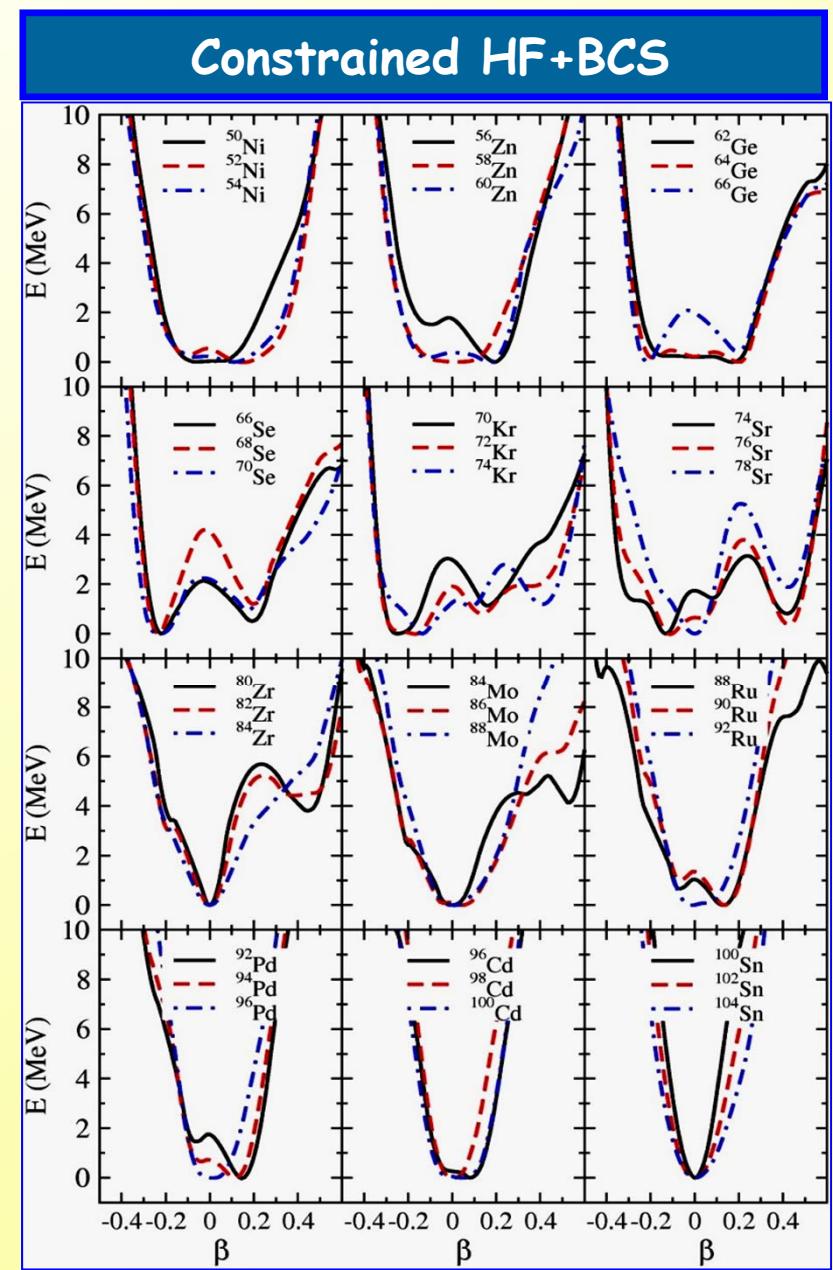
Light curve profile



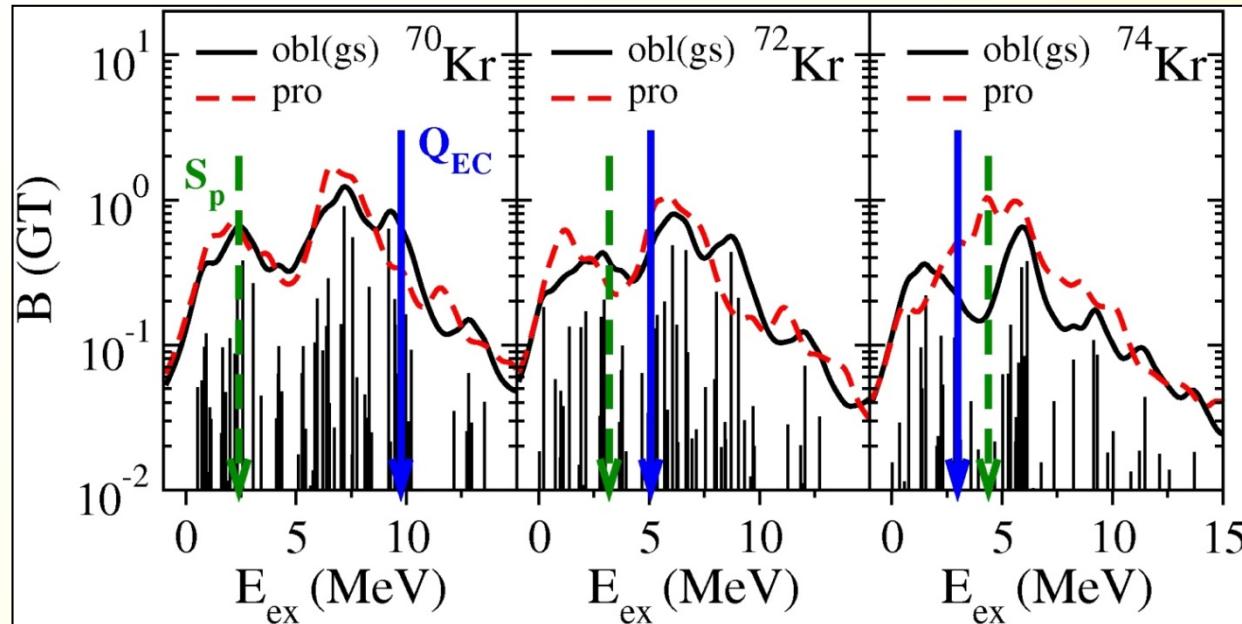
Medium mass neutron deficient isotopes



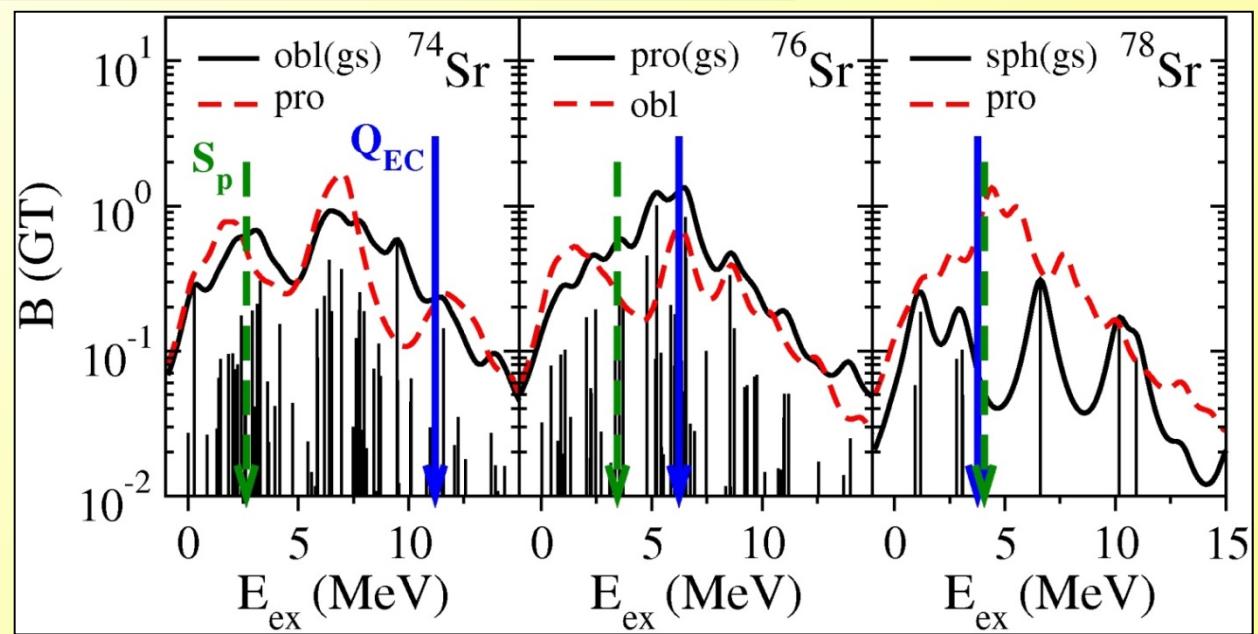
Waiting point nuclei in rp-processes
Shape coexistence
Beyond full Shell Model



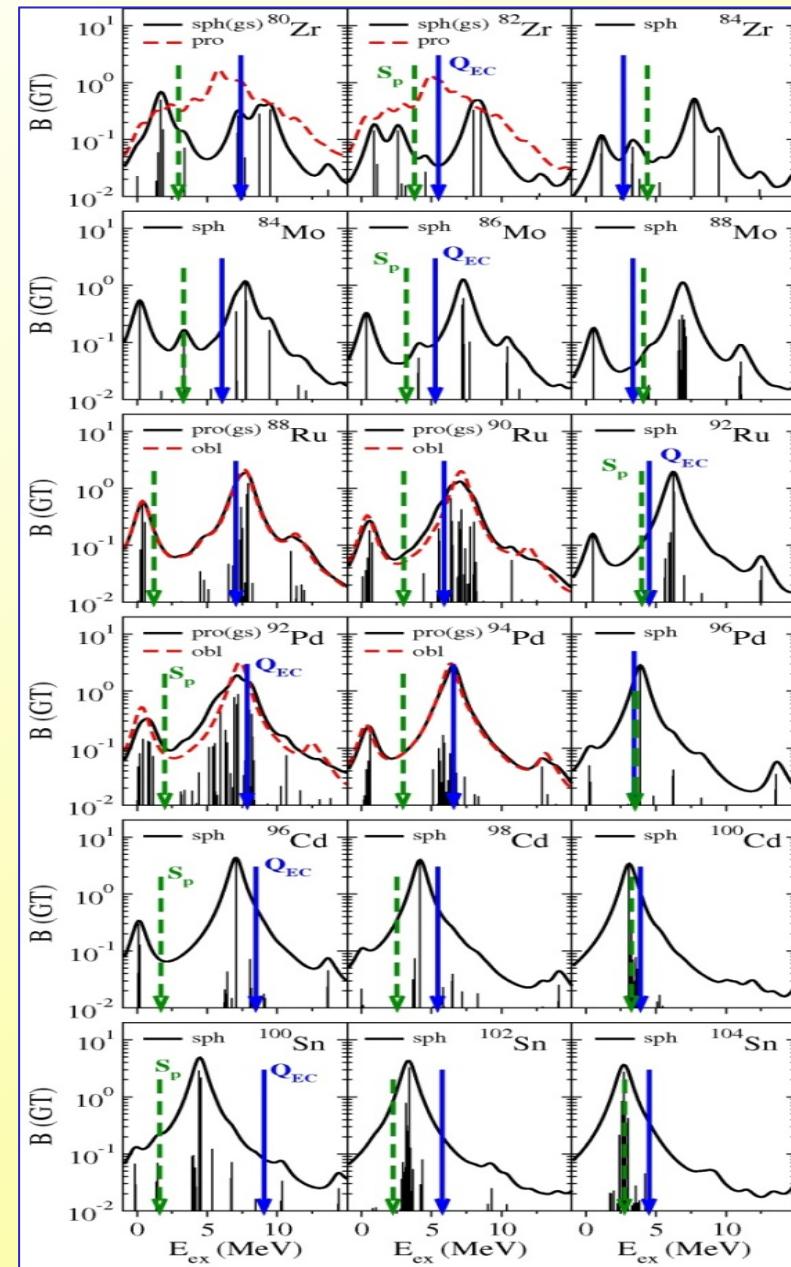
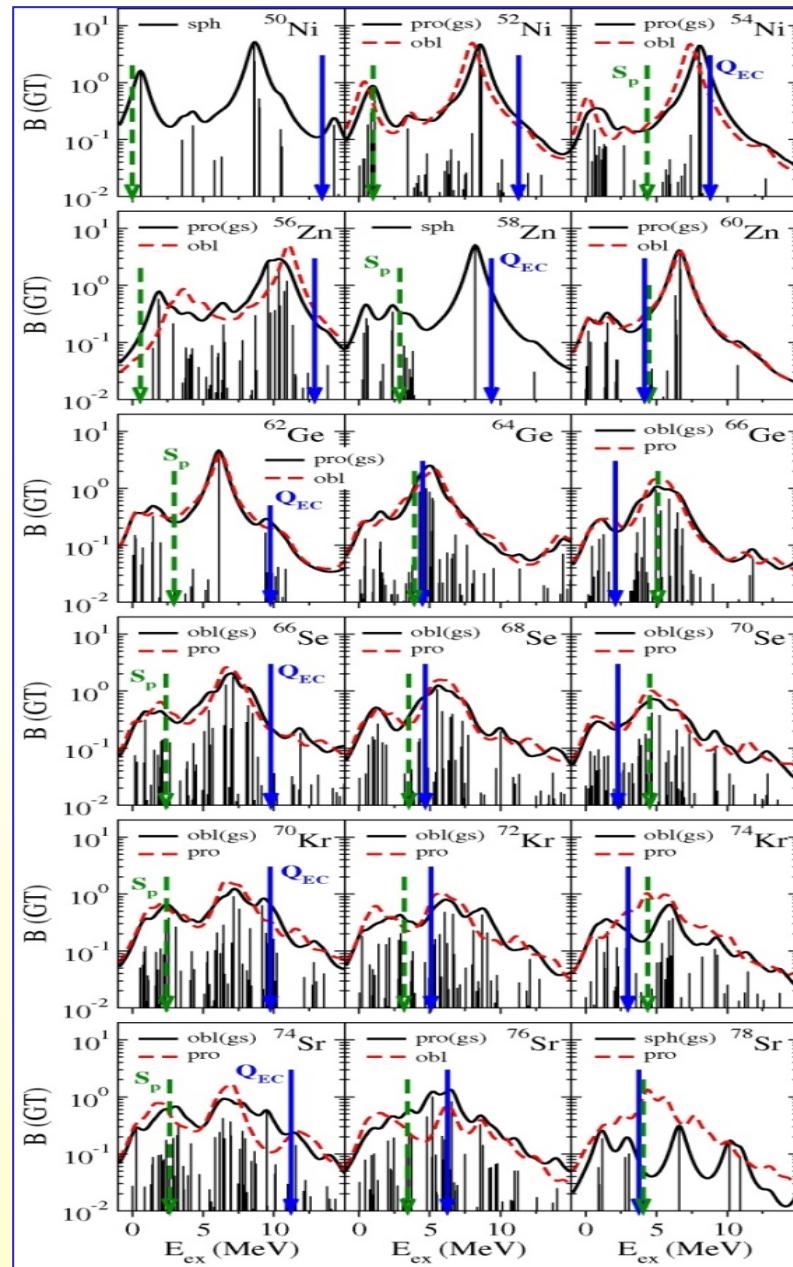
Gamow-Teller strength distribution



**Calculations for
Ni, Zn, Ge, Se,
Kr, Sr, Zr, Mo,
Ru, Pd, Cd, Sn
($N=Z$ and neighbors)**

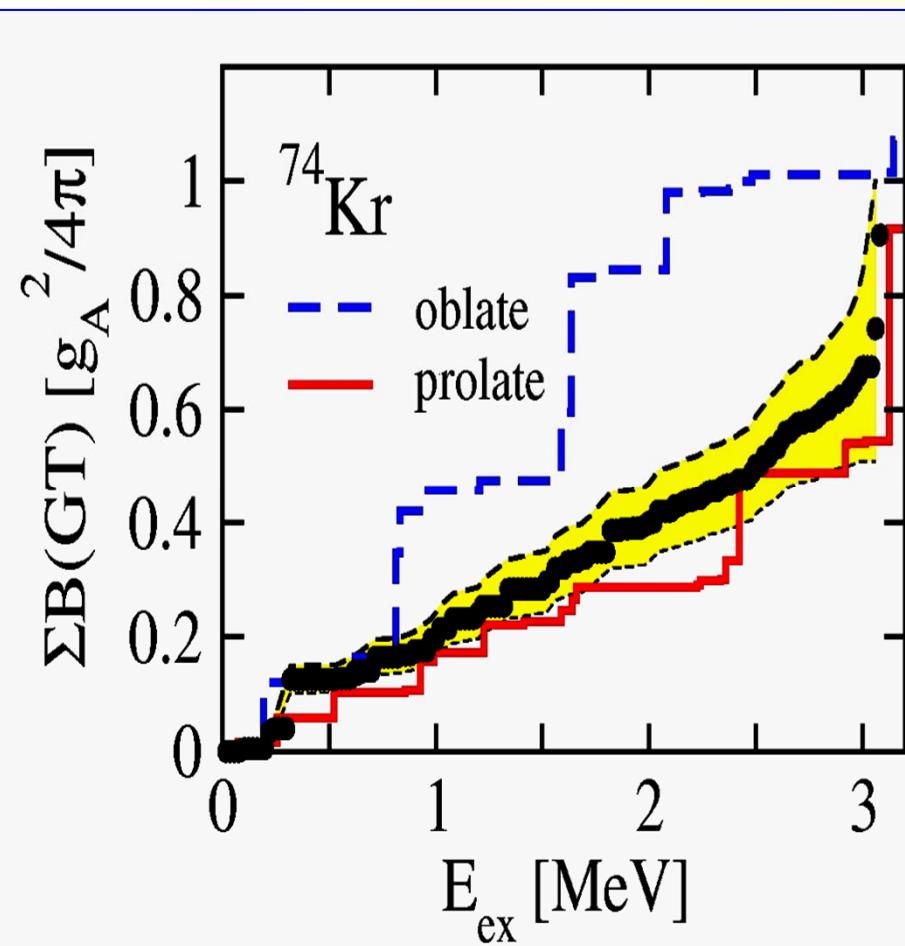


Gamow-Teller strength distribution

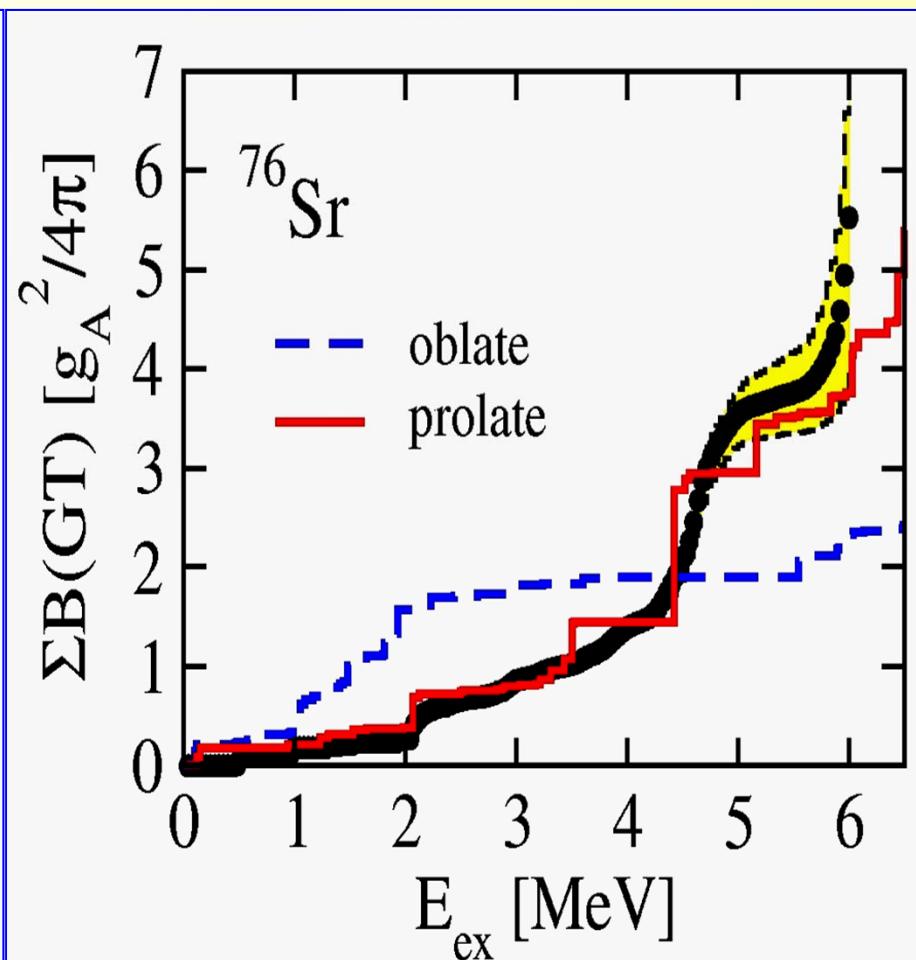


Gamow-Teller strength: Theory and Experiment

ISOLDE: Total absorption spectroscopy



Exp: Poirier et al. PRC69, 034307 (2004)



Exp: Nacher et al. PRL92, 232501 (2004)

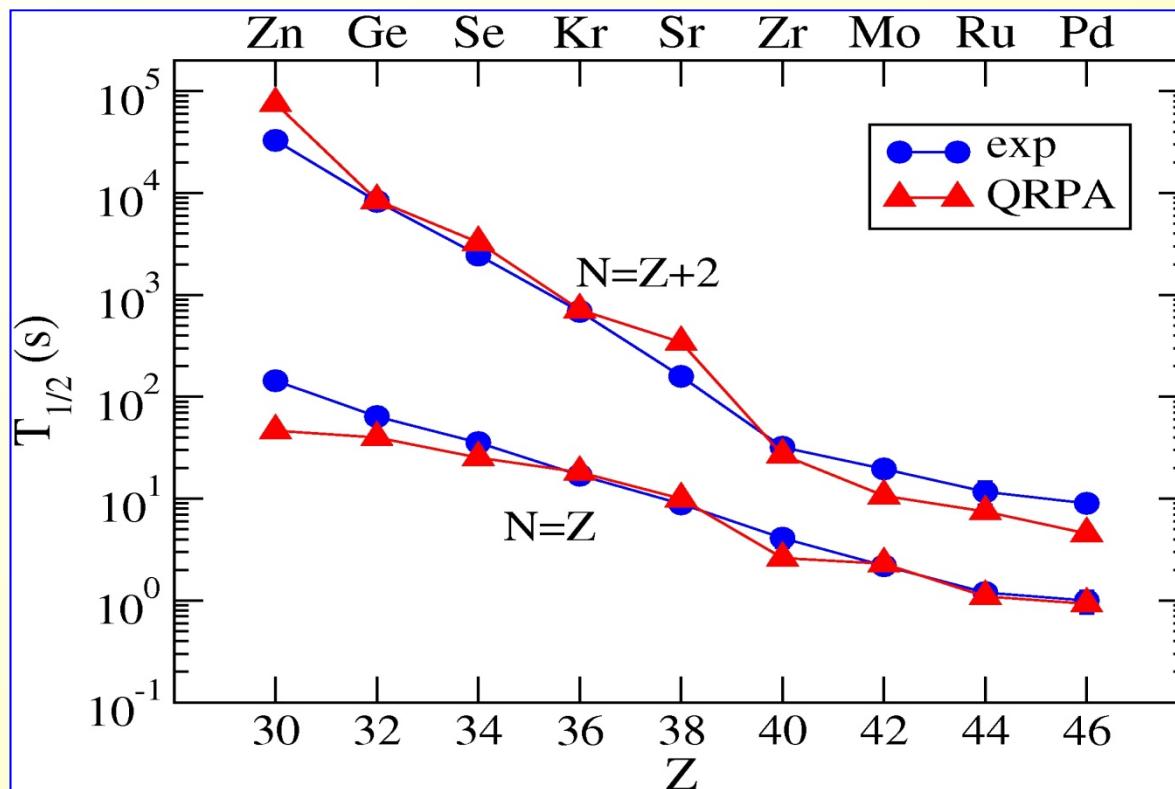
β^+/EC half-lives: Theory and Experiment

$$T_{1/2}^{-1} = \frac{(g_A / g_V)_{\text{eff}}^2}{6200} \sum_f \Phi^{\beta^+/\text{EC}} \left| \langle f | \beta^+ | i \rangle \right|^2$$

$$(g_A / g_V)_{\text{eff}} = 0.74 (g_A / g_V)_{\text{bare}}$$

$$\Phi_{if}^{\beta^+} = \int_1^{Q_{if}} \omega \sqrt{\omega^2 - 1} (Q_{if} - \omega)^2 F(Z, \omega) d\omega$$

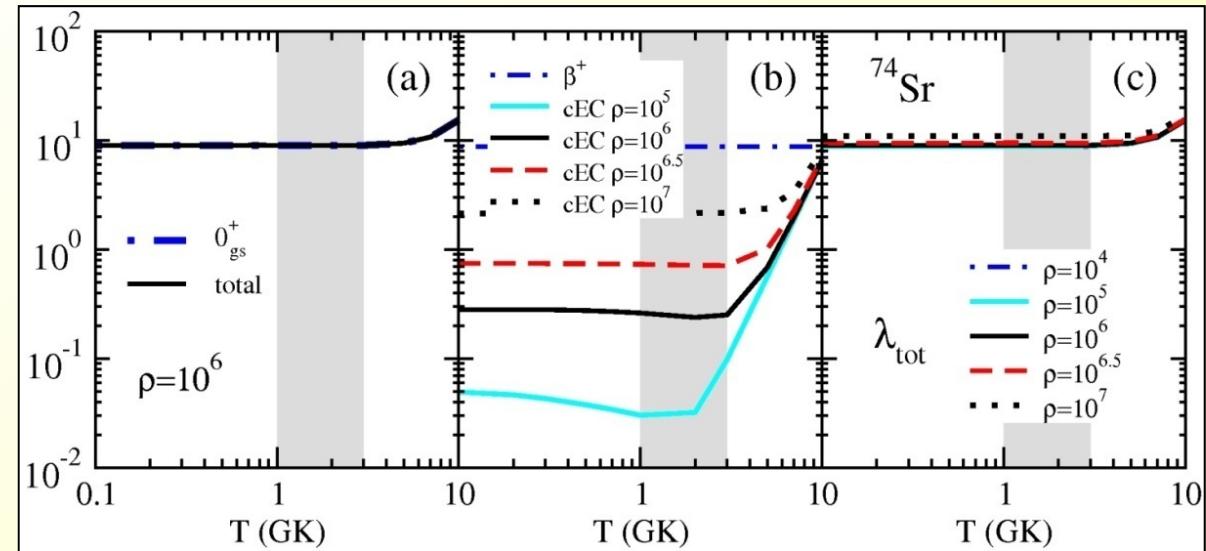
$$\Phi^{\text{EC}} = \frac{\pi}{2} \left[q_K^2 g_K^2 B_K + q_L^2 g_L^2 B_L + \dots \right]$$



Good agreement with experiment:
Reliable extrapolations to high ρ and T

Weak decay rates in rp-process

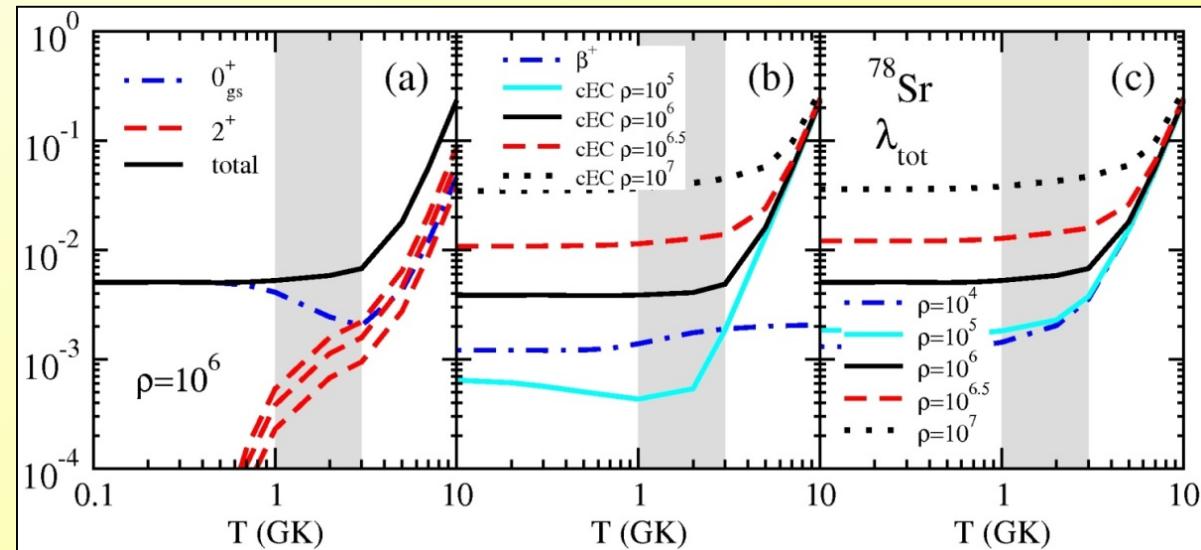
^{74}Sr
Deformed pn-QRPA
 $B(GT)$ and $T_{1/2}$: Good
agreement with
experiment



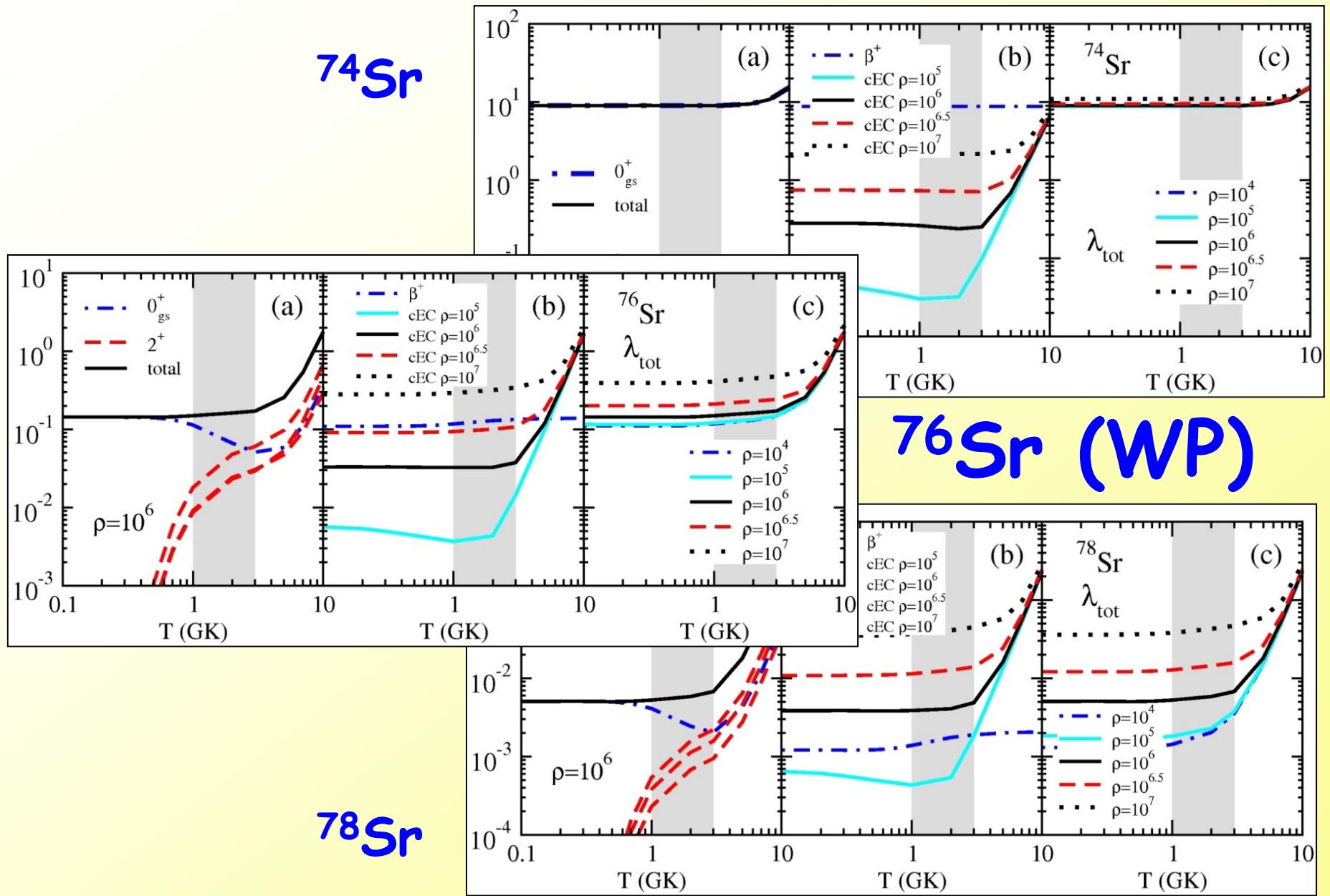
Competition β^+/EC

P.S. PRC83, 025801 (2011)

^{78}Sr

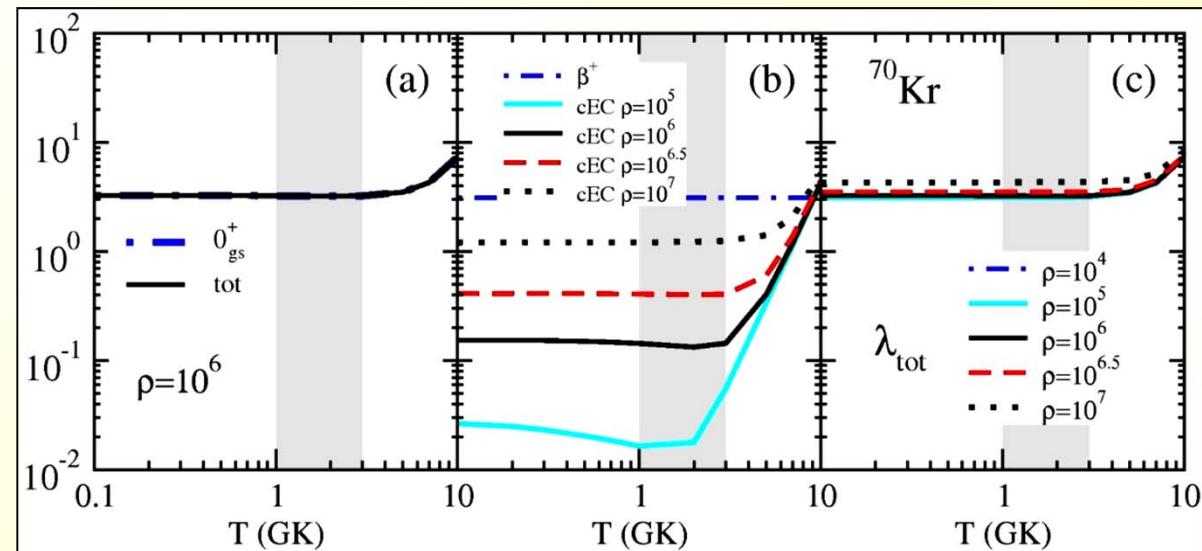


Weak decay rates in rp-process



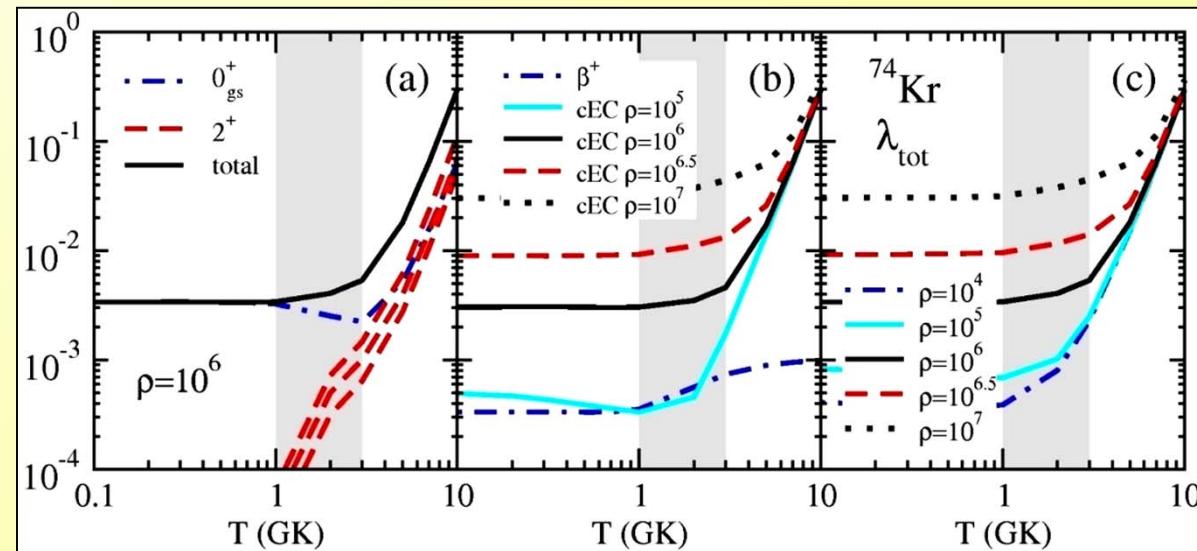
Weak decay rates in rp-process

^{70}Kr
(Large Q)

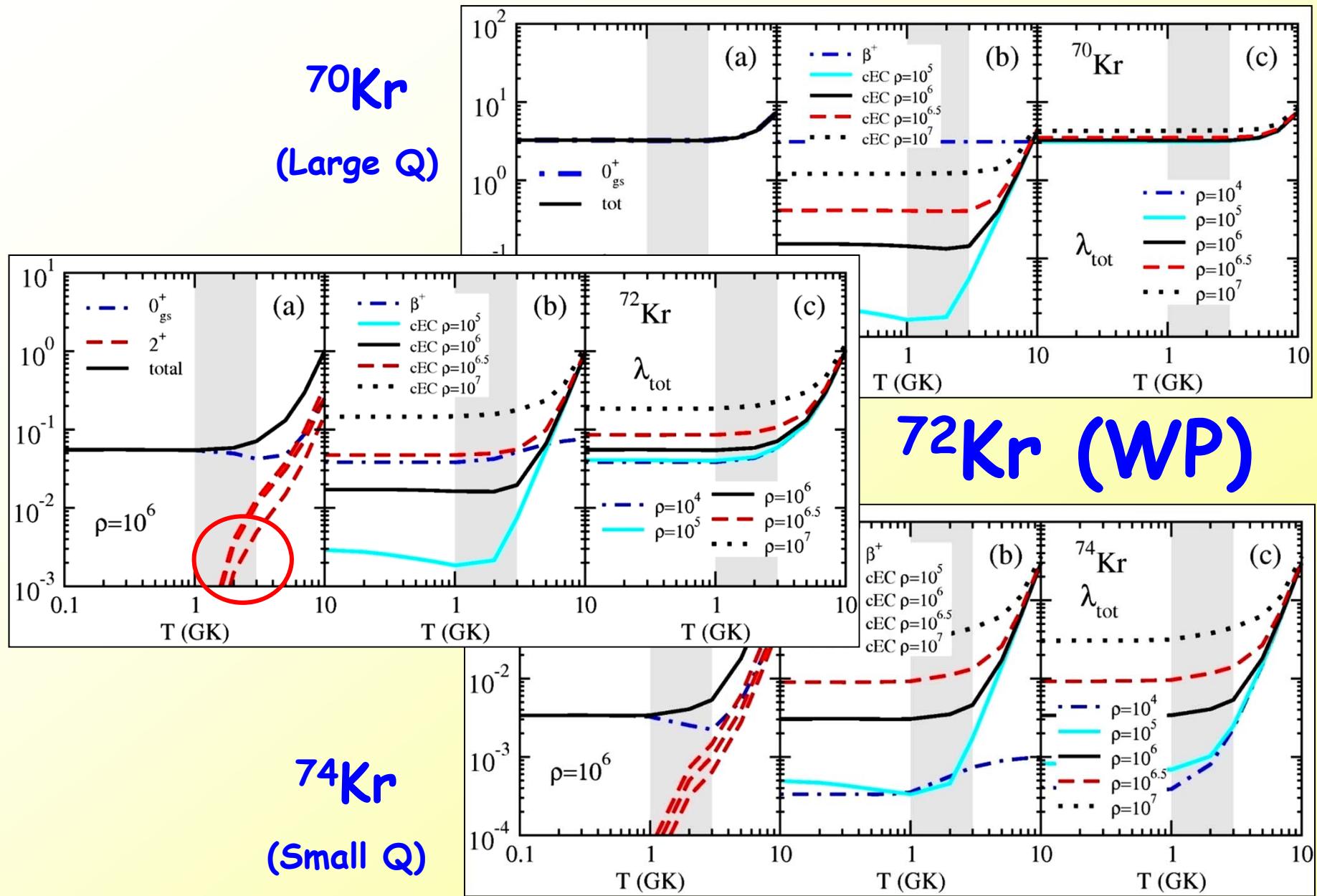


P.S. Phys. Rev. C 83, 025801 (2011)

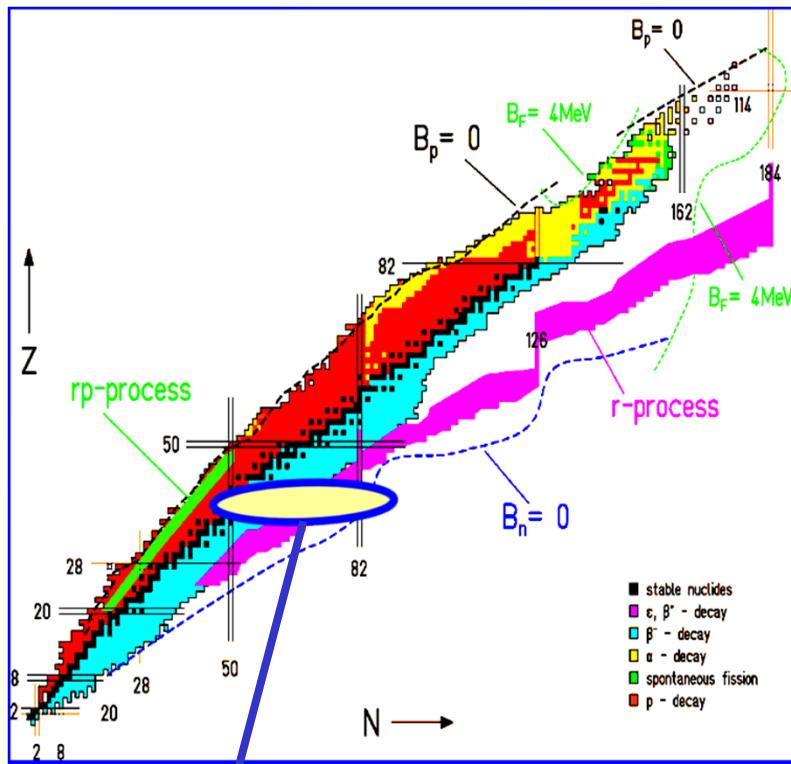
^{74}Kr
(Small Q)



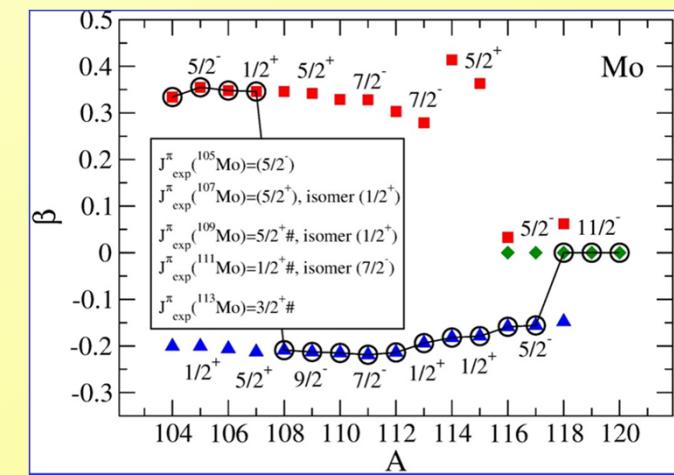
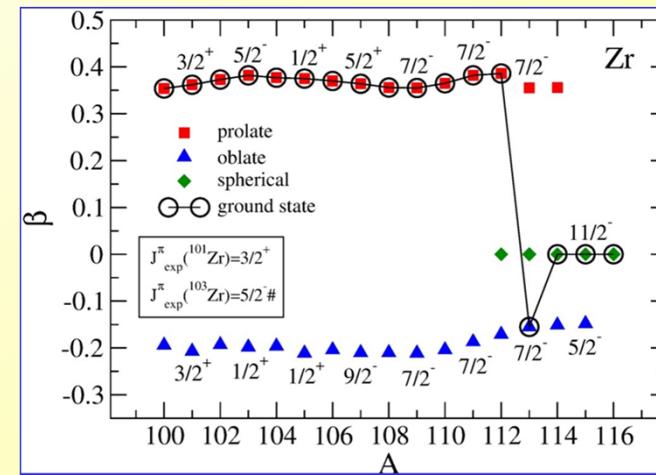
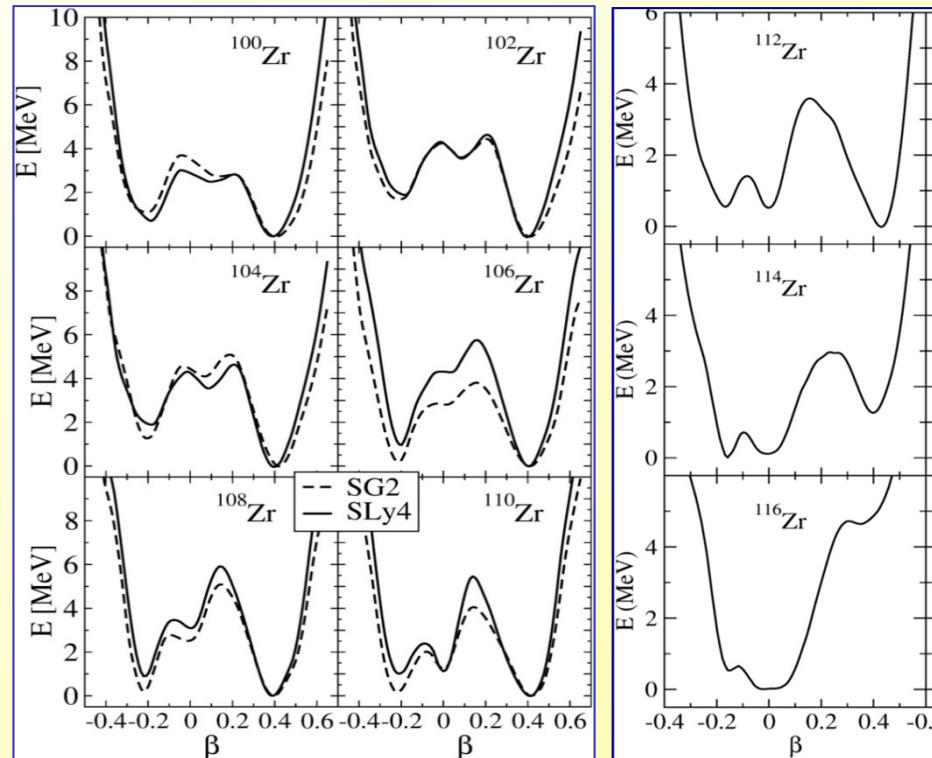
Weak decay rates in rp-process



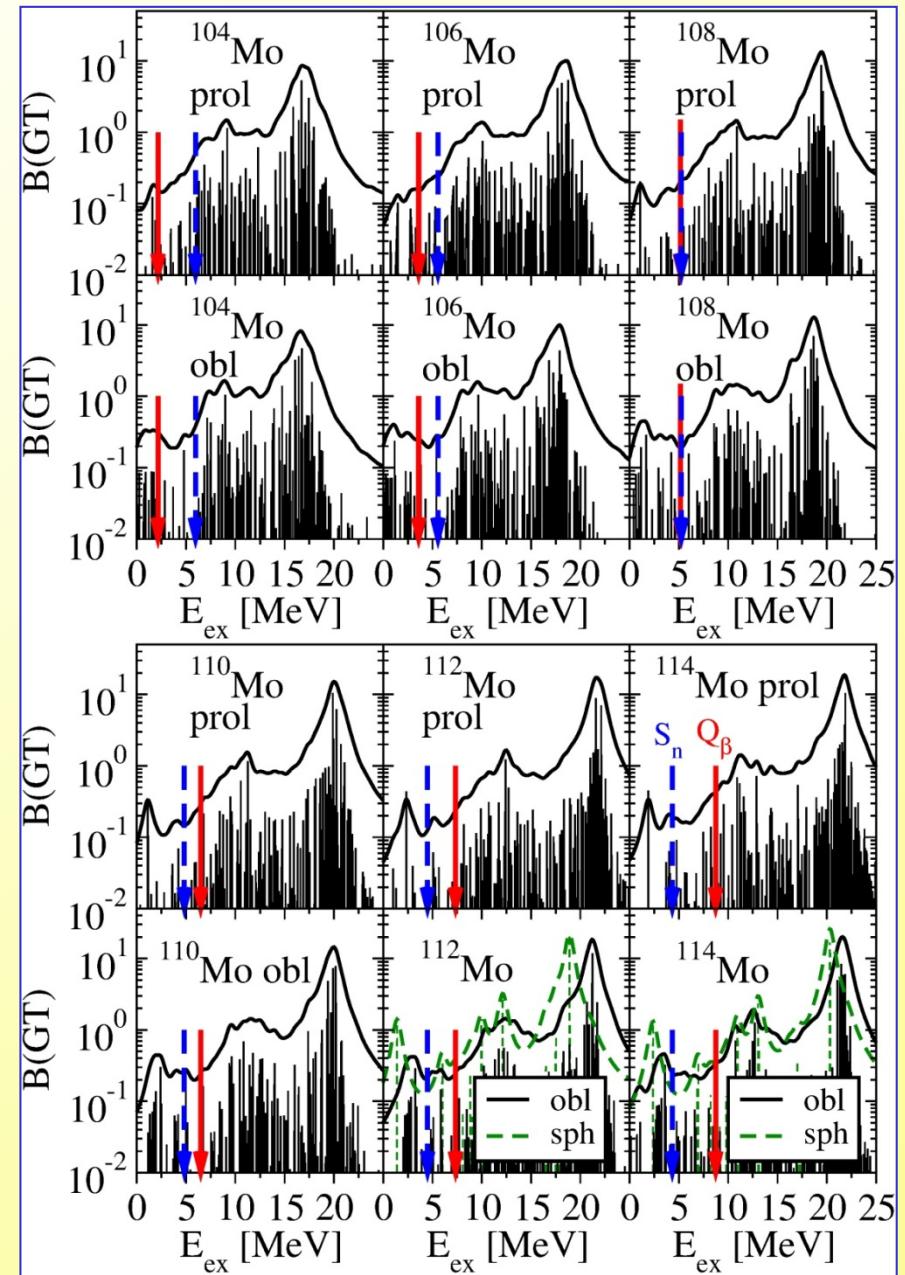
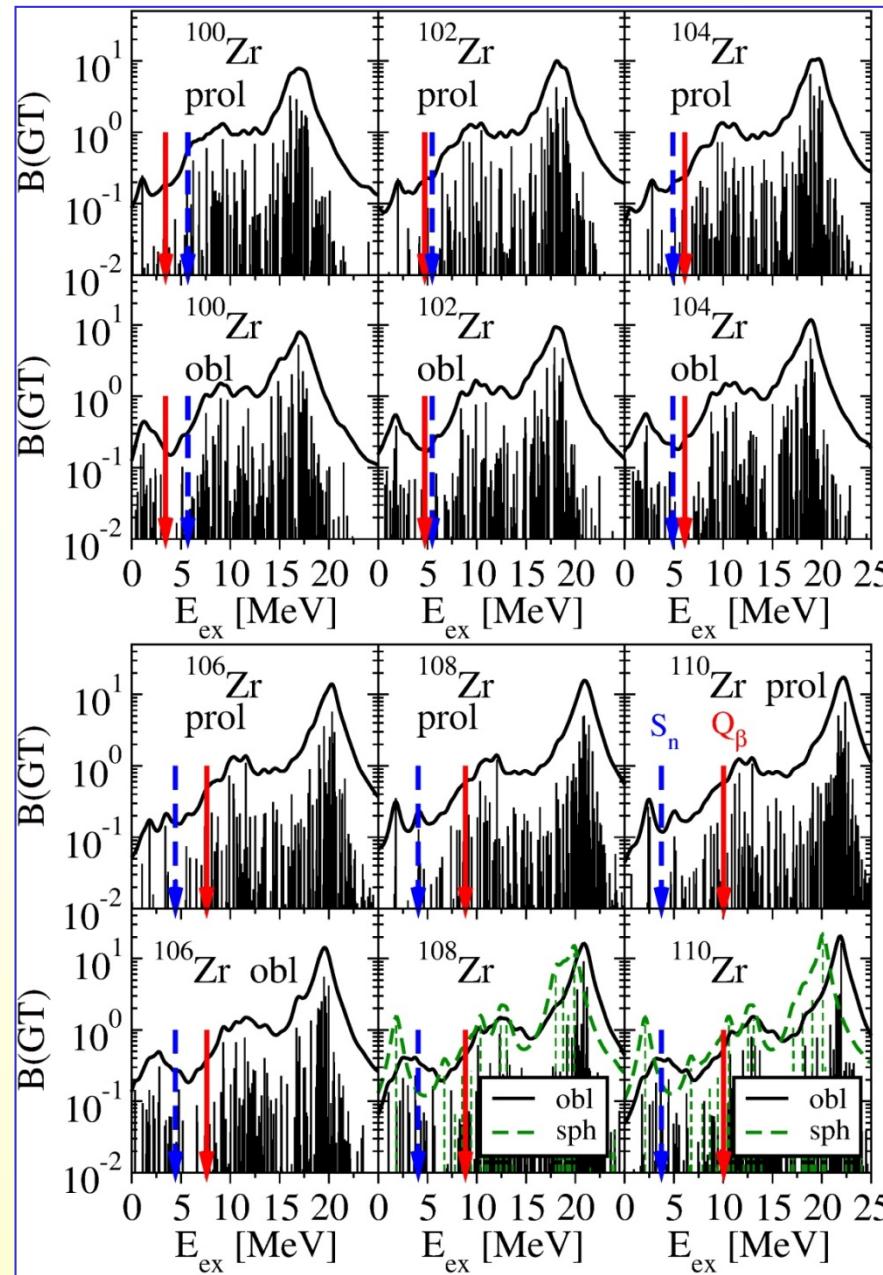
Zr-Mo neutron-rich isotopes



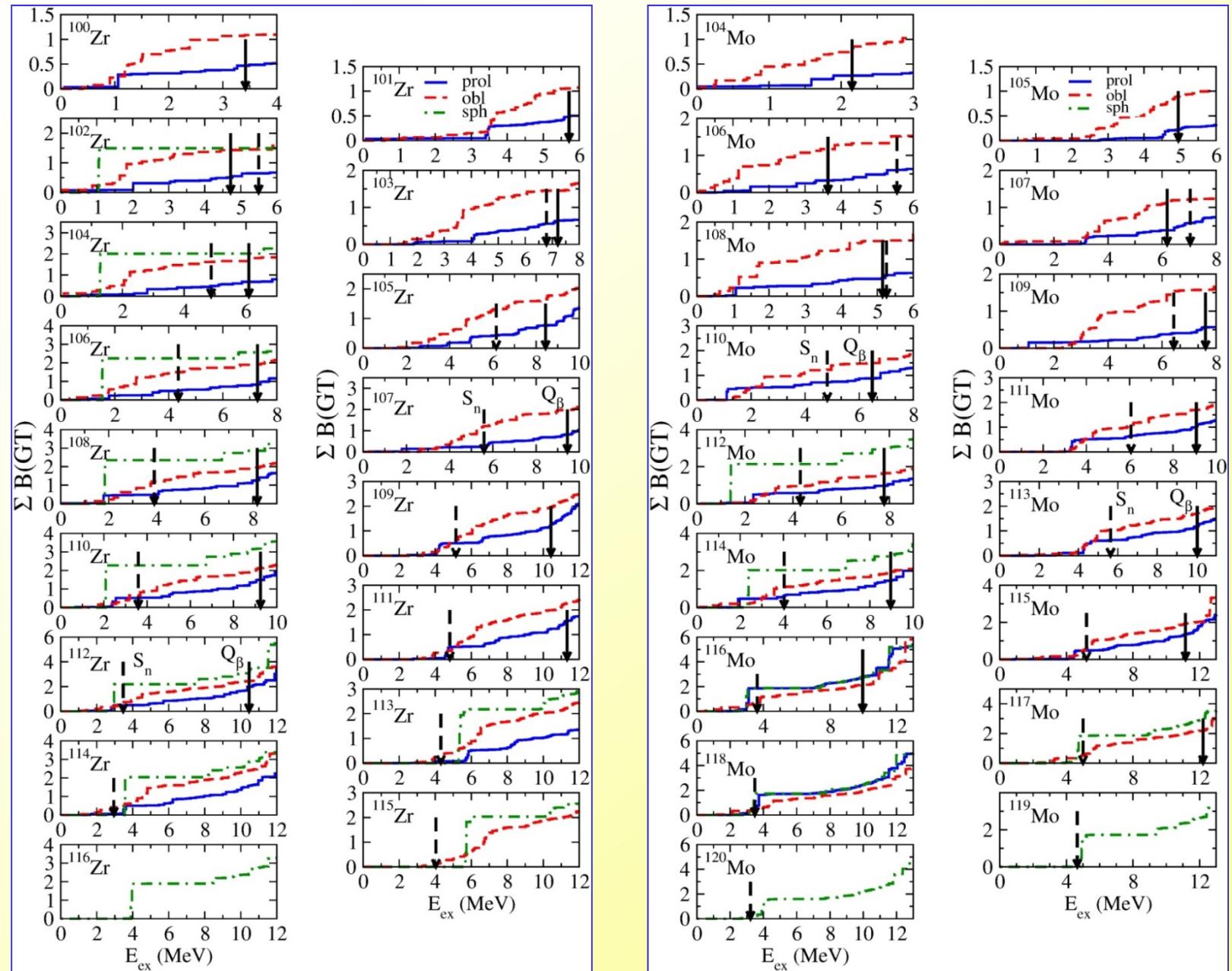
$^{100-116}\text{Zr}$
 $^{104-120}\text{Mo}$



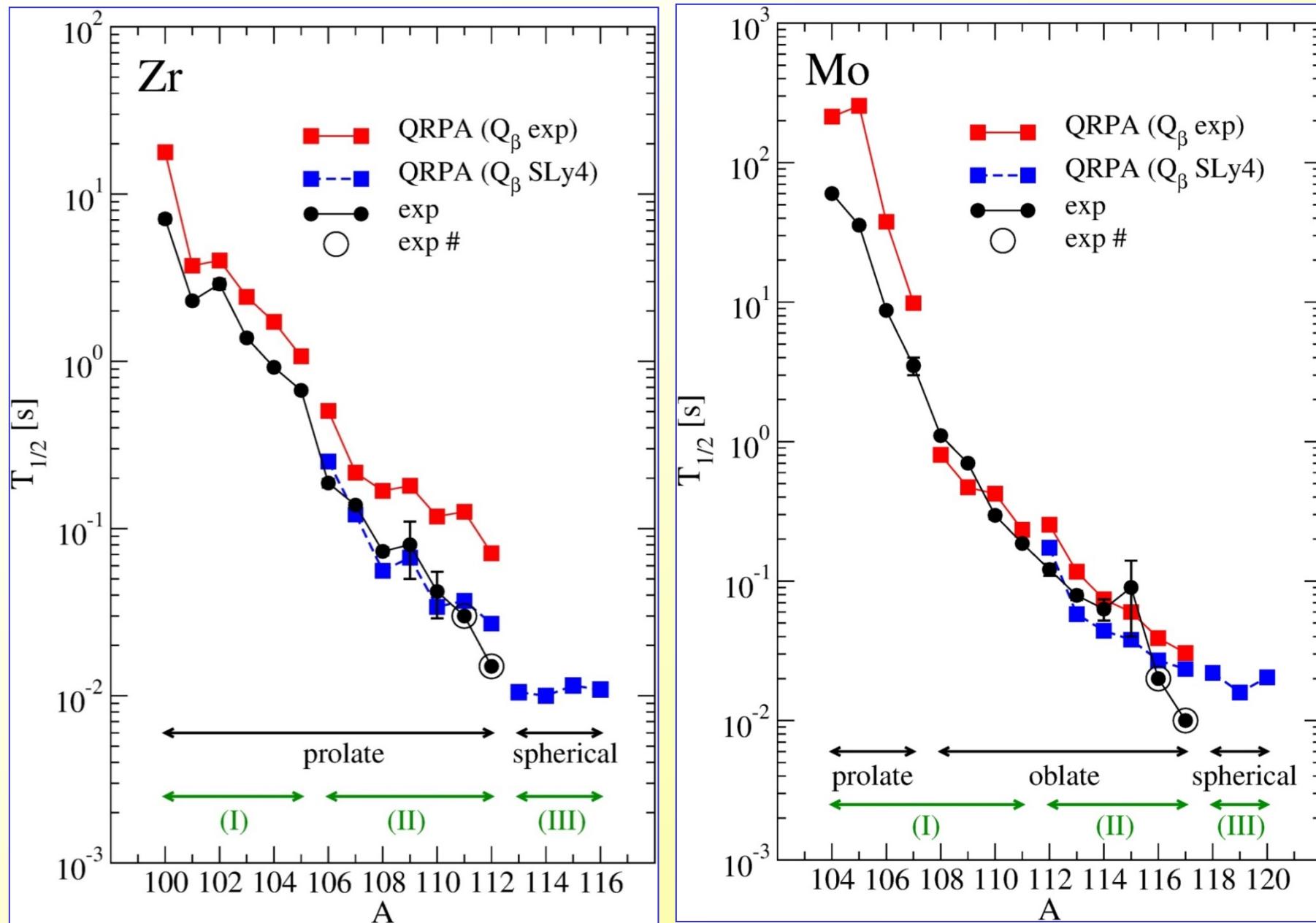
Zr-Mo B(GT)



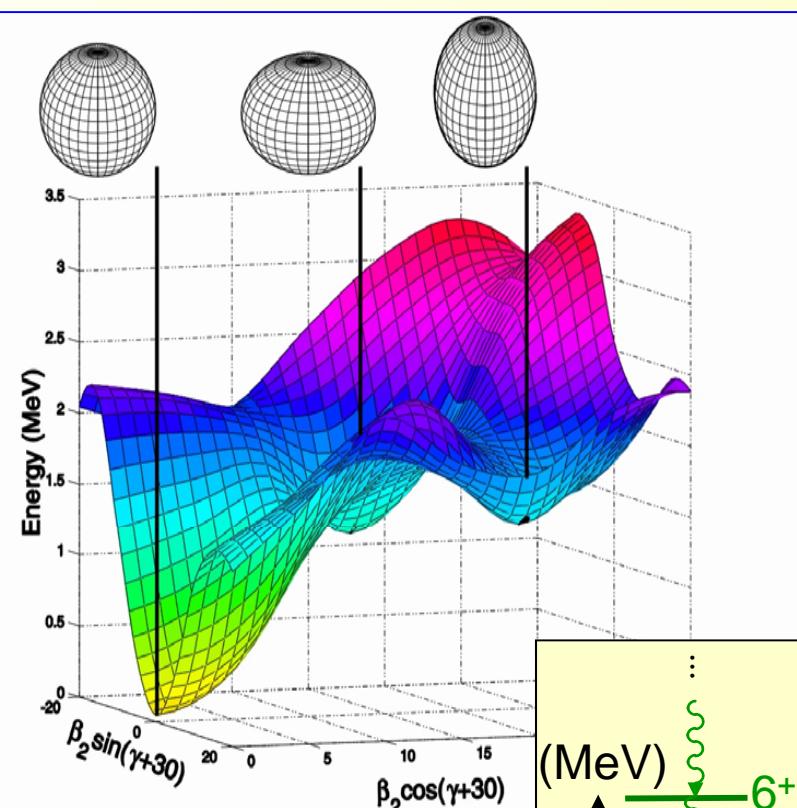
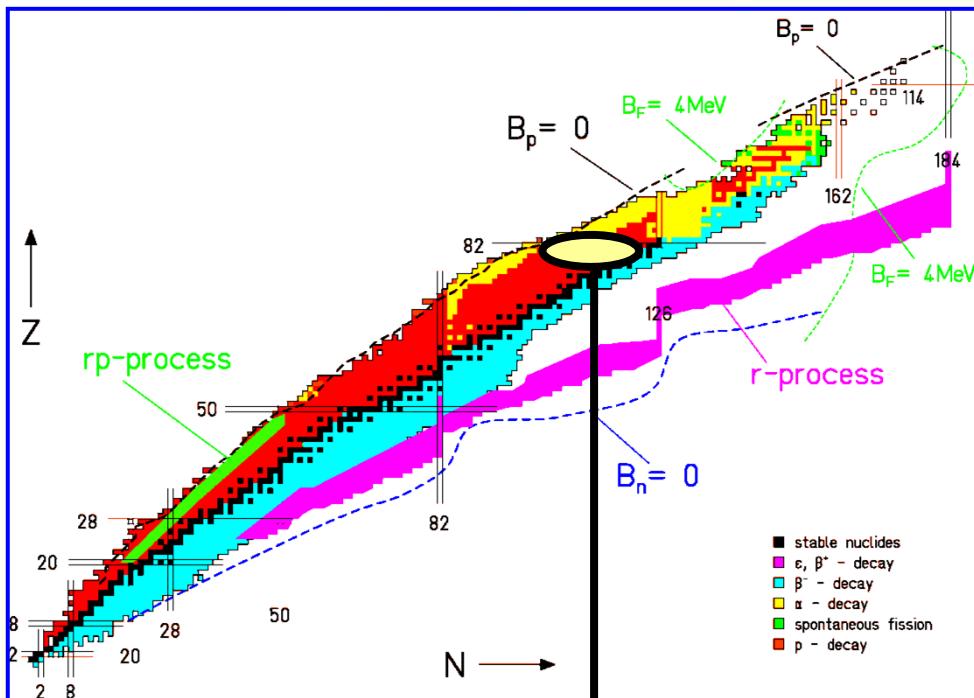
Zr-Mo B(GT)



Zr-Mo Half-lives

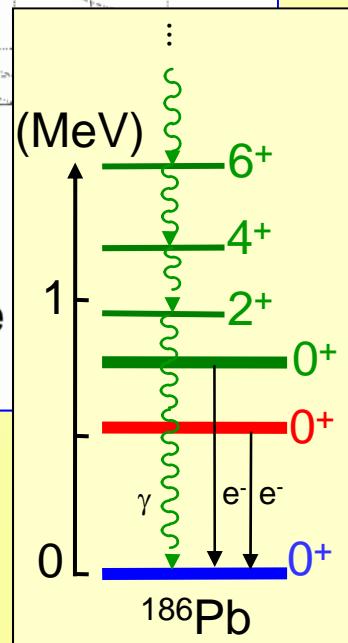


Shape dependence of GTdistributions in neutron-deficient Hg, Pb, Po isotopes

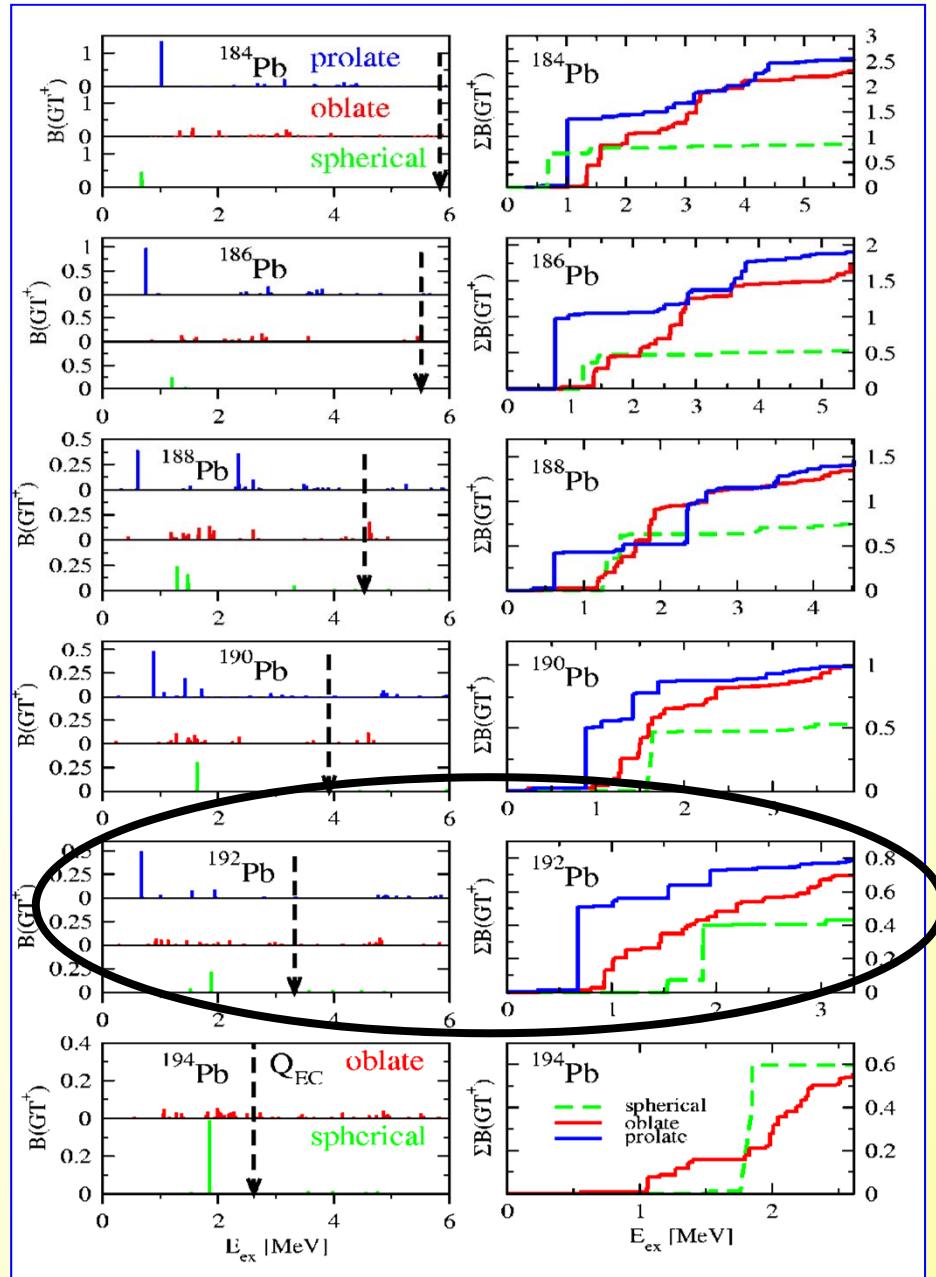


Potential Energy Surface

- Triple shape coexistence at low excitation energy
- Search for signatures of deformation on their beta-decay patterns



Shape dependence of GT distributions in neutron-deficient: Pb isotopes

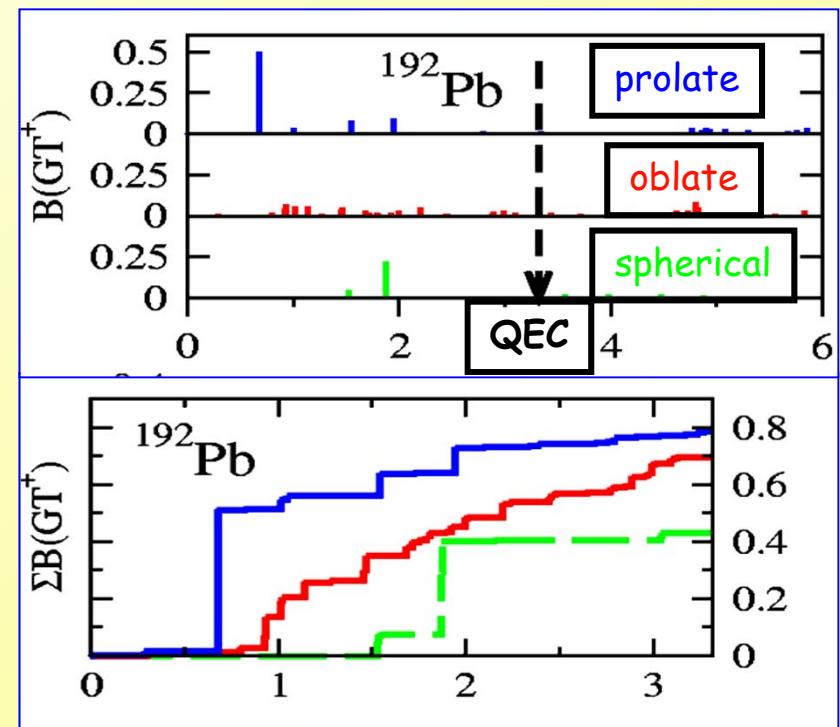


B(GT) strength distributions

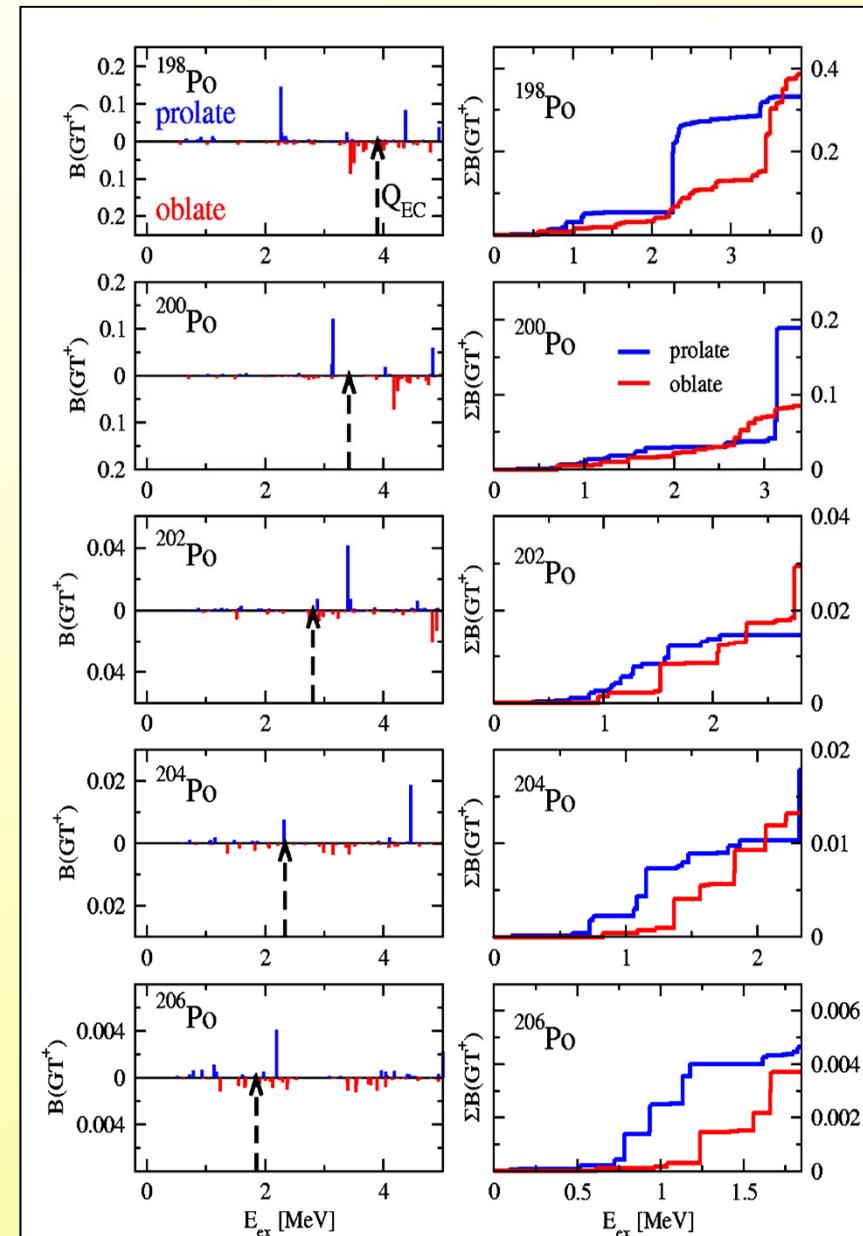
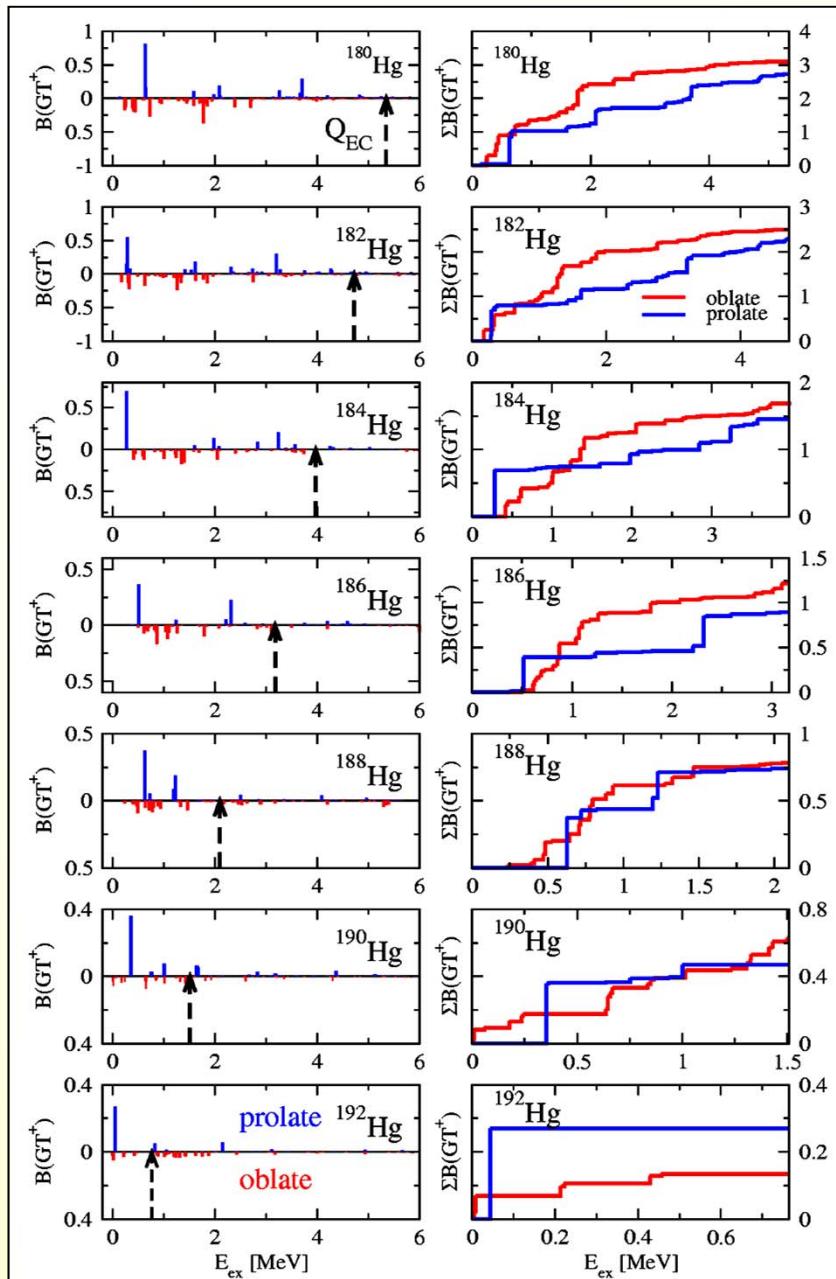
- Not very sensitive to : Skyrme force and pairing treatment
- Sensitive to : Nuclear shape

Signatures of deformation

PRC 72, 054317 (2005), PRC 73, 054302 (2006)



Shape dependence of GT distributions in neutron-deficient Hg, Po isotopes



Conclusions

Nuclear structure model (**deformed Skyrme HF+BCS+QRPA**)

- Nuclear structure in different mass regions, astrophysical applications.
- Reproduce half-lives and main features of GT strength distributions extracted from beta-decay and/or charge exchange reactions.
- Weak-decay rates at (ρ, T) typical of astrophysical scenarios:
 - pf-shell nuclei (presupernova): EC rates from QRPA comparable quality to benchmark SM calculations.
 - Neutron-deficient WP nuclei (rp-process): EC/ β^+ compete
 - Neutron-rich Zr-Mo isotopes (r process).