rプロセス研究における密度汎関数理論：ベータ崩壊を中心として

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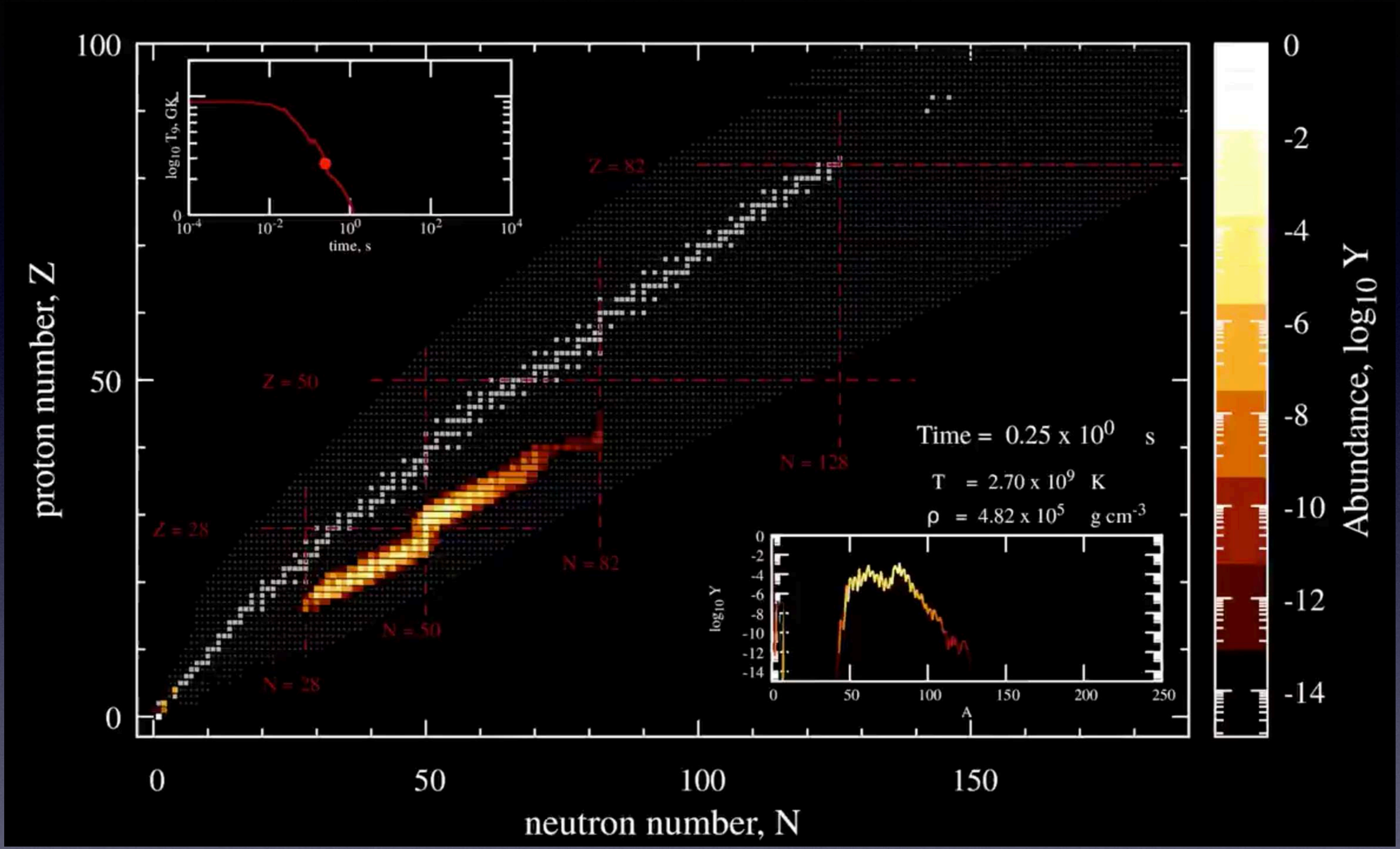
Nuclear data needed for describing r-process: initial stage



Cal.: N. Nishimura

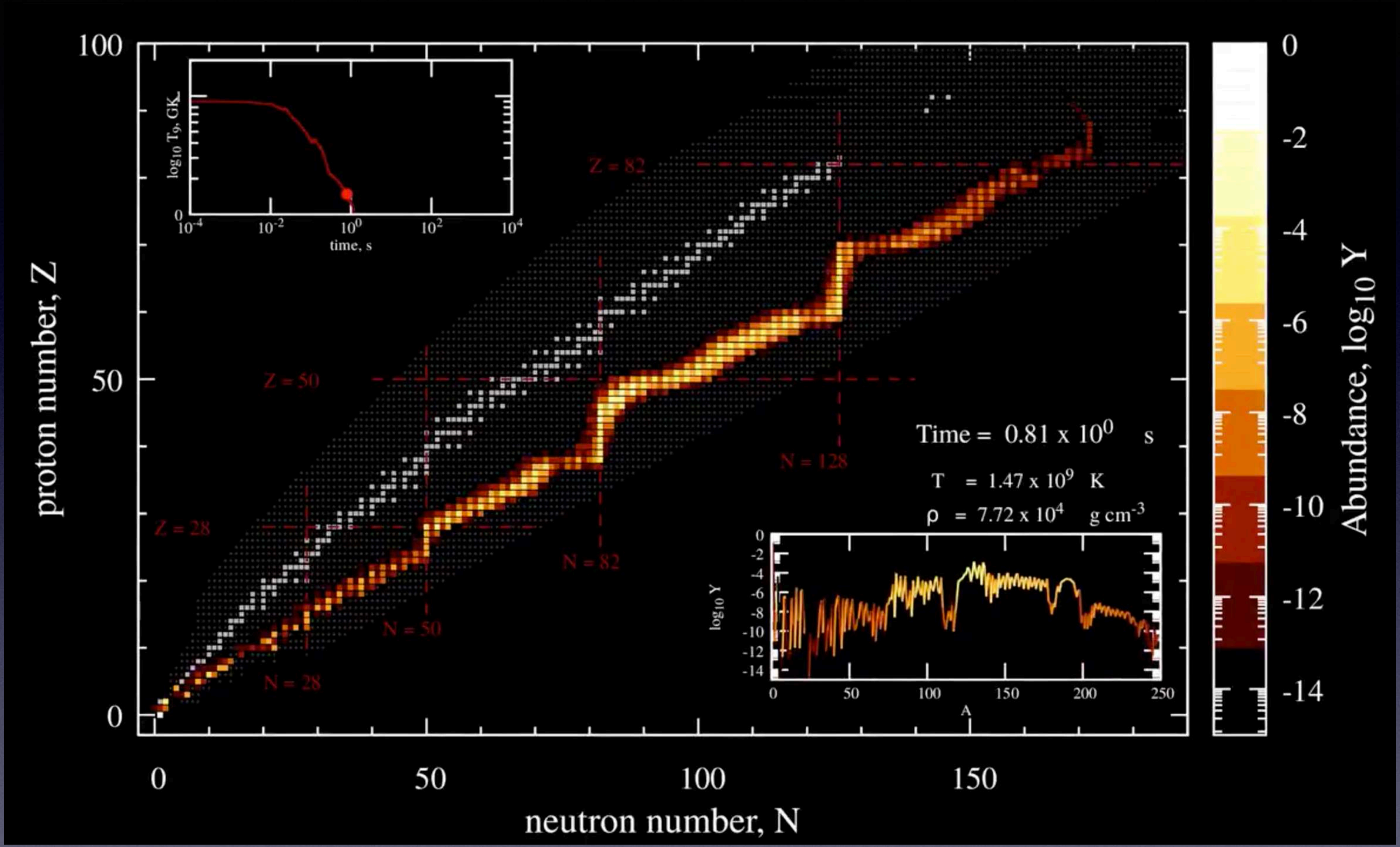
astrophysical conditions:

- neutron density
- temperature

↓ **mass**

seed nuclei

Nuclear data needed for describing r-process: early stage



Cal.: N. Nishimura

seed nuclei

neutron-capture rate
beta-decay rate

neutron-rich nuclei

reaching heavy region

fission rate

β-delayed fission

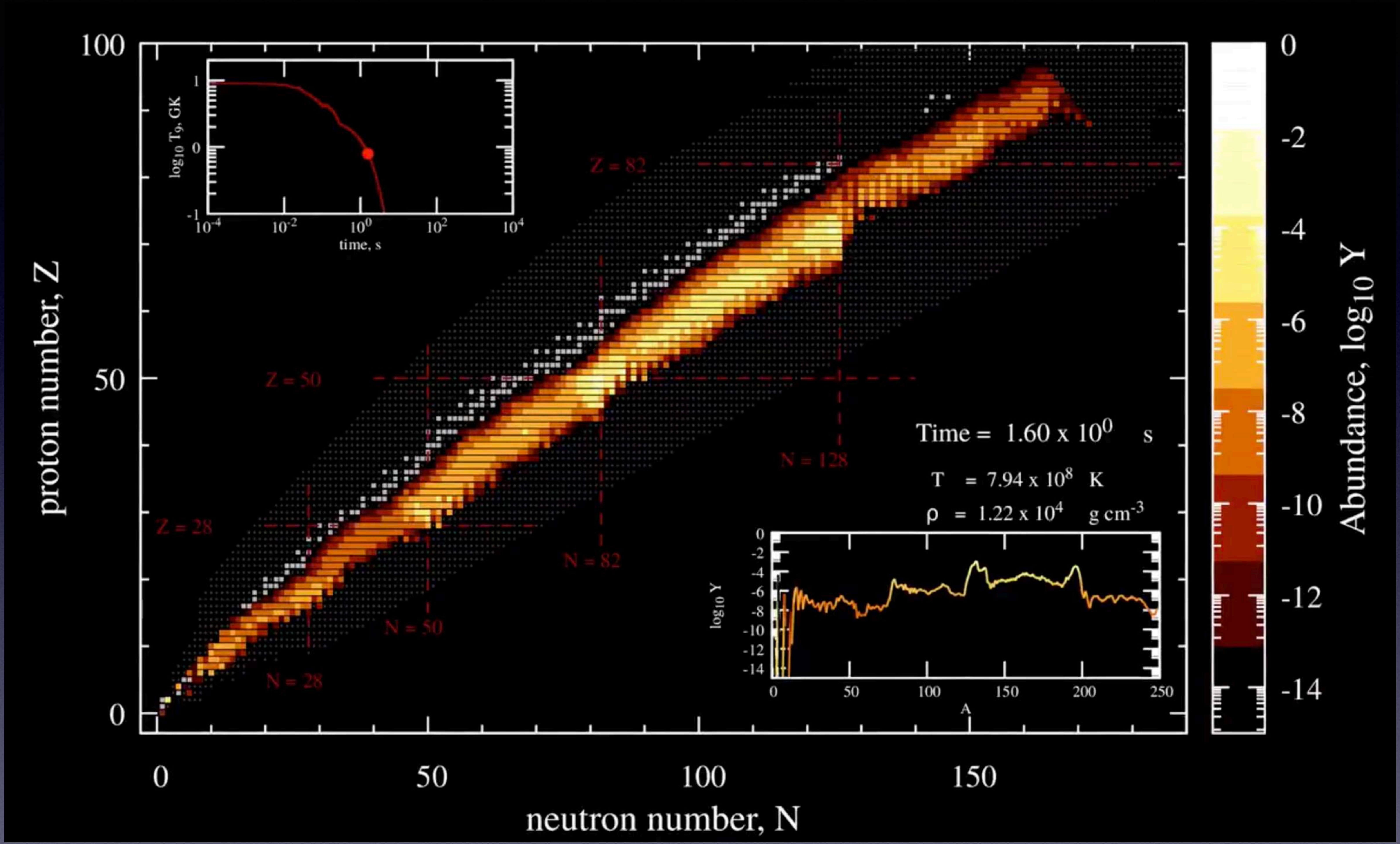
n-induced fission

fission after β-delayed neuron emission

ν-induced fission

fission fragment dis.

Nuclear data needed for describing r-process: late stage



Cal.: N. Nishimura

n-rich nuclei

β-decay rate

β-delayed n-emission

ν-scattering

stability line

Decisive roles by nuclear theory

Desirable nuclear data

- in a wide mass region; even close to the drip line
  - No experimental data available, nor reachable
- with high reliability and accuracy
  - To disentangle the uncertainties of astro/nuclear physics

solving the time-dependent many-body Sch. equation w/ appropriate B.C.

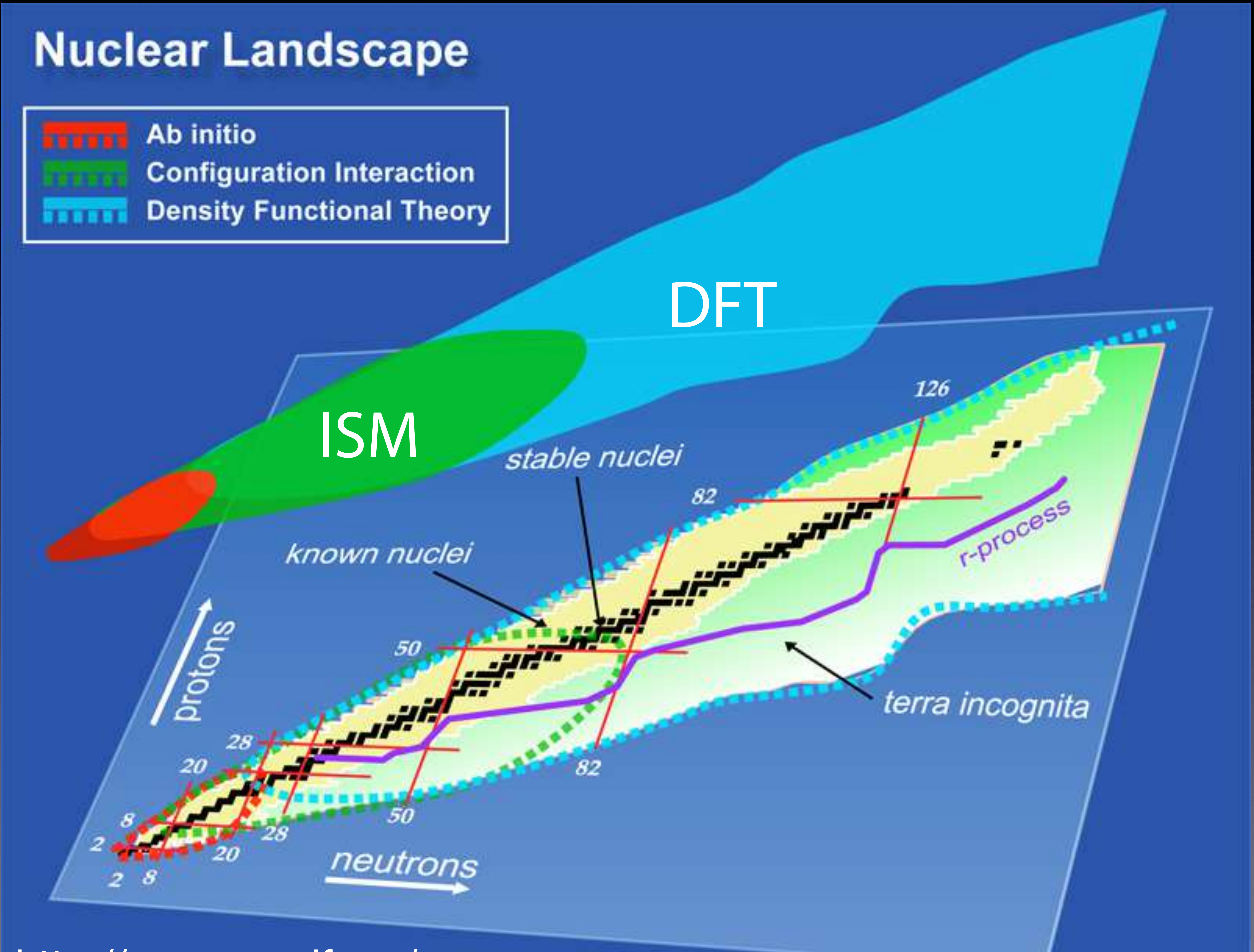
hyper-ambitious

↓

find a pragmatic way

Microscopic theory for nuclear many-body systems

in terms of a nucleonic d.o.f.



http://www.unedf.org/

For medium-heavy and heavy nuclei

Interacting Shell Model

talk by Y. Tsunoda

Density Functional Theory

DFT: Quantum many-body theory

1998 化学賞

W. Kohn
Nobelprize.org

variational principle with respect to the density as a variational parameter

$$\delta\langle \hat{H} - \lambda \hat{Q} \rangle = 0 \;\Rightarrow\; E = E(Q), \quad Q = \langle \hat{Q} \rangle$$

δQ

$$\delta\langle \hat{H} - \sum_k \lambda_k \hat{Q}_k \rangle = 0 \;\Rightarrow\; E = E(Q_k)$$

exact g.s. energy

E_0

$$\delta\langle \hat{H} - \int d\alpha \lambda(\alpha) \hat{Q}(\alpha) \rangle = 0 \;\Rightarrow\; E = E[Q(\alpha)]$$

$$\delta\langle \hat{H} - \int d\vec{x}\, v(\vec{x}) \hat{\rho}(\vec{x}) \rangle = 0 \;\Rightarrow\; E = E[\rho(\vec{x})]$$

$$\hat{\rho}(\vec{x}) = \hat{\psi}^\dagger(\vec{x}) \hat{\psi}(\vec{x})$$

energy density functional

DFT for excitation and dynamics

$$\hat{H}(t) = \hat{T} + \hat{V}(t) + \hat{W}$$

通常の量子力学

$$A(t_1, t_0) \equiv \int_{t_0}^{t_1} dt \langle \Psi(t) | i\partial_t - \hat{H}(t) | \Psi(t) \rangle$$

最小作用 $\frac{\delta A}{\delta \langle \Psi(t) |} = [i\partial_t - \hat{H}(t)] | \Psi(t) \rangle = 0$ ⟺ $| \Psi(t) \rangle$ は時間依存Sch. eqの解

時間依存密度汎関数理論: Time-dependent DFT

E. Runge and E. K. U. Gross, PRL52(1984)997

定理１：状態・作用は密度と初期状態の汎関数

$$| \Psi(t) \rangle = | \Psi[\rho, \Psi_0](t) \rangle$$

$$A = A[\rho, \Psi_0]$$

$$\rho(\vec{r}, t) \Longleftrightarrow v(\vec{r}, t) \Longleftrightarrow \Psi(\vec{r}, t)$$

定理２：密度変分原理

$\frac{\delta A}{\delta \rho(\vec{r}, t)} = 0$ ⟺ $\rho(\vec{r}, t)$ 時間依存Sch. eqの解から作られる密度

DFT for weak-interaction processes

beta-decay $\,^{A}_{Z}A \rightarrow e^- + \bar{\nu}_e + \,^{A}_{Z+1}B^*$

decay rate $d\Gamma = \sum_{\bar{i},f} 2\pi\delta(M_A - \epsilon_e - p_\nu - M_{B^*})\,|\langle f|H_W|i\rangle|^2 \frac{d\vec{p}_\nu d\vec{p}_e}{(2\pi)^6}$

$$\langle f|H_W|i\rangle = \langle B^*|\int d\vec{x}\,\frac{G_F V_{ud}}{\sqrt{2}}[\bar{\psi}_e(\vec{x})\gamma^\mu(1-\gamma_5)v(\vec{p}_\nu)e^{-i\vec{p}_\nu\cdot\vec{x}}]J_\mu(\vec{x})|A\rangle$$

hadronic current

$$J_\mu(x) = \bar{\psi}_{\rm p}(x)[V_\mu^+ - A_\mu^+]\psi_{\rm n}(x)$$

half-life $t = \frac{\ln 2}{\Gamma}$

$$ft = \frac{2\pi^3\hbar^7\ln 2}{m_e^5 c^4 (G_F V_{ud})^2} = \text{const}\,.$$

DFT

nuclear structure information

Linear-response TDDFT

response to the weak external field: $e^{-i\omega t}\hat{F} = e^{-i\omega t}\int d\mathbf{r} f(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$

$$\delta\rho(\mathrm{r},t) \sim \delta\rho(\mathrm{r})e^{-i\omega t} \qquad \delta\rho(\mathbf{r}) = \int d\mathbf{r}'\chi_0(\mathbf{r},\mathbf{r}')\left[\frac{\delta^2 E[\rho]}{\delta^2\rho}\delta\rho(\mathbf{r}') + f(\mathbf{r}')\right]$$

equivalent to

(Quasiparticle)-RPA $\quad v_{\mathrm{res}} = \dfrac{\delta^2 E[\rho]}{\delta^2\rho} \qquad \delta\rho = \dfrac{\chi_0}{1-\chi_0 v_{\mathrm{res}}} f = \chi_{\mathrm{RPA}} f$

transition matrix element : $\langle\Psi_\lambda|\hat{F}|\Psi_0\rangle = \int d\mathbf{r}\delta\rho(\mathbf{r};\omega_\lambda)f(\mathbf{r})$

neutral current:

$$\hat{F} = \sum_{\tau,\tau'} f(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}\tau)\hat{\psi}(\mathbf{r}\tau')\delta_{\tau,\tau'}$$

$$\hat{F} = \sum_{\tau,\tau'} f(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}\tau)\hat{\psi}(\mathbf{r}\tau')\langle\tau|\tau_z|\tau'\rangle$$

like-particle (Q)RPA

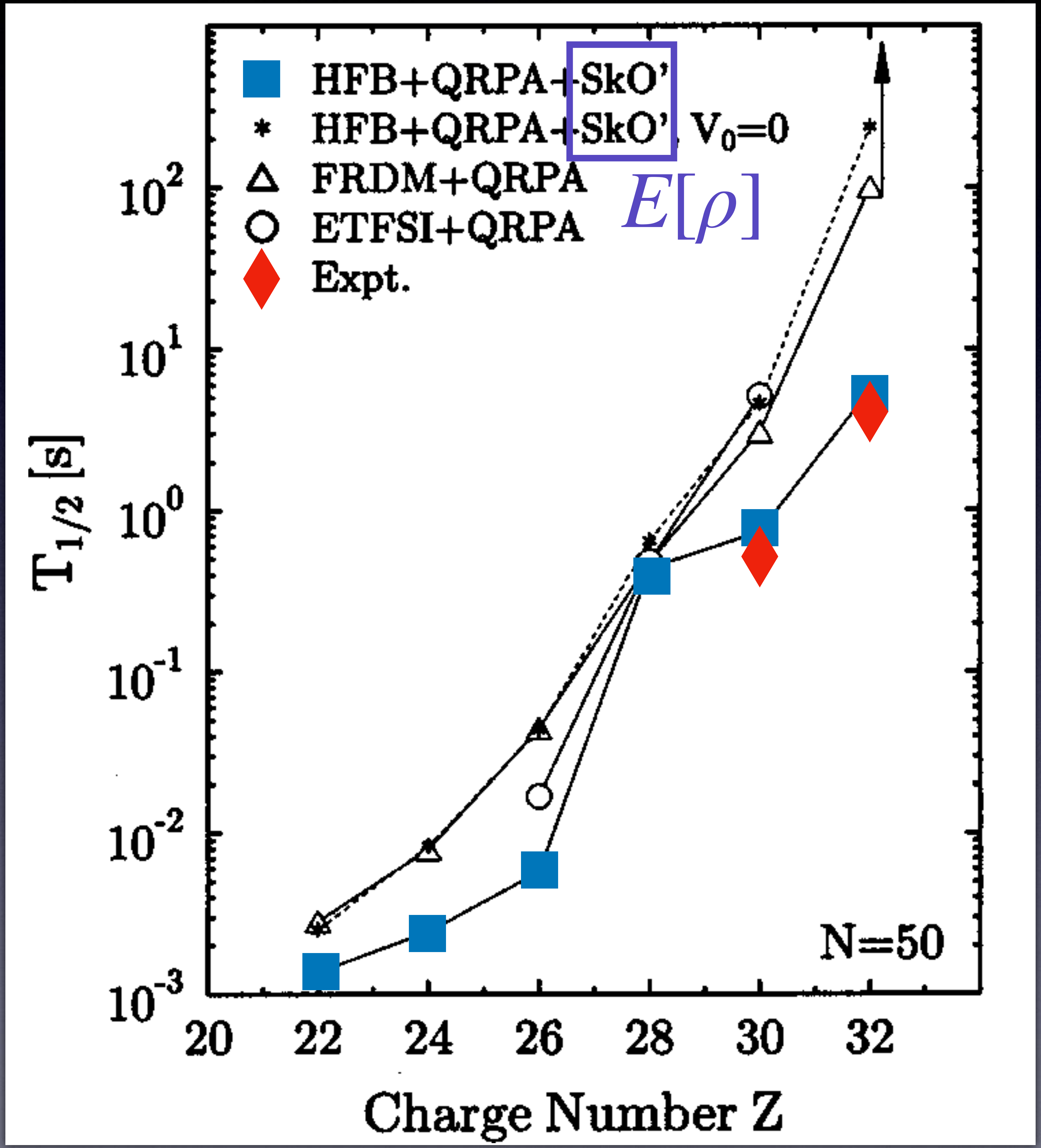
charged current:

$$\hat{F} = \sum_{\tau,\tau'} f(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}\tau)\hat{\psi}(\mathbf{r}\tau')\langle\tau|\tau_\pm|\tau'\rangle$$

proton-neutron (Q)RPA

Pioneering cal.: spherical nuclei

J. Engel *et al.*, PRC60(1999)014302



Hadronic current

$$J_\mu(x) = \bar{\psi}_p(x)[V_\mu^+ - A_\mu^+]\psi_n(x)$$

$$V_\mu^+ = g_V(q^2)\gamma_\mu + \sout{ig_M(q^2)\frac{\sigma_{\mu\nu}}{2m_n}q^\nu}$$

$$A_\mu^+ = g_A(q^2)\gamma_\mu\gamma_5 + \sout{ig_P(q^2)q_\mu\gamma_5}$$

$$g_V(q^2=0) = g_V = 1$$
$$g_A(q^2=0) = g_A \simeq 1.27$$

Fermi (allowed, vector)

$$\hat{F} = \sum_{\sigma,\sigma'} \int d\mathbf{r}\hat{\psi}_\pi^\dagger(\mathbf{r}\sigma)\hat{\psi}_\nu(\mathbf{r}\sigma')\delta_{\sigma,\sigma'}$$

Gamow-Teller (allowed, axial-vector)

$$\hat{F} = \sum_{\sigma,\sigma'} \int d\mathbf{r}\hat{\psi}_\pi^\dagger(\mathbf{r}\sigma)\langle\sigma|\vec{\sigma}|\sigma'\rangle\hat{\psi}_\nu(\mathbf{r}\sigma')$$

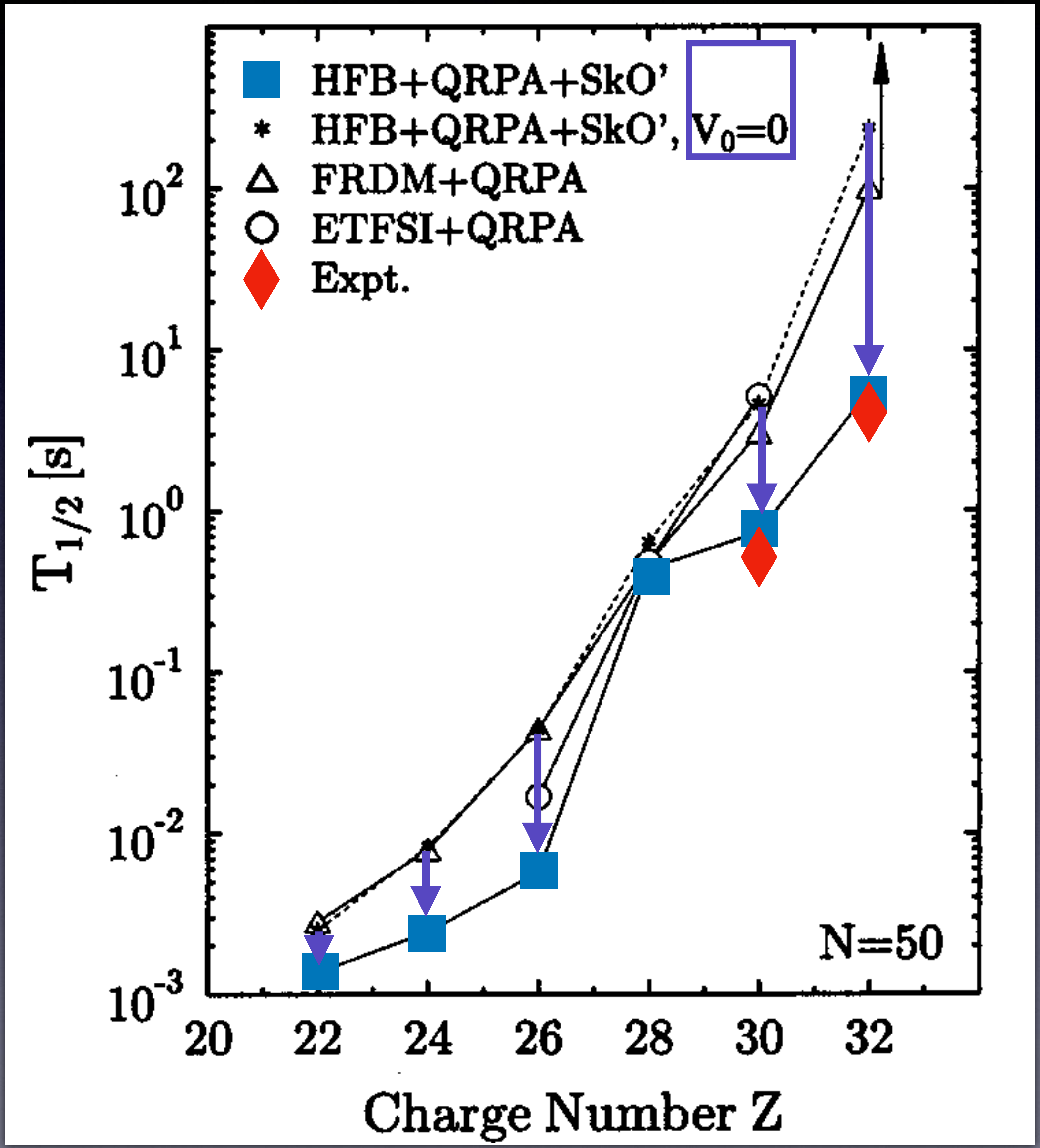
quenching

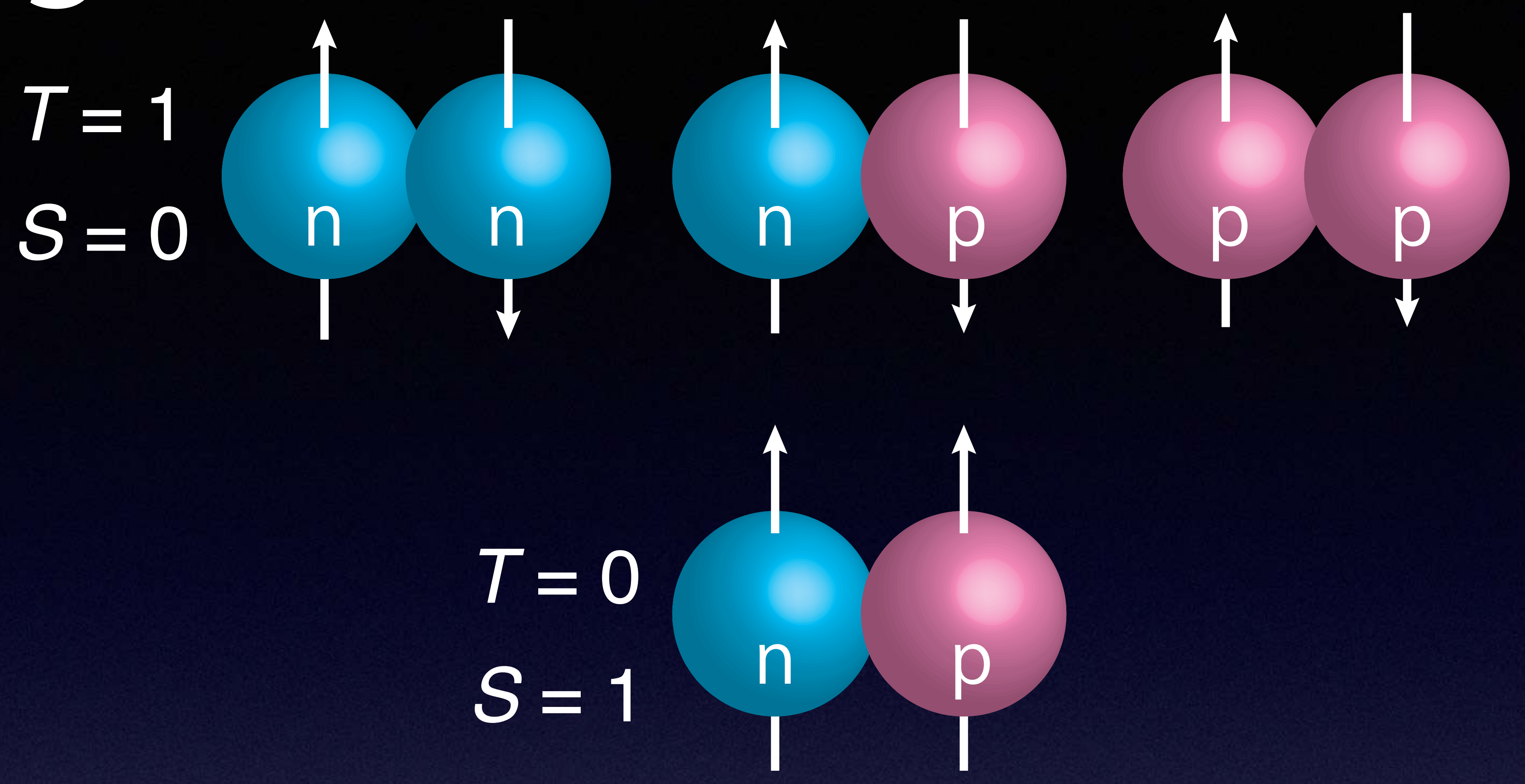
$$g_A^{\text{eff}} = qg_A$$
$$q \sim 0.78$$

non-nucleonic d.o.f.
two-body currents
short-range correlation
truncation of many-body space

Spin-triplet proton-neutron pairing

J. Engel *et al.*, PRC60(1999)014302





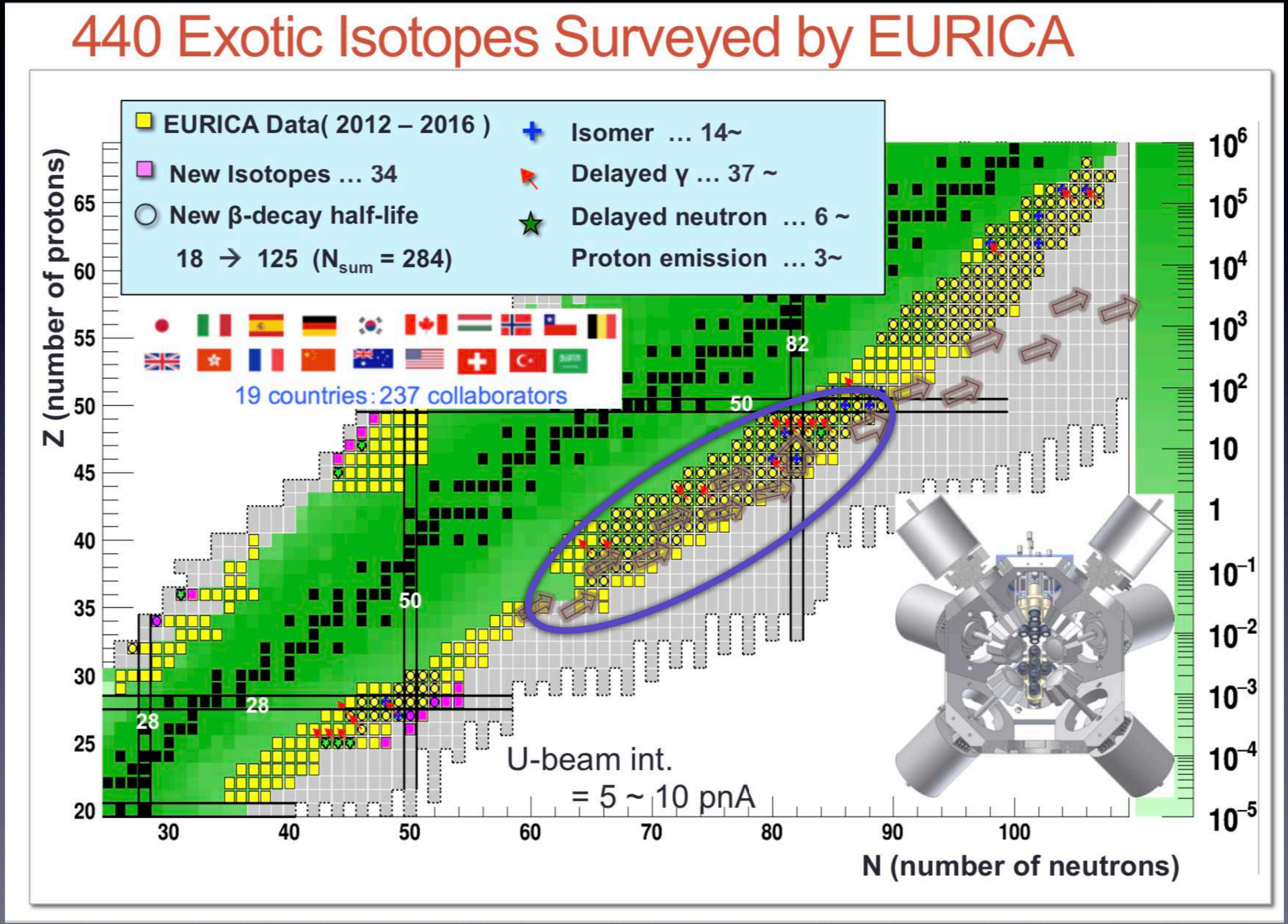
- ✓ being not included in FRDM
- ✓ shortens the half-lives
- ✓ sensitive to the shell structure

has no connection to the g.s. property

how to determine?

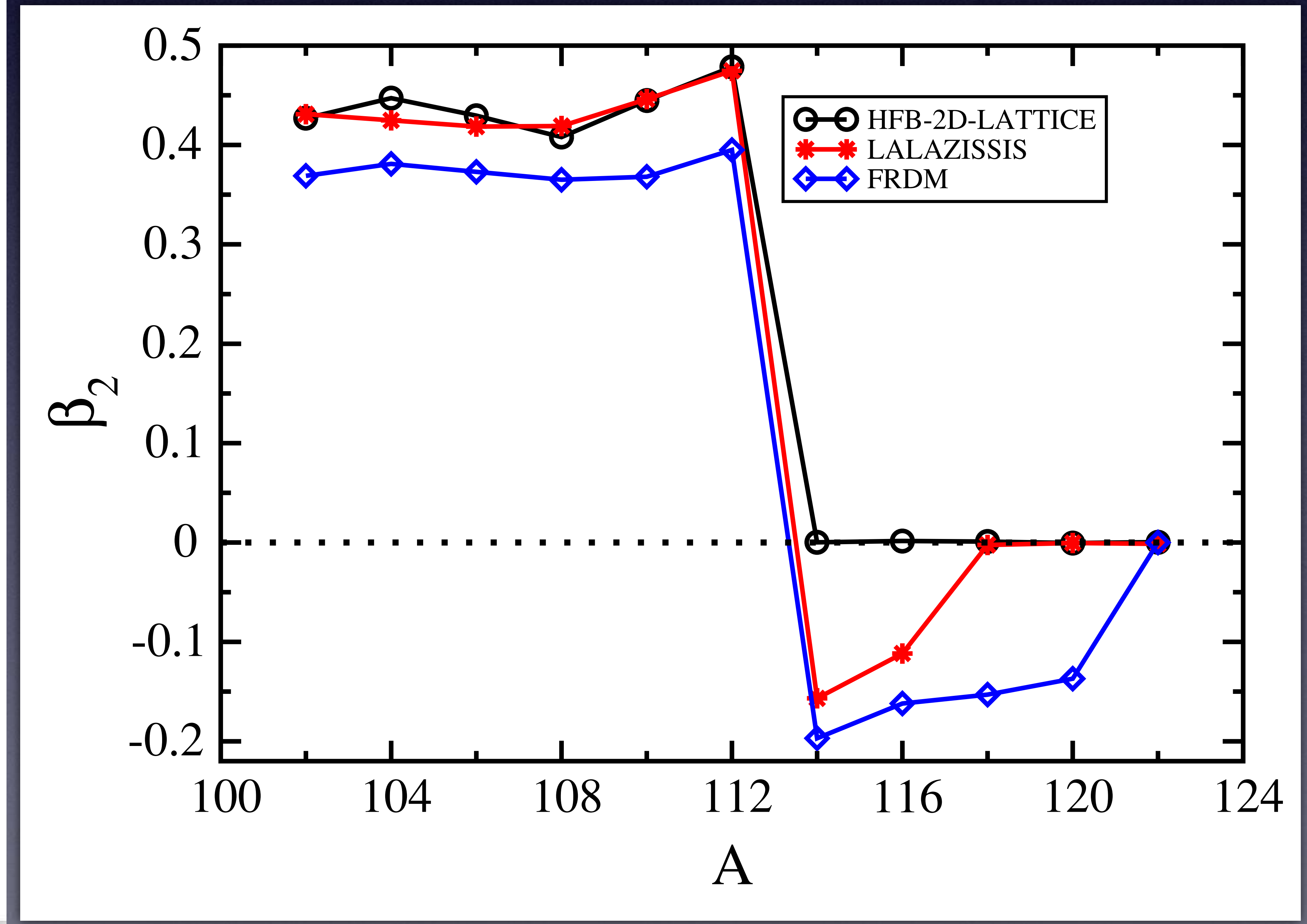
RIBF-experiment stimulating DFT-development

S. Nishimura



β-decay half-lives of r-process nuclei

predicted to be well deformed by DFT cal.



A. Blazkiewicz *et al.*, PRC71(2005)054321

RIBF-experiment stimulating DFT-development

Deformed Kohn-Sham-Bogoliubov-de Gennes: unperturbed ground state

Linear-response charge-exchange TDDFT: nuclear matrix element

PTEP
Prog. Theor. Exp. Phys. **2013**, 113D02 (17 pages)
DOI: 10.1093/ptep/ptt091

Spin–isospin response of deformed neutron-rich nuclei in a self-consistent Skyrme energy-density-functional approach

Kenichi Yoshida*

Matrix QRPA

Skyrme

PHYSICAL REVIEW C **87**, 064302 (2013)

Large-scale calculations of the double-β decay of ^{76}Ge, ^{130}Te, ^{136}Xe, and ^{150}Nd in the deformed self-consistent Skyrme quasiparticle random-phase approximation

M. T. Mustonen[1,2,*] and J. Engel[1,†]

Matrix QRPA

PHYSICAL REVIEW C **90**, 024308 (2014)

Finite-amplitude method for charge-changing transitions in axially deformed nuclei

M. T. Mustonen,[1,*] T. Shafer,[1,†] Z. Zenginerler,[2,‡] and J. Engel[1,§]

FAM-QRPA

PHYSICAL REVIEW C **89**, 044306 (2014)

Gamow-Teller strength in deformed nuclei within the self-consistent charge-exchange quasiparticle random-phase approximation with the Gogny force

M. Martini,[1,2,3] S. Péru,[3] and S. Goriely[1]

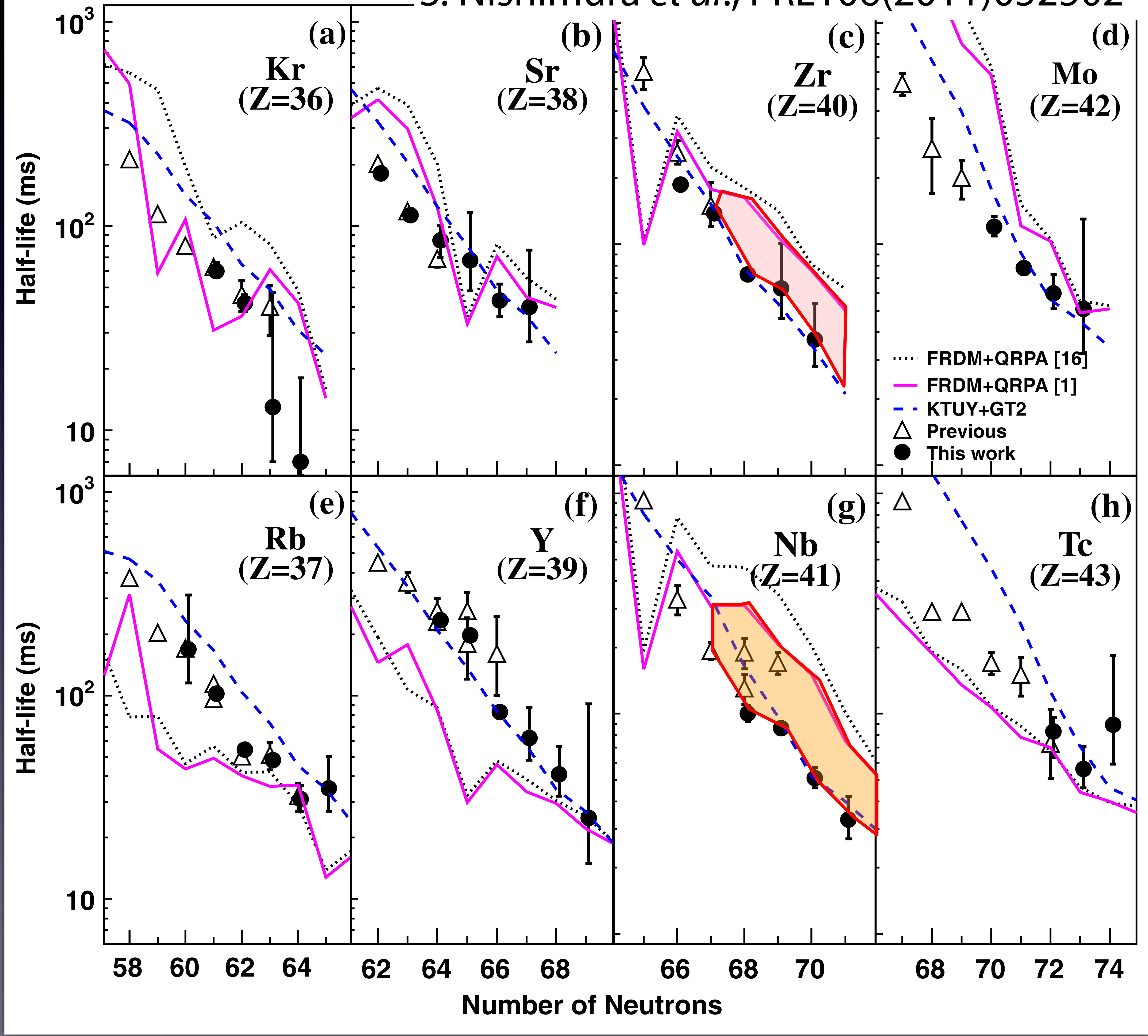
Matrix QRPA

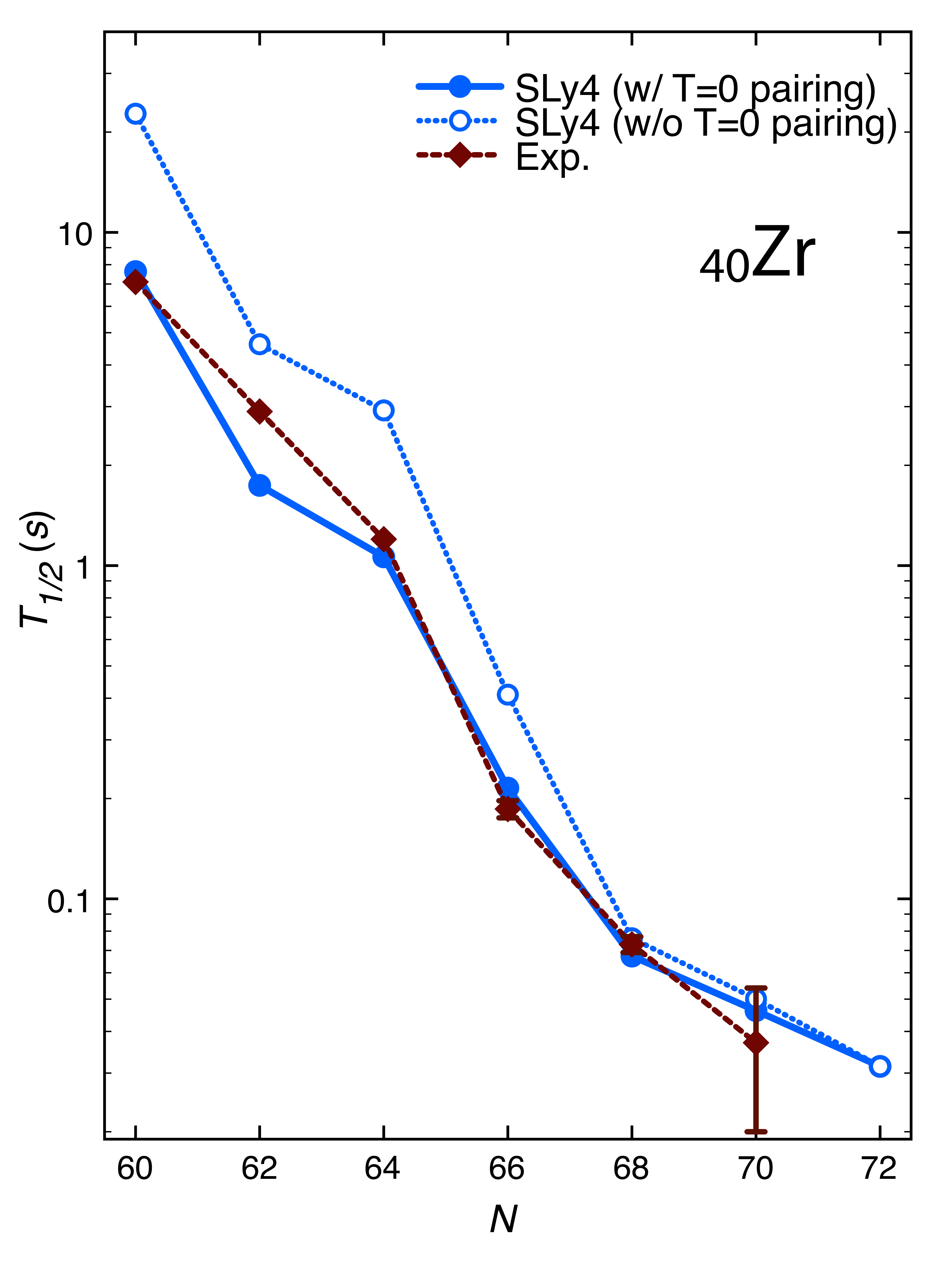
Gogny

Short half-lives found in the Zr region

KY, PTEP(2013)113D02

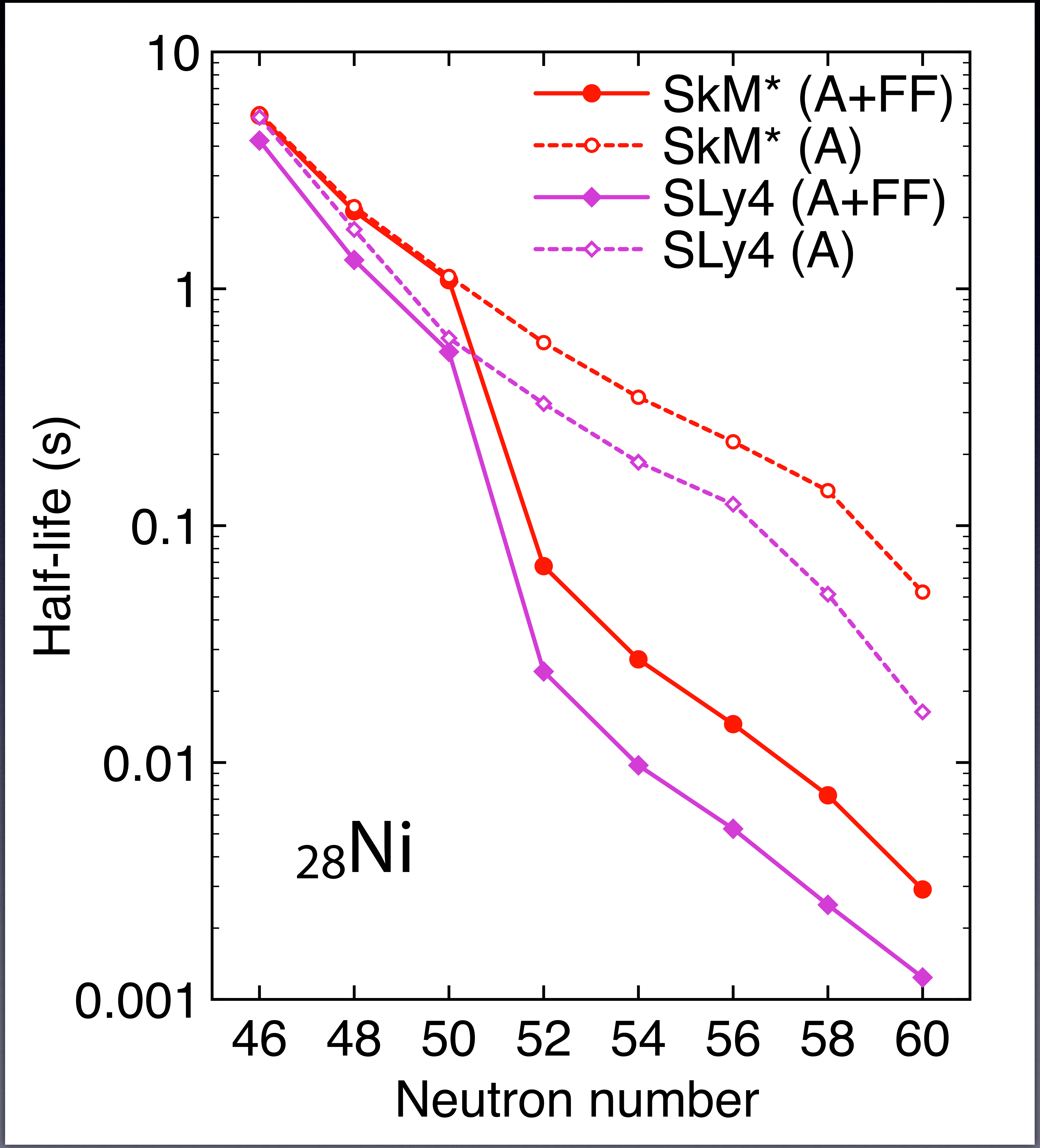
S. Nishimura *et al.*, PRL106(2011)052502



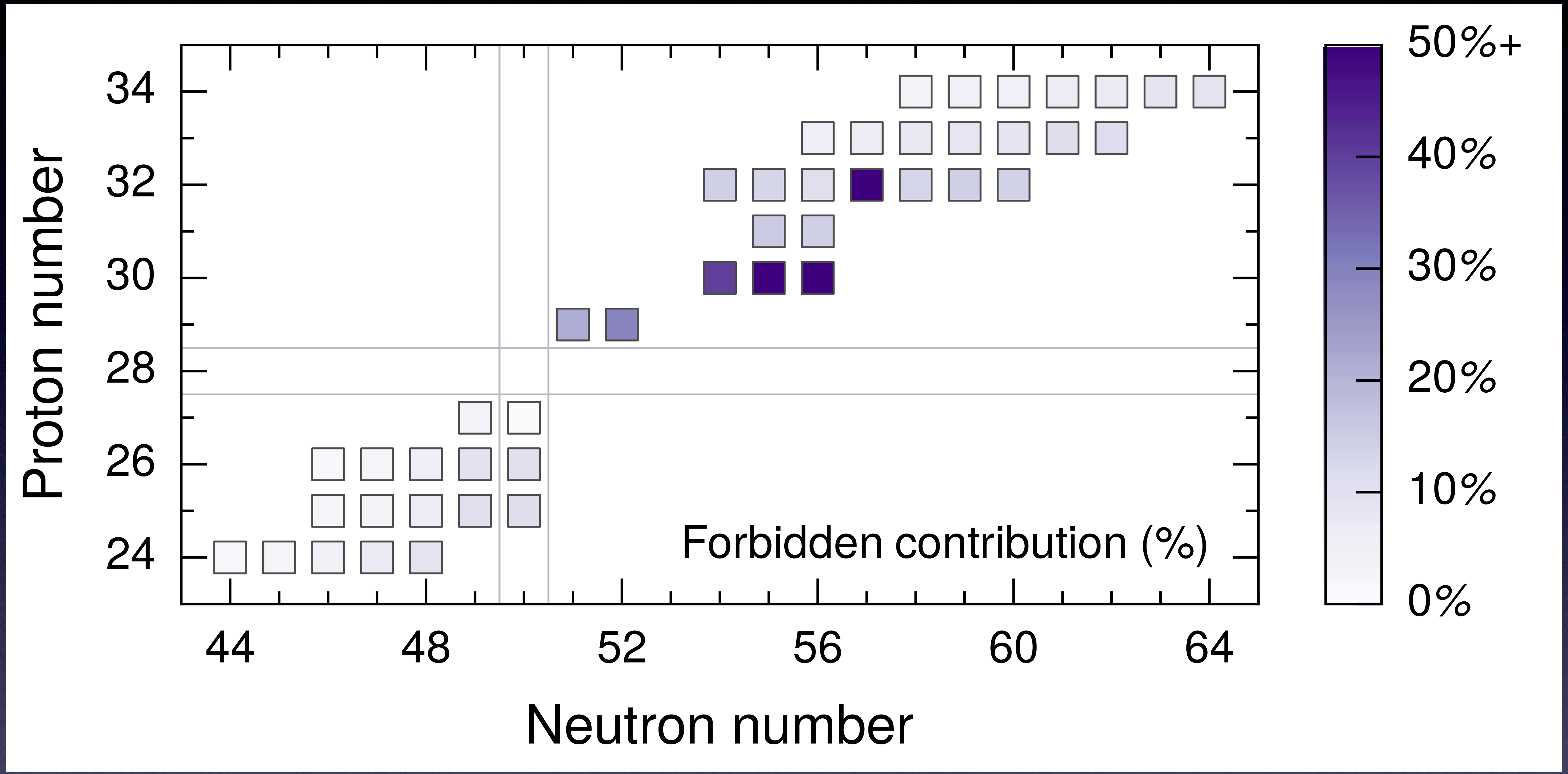


Including the forbidden transitions

KY, arXiv: 1903.03310



T. shafer, J. Engel *et al.*, PRC94(2016)055802

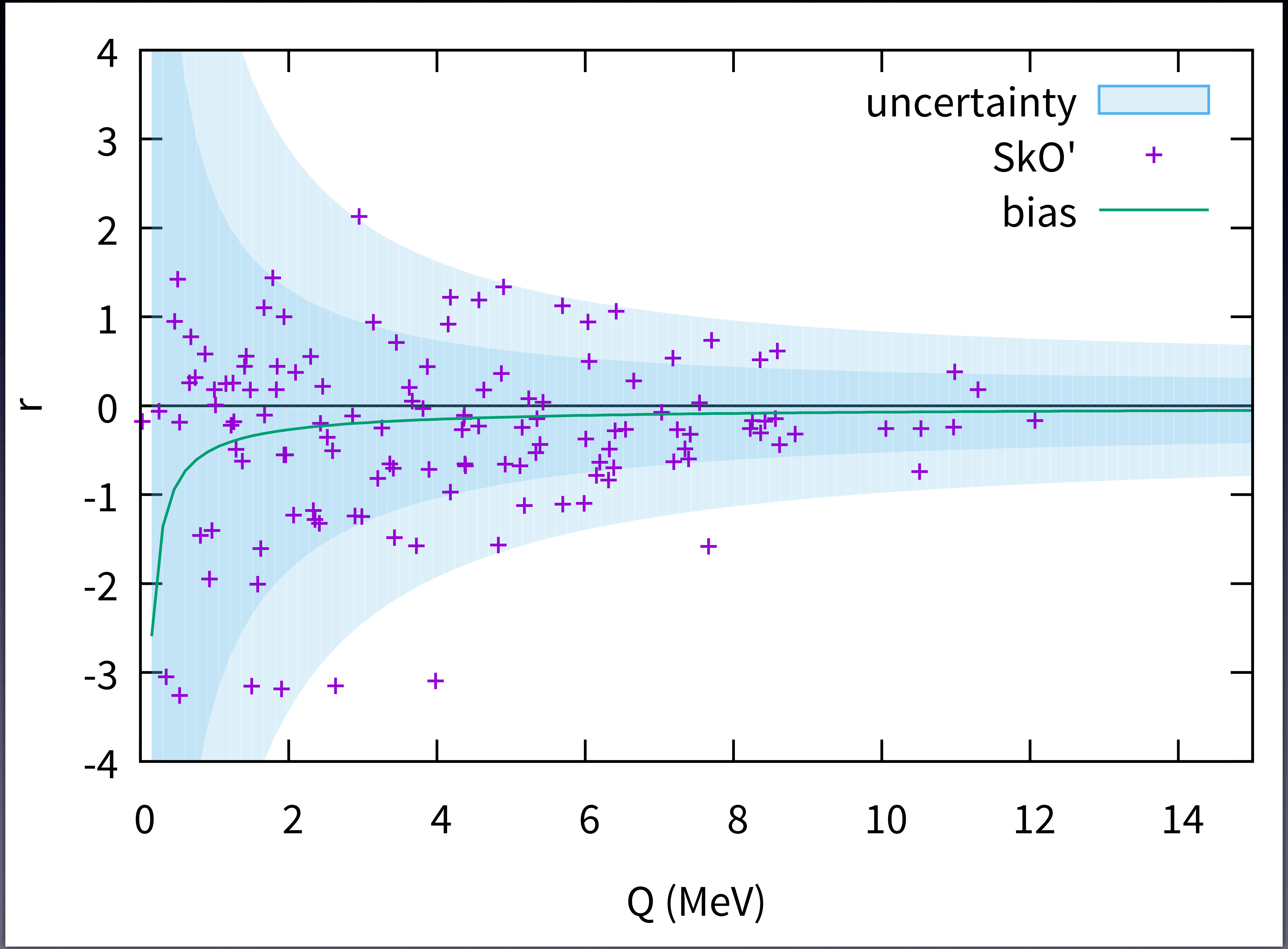


Shell effect (purely quantal!)
determines the β-decay half-life.

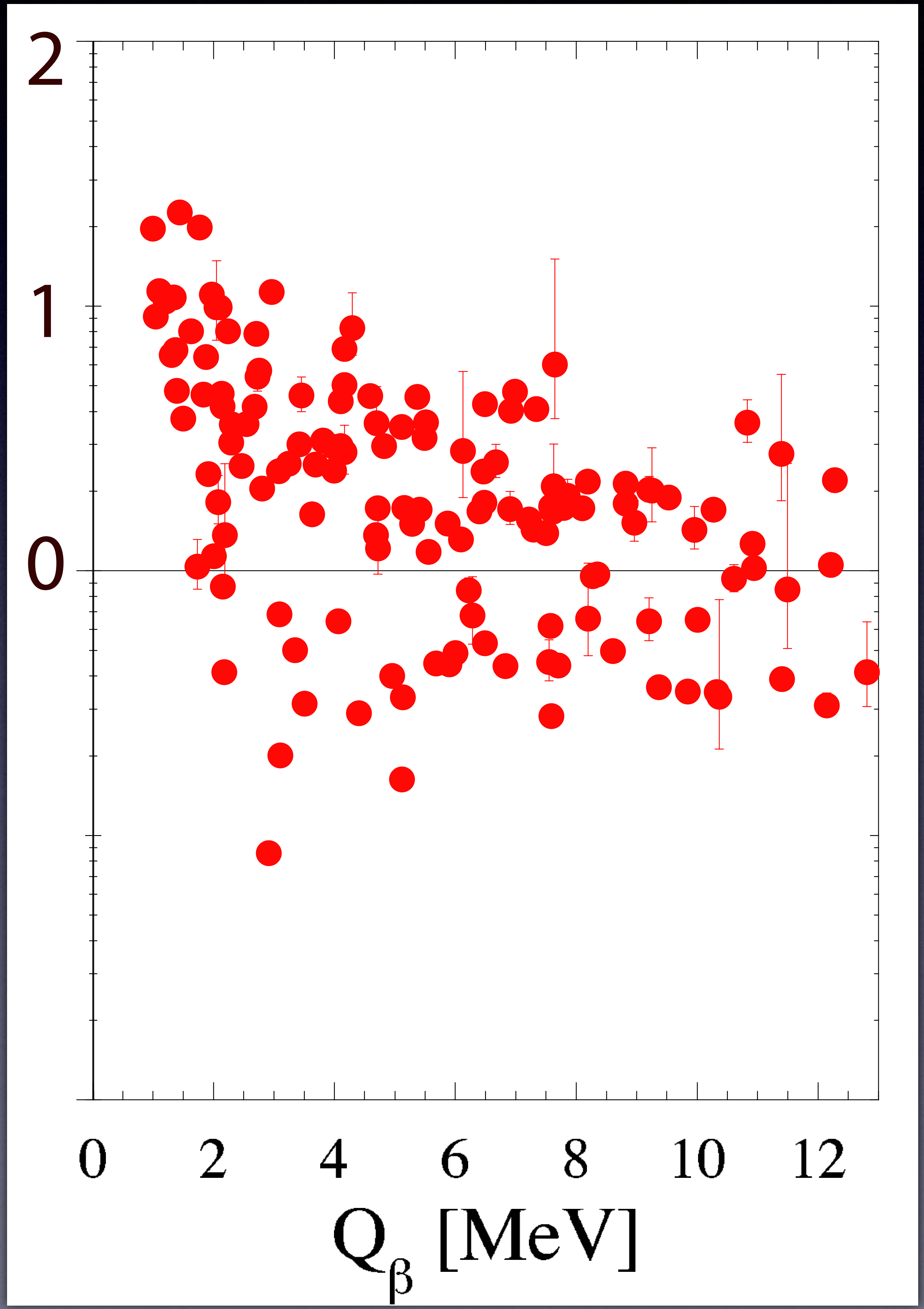
Microscopic approach is necessary.

Theory works better for exotic nuclei: complementary to experiment

$r = T_{\rm cal}/T_{\rm exp}$



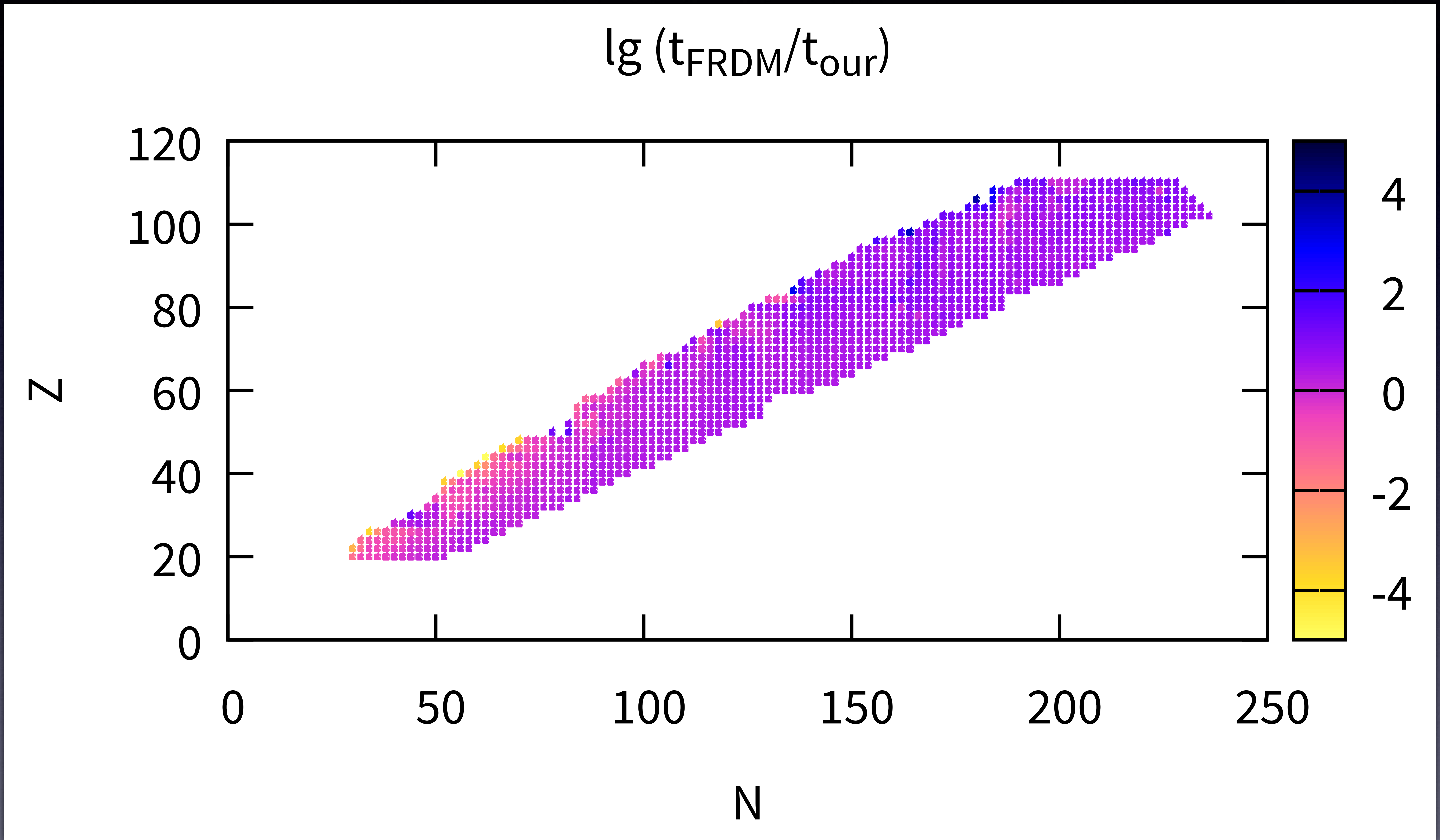
M. T. Mustonen, J. Engel, PRC93(2016)014304



M. Martini *et al.*, PRC89(2014)044306

Global DFT calculation

M. T. Mustonen, J. Engel, PRC93(2016)014304

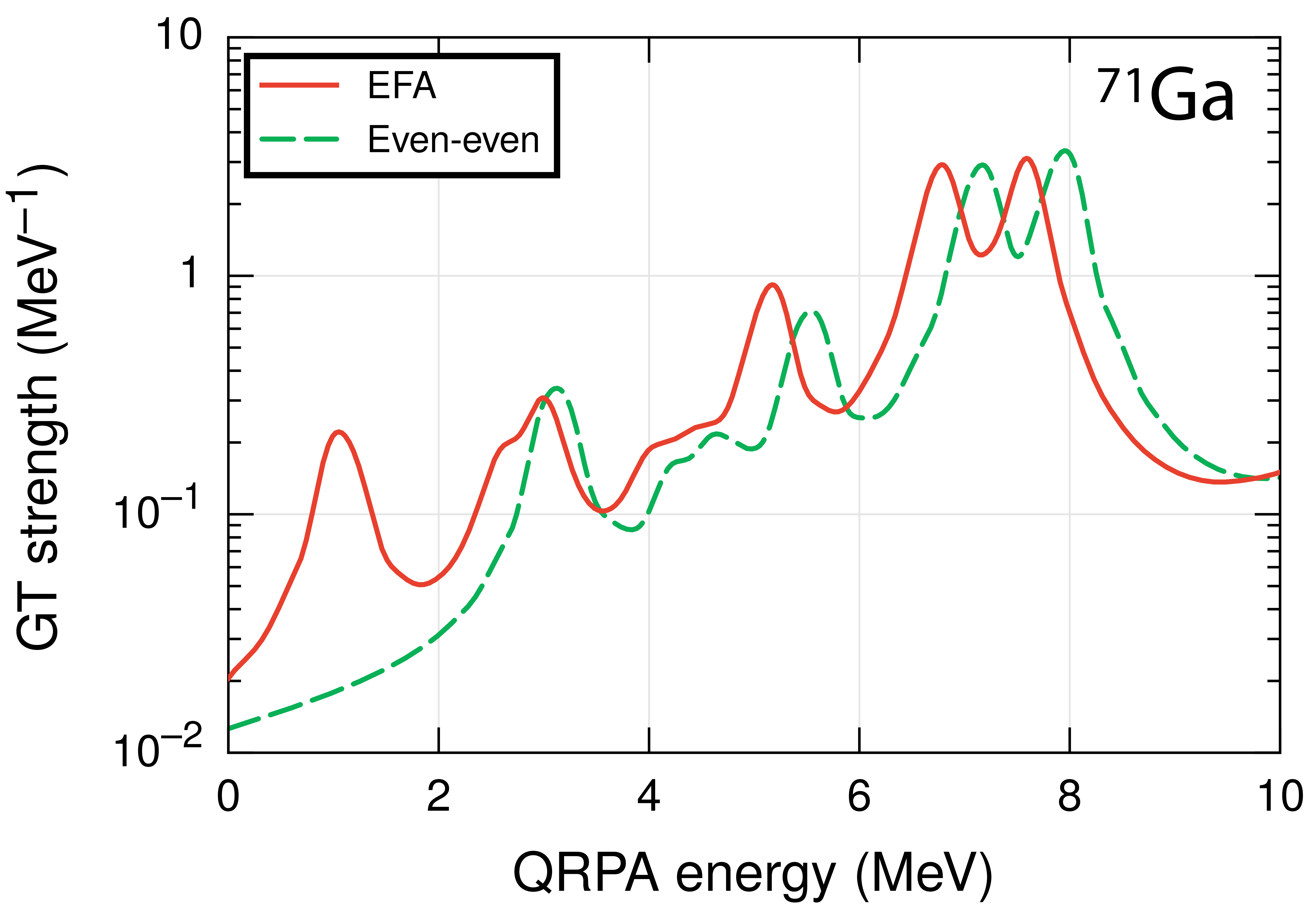


DFT(SkO') gives mostly shorter half-lives than FRDM

lack of calculation for odd-mass and odd-odd nuclei

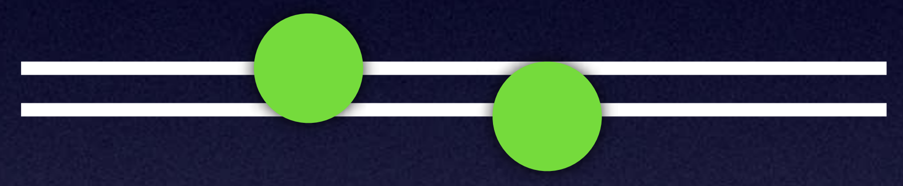
β-decay from odd-mass mothers

T. shafer, J. Engel *et al.*, PRC94(2016)055802



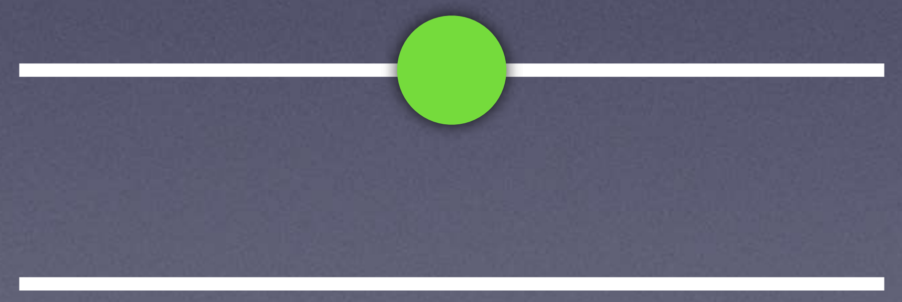
EFA: equal-filling approximation

two "0.5" particles occupy the paired orbitals



Actually, for finite spin,
intrinsic time-reversal sym. is broken

Kramers degeneracy is broken



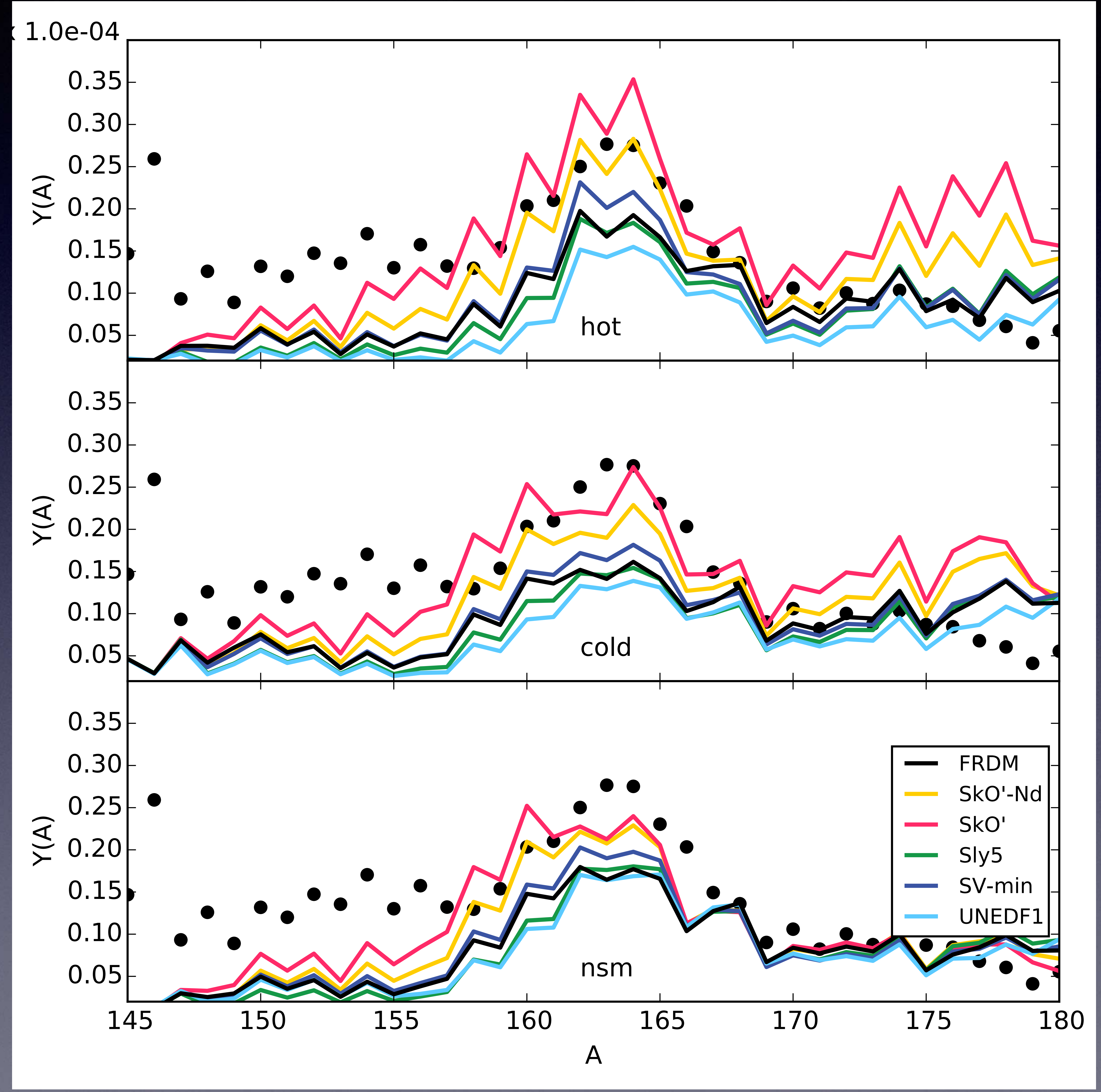
orbital $|\alpha\rangle$

$|\bar{\alpha}\rangle$

one nucleon occupies either orbital

DFT calculation for r-process

T. shafer, J. Engel *et al.*, PRC94(2016)055802



A~150-160

decay-rates affect the distribution

height

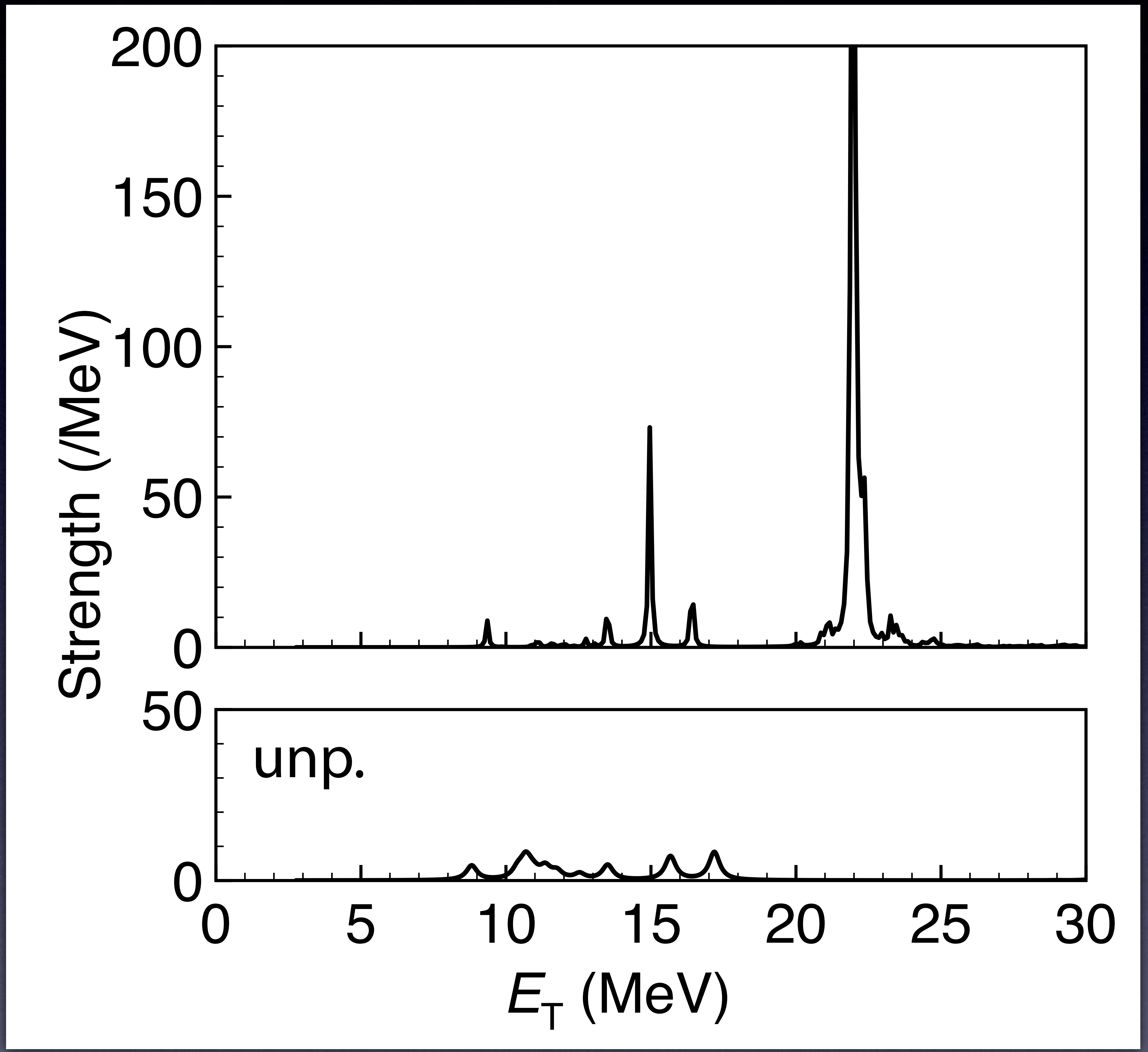
width

toward a systematic calculation

need to control the uncertainty w.r.t. the EDF

Need to go beyond RPA near the magic numbers in particular

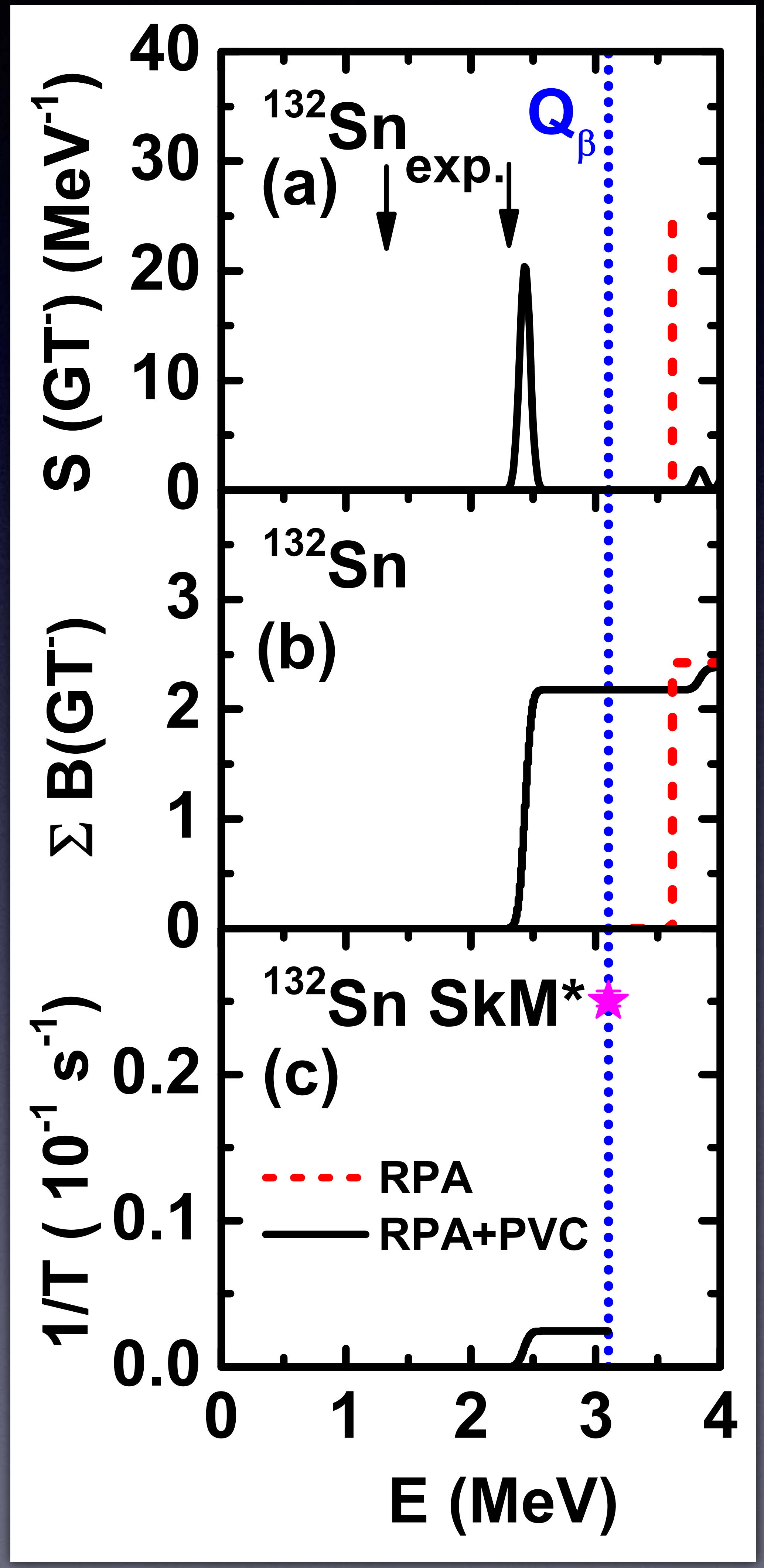
^{208}Pb, SGII



Most of the strengths are gathered in the high-energy giant resonance

tiny low-lying strengths should be described

^{132}Sn spherical and normal-fluid nucleus



RPA
single peak
↓ Phonon coupling
spreading
lowering

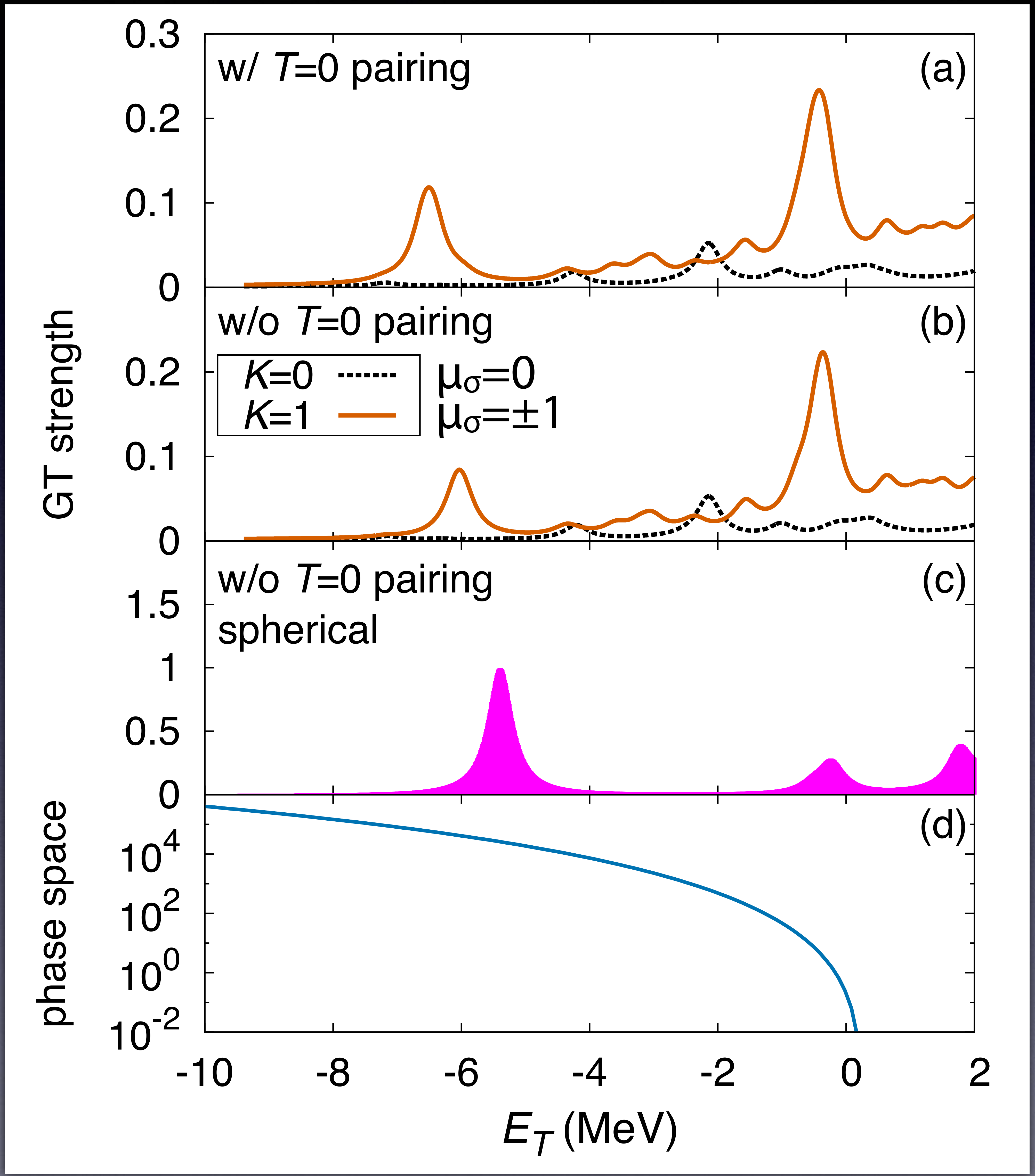
$T_{1/2}$: ∞ → finite

Y. F. Niu *et al.*, PRL114(2015)142501

Pairing and deformation for low-lying GT states

S. Nishimura *et al.*, PRL106(2011)052502

^{106}Zr



KY, JPS Conf. Proc. 6(2015)020017

SLy4

$T_{1/2} = 0.21$ s

$T_{1/2} = 0.41$ s

deformation
superfluidity

$T_{1/2} = 0.07$ s

Exp.

$T_{1/2} = 0.186(11)$ s

β-decay rate is quite sensitive to the details of nuclear structure

Summary and perspectives

Energy density functional: input for DFT cal.

$E[\rho]$ ↓

weak-interaction rate: beta-decay rate,…
nuclear mass, neutron-capture rate, fission dynamics

microscopic construction

quantum many-body method

Systematic and consistent calculation for nuclear data

CPU-less demanding   for a given EDF

Uncertainty quantification