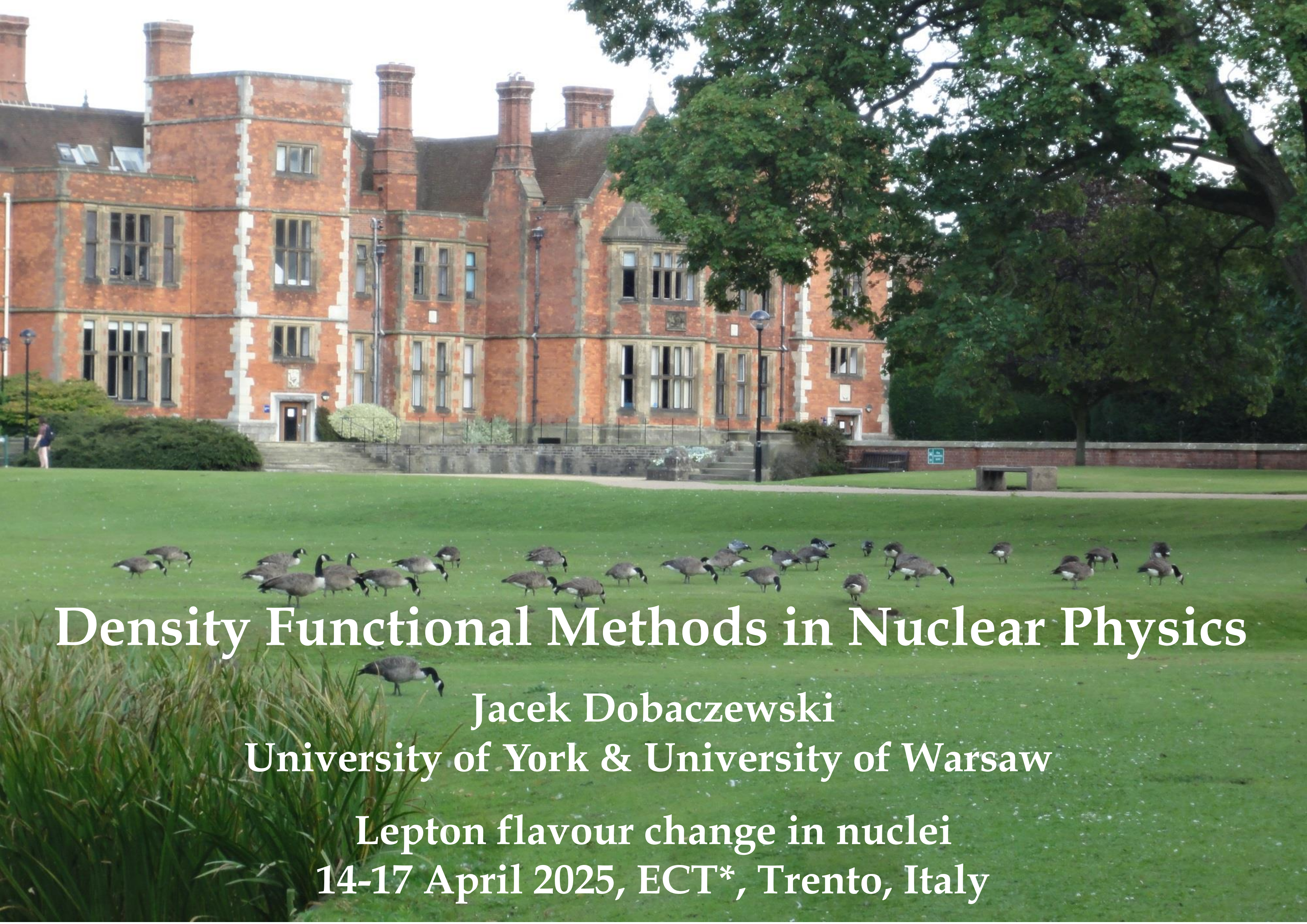

Density Functional Methods in Nuclear Physics

Jacek Dobaczewski
University of York & University of Warsaw

Lepton flavour change in nuclei
14-17 April 2025, ECT*, Trento, Italy

University of York

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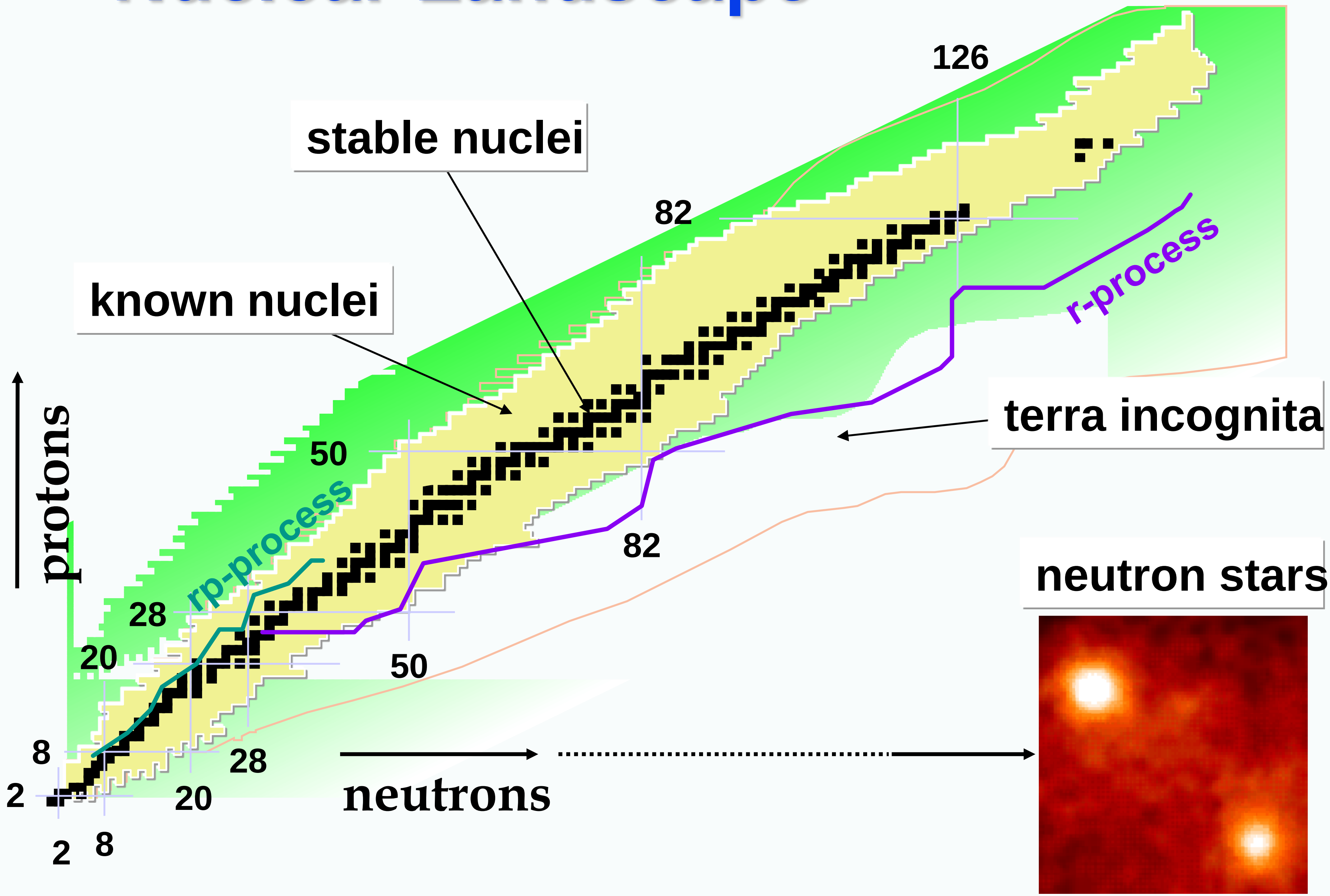
Introduction

Nuclear Landscape



Nuclear Landscape

Lessons learnt

There are only less than 300 stable nuclides in nature (black squares), while already about 3000 other ones have been synthesized and studied in nuclear structure laboratories (yellow zone). However, the nuclear landscape extends further away into uncharted territories (green zone), where probably double of that await discovery. Properties of these exotic systems cannot be at present reliably derived from theoretical models, because our knowledge of basic ingredients thereof is still quite rudimentary. Derivations form first principles allow us already now to recognize general features of nuclear forces, energy-density functionals, or shell-model interactions, however, plenty of these features require careful adjustment to precise nuclear data. Such adjustments, especially when performed for exotic, extreme systems, provide invaluable information, and then in turn allow for more reliable extrapolations.

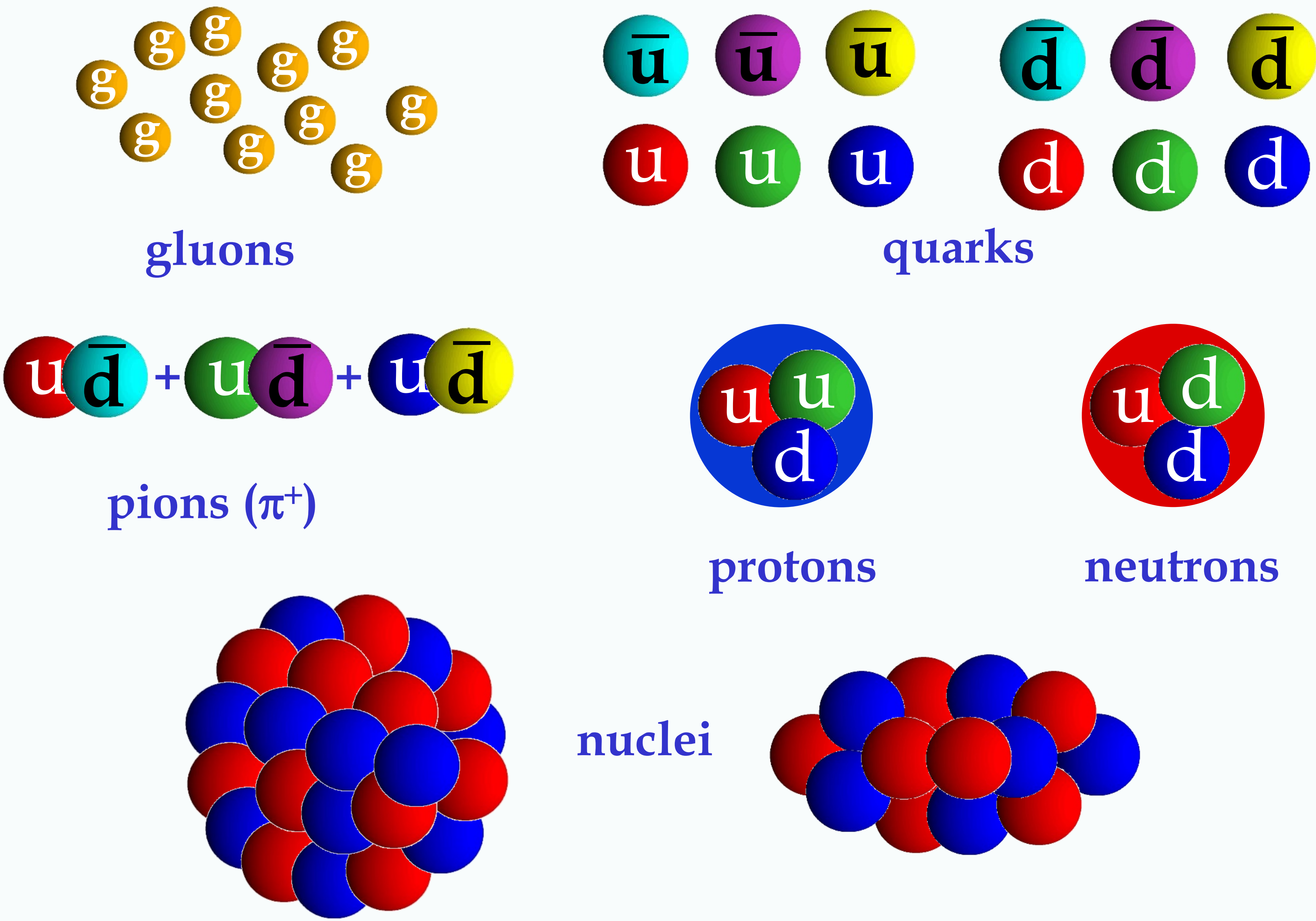
Contents:

1. Fundamentals. QCD and all that in 3 slides
2. Nuclear energy density functionals, 7 slides
3. Spontaneous symmetry breaking, 10 slides
    - Doubly symmetric potential well
    - Parity – NH_3 molecule
    - Nuclear deformations
4. What do the energy density functionals give us?
5. Muon-nucleus coupling, a project, 4 slides

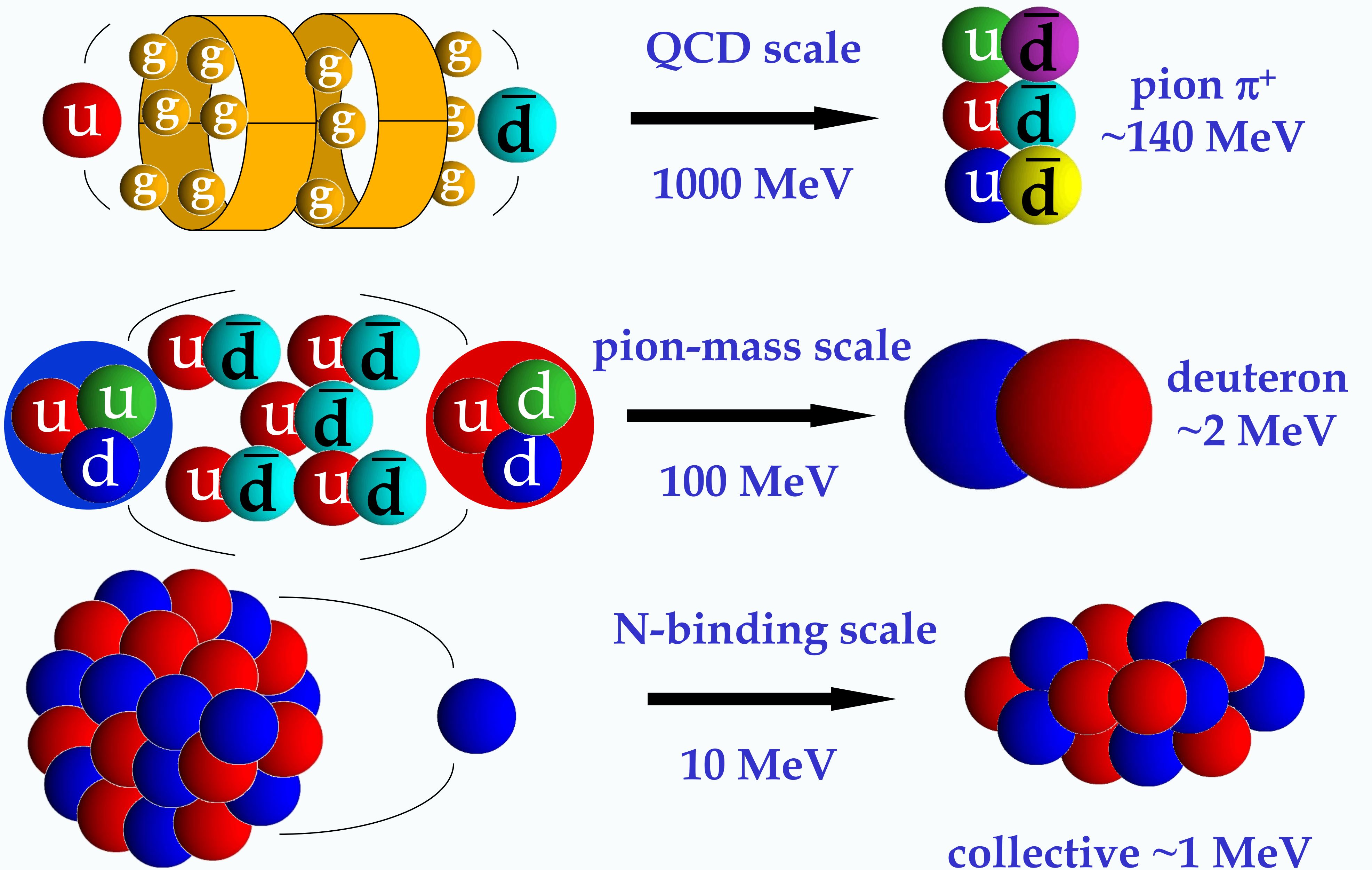
Home page: http://www.fuw.edu.pl/~dobaczew/

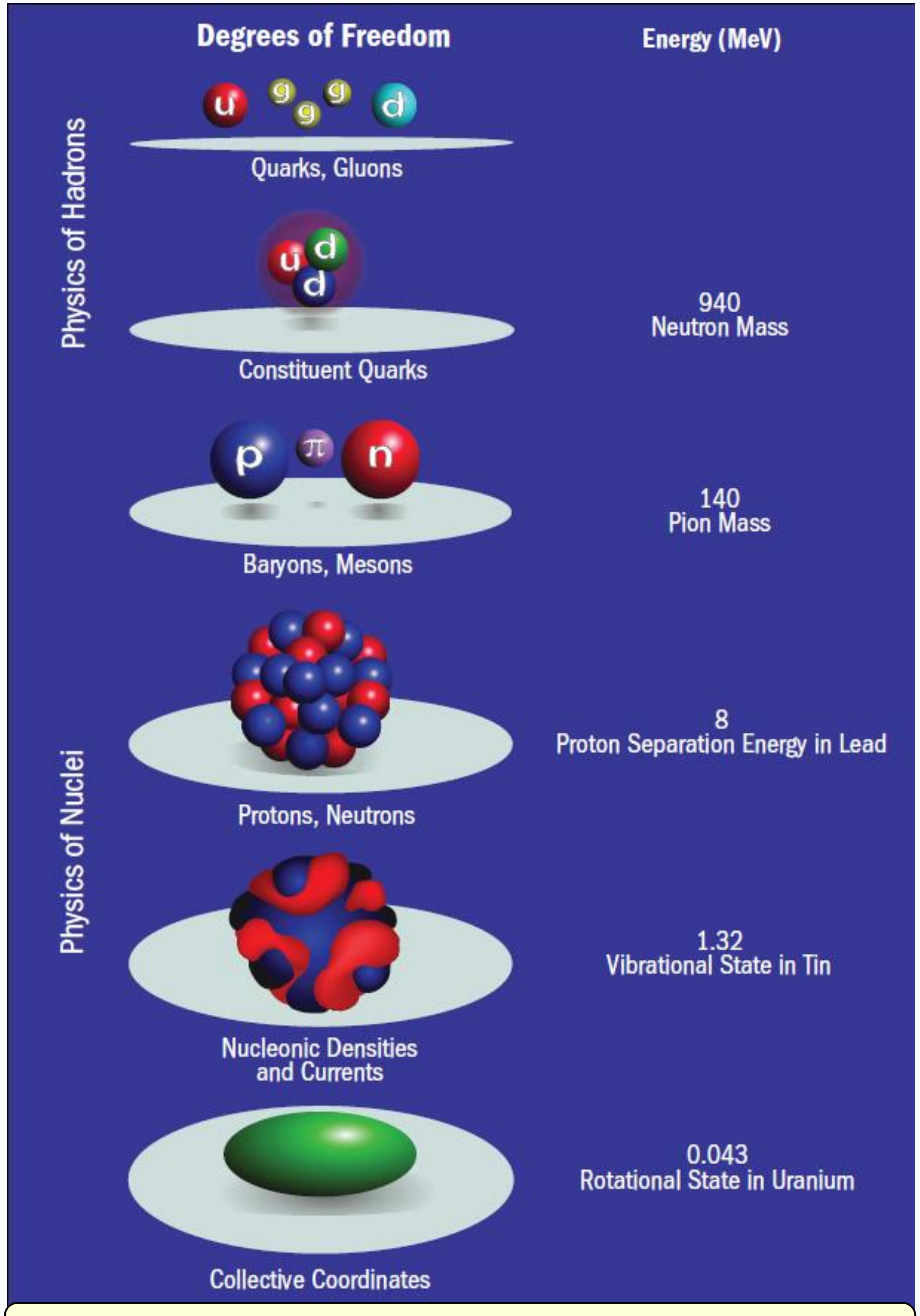
Fundamentals

Main players in Nuclear Physics



Scales of energy in Nuclear Physics





G.F. Bertsch, *et al.*, Scidac Review 6, 42 (2007)

- An effective theory (ET) is a theory which "effectively" captures what is physically relevant in a given domain.
- The most appropriate description of particle interactions in the language of quantum field theory (QFT) depends on the energy at which the interactions are studied.
- Objective reductionism (Weinberg): the convergence of arrows of scientific explanation.
- Emergence (Anderson): "at each new level of complexity entirely new properties appear and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other".

Elena Castellani, physics/0101039

Nuclear energy density functionals

Rayleigh-Ritz Variational Principle

$$\hat{H}|\Psi_i\rangle = E_i|\Psi_i\rangle$$

$$\Downarrow$$

$$|\Psi\rangle = a_0|\Psi_0\rangle + a_1|\Psi_1\rangle + a_2|\Psi_2\rangle + \ldots$$

$$\langle\Psi|\hat{H}|\Psi\rangle = E_0|a_0|^2 + E_1|a_1|^2 + E_2|a_2|^2 + \ldots$$

$$\Downarrow$$

$$\min_{a_0,a_1,a_2\ldots} \langle\Psi|\hat{H}|\Psi\rangle = E_0 \quad \Longleftarrow$$

Rayleigh-Ritz variational principle

$$\Downarrow$$

$$\min_{\alpha} \langle\Phi(\alpha)|\hat{H}|\Phi(\alpha)\rangle = E_0^{\text{var}} \geq E_0 \quad \Longleftarrow$$

variational approximation

What is DFT?

Density Functional Theory:

A variational method that uses observables as variational parameters.

$$\delta\langle\hat{H} - \lambda\hat{Q}\rangle = 0$$
$$\Downarrow$$
$$E = E(Q)$$

for $E(\lambda) \equiv \langle\hat{H}\rangle$ and $Q(\lambda) \equiv \langle\hat{Q}\rangle$

J. D., J. Phys.: Conf. Ser. 312, 092002 (2011)

What is the DFT good for?

$$\delta\langle\hat{H} - \lambda\hat{Q}\rangle = 0$$
$$\Downarrow$$
$$E = E(Q)$$

Energy E is a function(al) of Q

1) **Exact:** Minimization of E(Q) gives the exact E and exact Q
2) **Impractical:** Derivation of E(Q) requires the full variation δ (bigger effort than to find the exact ground state)
3) **Inspirational:** Can we build useful models E′(Q) of the exact E(Q)?
4) **Experiment-driven:** E′(Q) works better or worse depending on the physical input used to build it.

Which DFT?

$$\delta\langle\hat{H}-\lambda\hat{Q}\rangle=0 \implies E=E(Q)$$

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

$$\delta\langle\hat{H}-\int\mathrm{d}q\,\lambda(q)\hat{Q}(q)\rangle=0 \implies E=E[Q(q)]$$

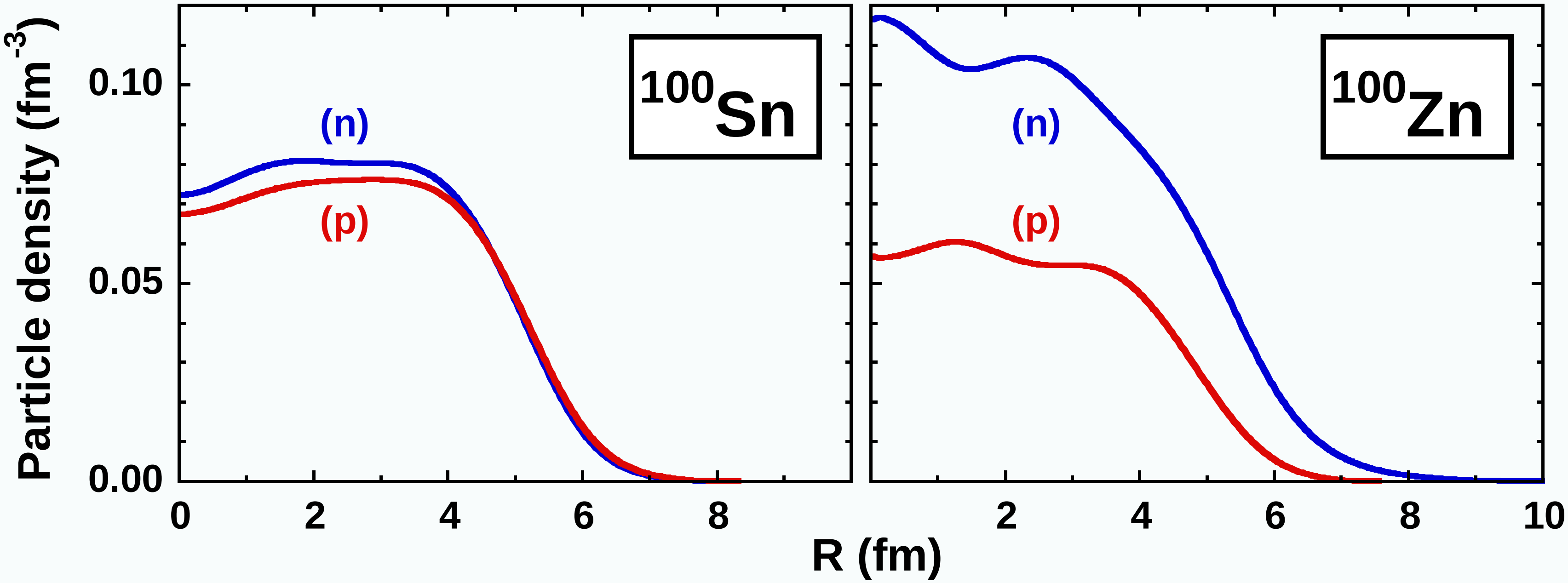
$$\delta\langle\hat{H}-\int\mathrm{d}\vec{r}\,\lambda(\vec{r})\hat{\rho}(\vec{r})\rangle=0 \implies E=E[\rho(\vec{r})]$$

$$\text{for}\quad\hat{\rho}(\vec{r}) \;=\; \textstyle\sum_{i=1}^{A}\delta(\vec{r}-\vec{r}_i)$$

$$\delta\langle\hat{H}-\int\!\!\int\mathrm{d}\vec{r}\mathrm{d}\vec{r}\,'\,\lambda(\vec{r},\vec{r}\,')\hat{\rho}(\vec{r},\vec{r}\,')\rangle=0 \implies E=E[\rho(\vec{r},\vec{r}\,')]$$

J. D., J. Phys.: Conf. Ser. 312, 092002 (2011)

Nuclear densities as composite fields



Modern Mean-Field Theory ≡ Energy Density Functional

ρ, τ, $\overleftrightarrow{J}$, $\vec{j}$, $\vec{T}$, $\vec{s}$, $\vec{F}$,

- Hohenberg-Kohn
- Kohn-Sham
- Negele-Vautherin
- Landau-Migdal
- Nilsson-Strutinsky

mean field ⇒ one-body densities

zero range ⇒ local densities

finite range ⇒ non-local densities

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Nuclear densities as composite fields

Density matrix:

$$\rho(\vec{r}\sigma,\vec{r}'\sigma') = \langle\Phi|a^+(\vec{r}'\sigma')a(\vec{r}\sigma)|\Phi\rangle$$

Scalar and vector part:

$$\begin{aligned}\rho(\vec{r},\vec{r}') &= \sum_\sigma \rho(\vec{r}\sigma,\vec{r}'\sigma)\\ \vec{s}(\vec{r},\vec{r}') &= \sum_{\sigma\sigma'} \rho(\vec{r}\sigma,\vec{r}'\sigma')\langle\sigma'|\vec{\sigma}|\sigma\rangle\end{aligned}$$

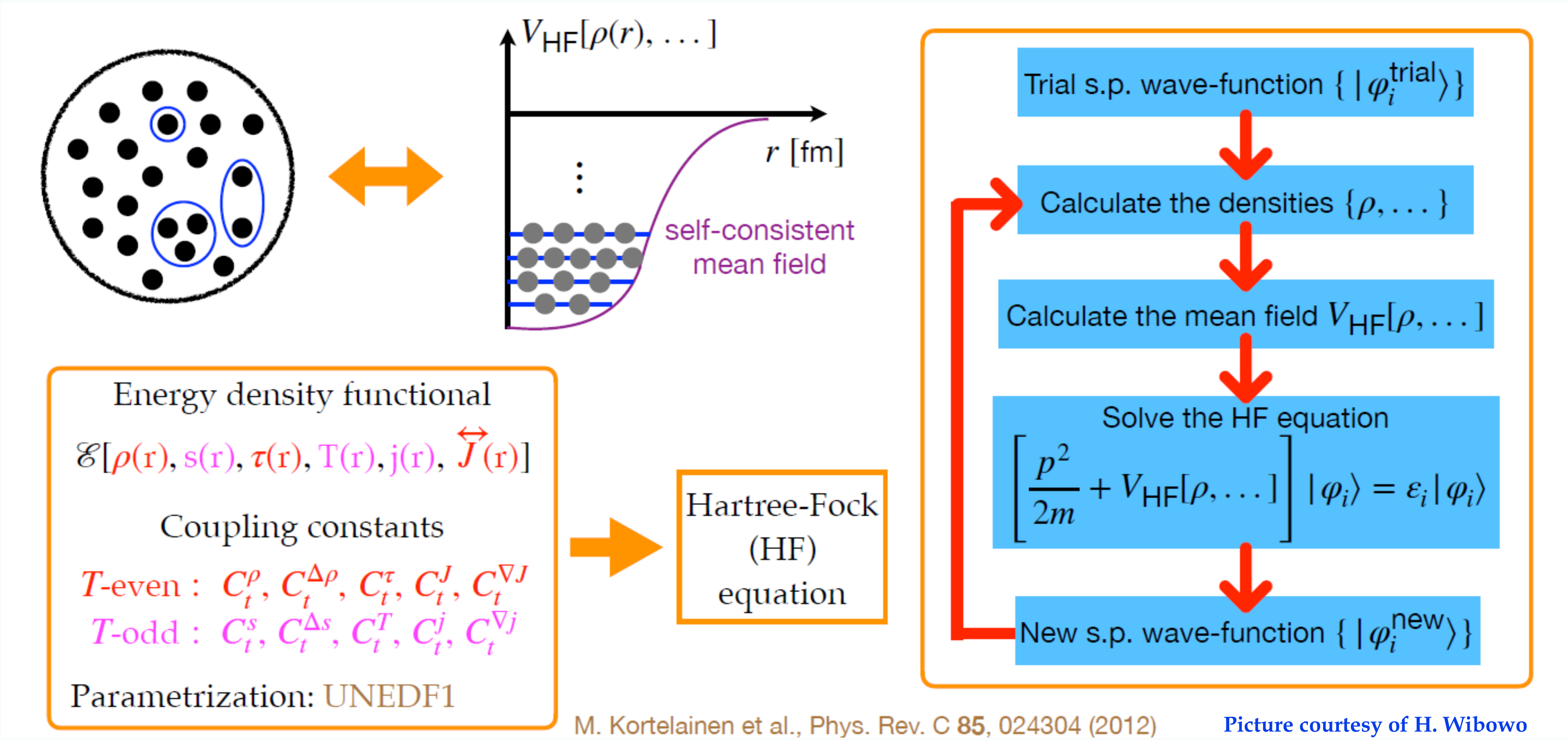
Symmetries:

$$\begin{aligned}\rho^T(\vec{r},\vec{r}') &= \rho^*(\vec{r},\vec{r}') &= \rho(\vec{r}',\vec{r})\\ \vec{s}^T(\vec{r},\vec{r}') &= -\vec{s}^*(\vec{r},\vec{r}') &= -\vec{s}(\vec{r}',\vec{r})\end{aligned}$$

Local densities:

Matter:	$\rho(\vec{r}) = \rho(\vec{r},\vec{r})$
Momentum:	$\vec{j}(\vec{r}) = (1/2i)[(\vec{\nabla}-\vec{\nabla}')\rho(\vec{r},\vec{r}')]_{r=r'}$
Kinetic:	$\tau(\vec{r}) = [\vec{\nabla}\cdot\vec{\nabla}'\rho(\vec{r},\vec{r}')]_{r=r'}$
Spin:	$\vec{s}(\vec{r}) = \vec{s}(\vec{r},\vec{r})$
Spin momentum:	$J_{\mu\nu}(\vec{r}) = (1/2i)[(\nabla_\mu-\nabla'_\mu)s_\nu(\vec{r},\vec{r}')]_{r=r'}$
Spin kinetic:	$\vec{T}(\vec{r}) = [\vec{\nabla}\cdot\vec{\nabla}'\vec{s}(\vec{r},\vec{r}')]_{r=r'}$
Tensor kinetic:	$\vec{F}(\vec{r}) = \frac{1}{2}[(\vec{\nabla}\otimes\vec{\nabla}'+\vec{\nabla}'\otimes\vec{\nabla})\cdot\vec{s}(\vec{r},\vec{r}')]_{r=r'}$

Nuclear density functional theory

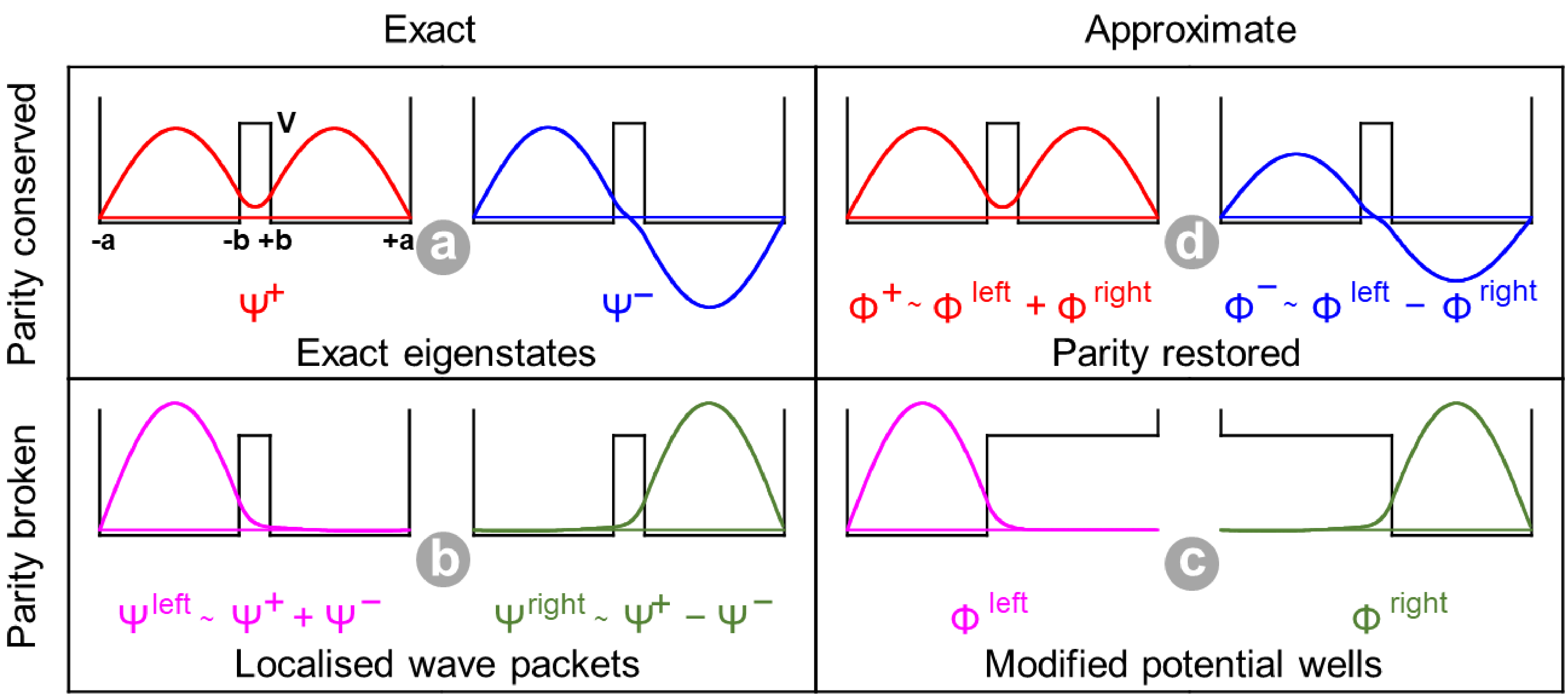


Self-consistent equations are solved iteratively, which includes the polarization effects summed up to all orders without recurring to the lowest order perturbative coupling.

Spontaneous symmetry breaking

Doubly symmetric potential well

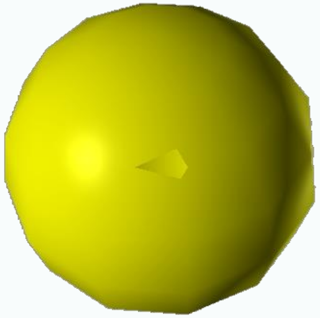
Symmetry breaking → Symmetry restoration



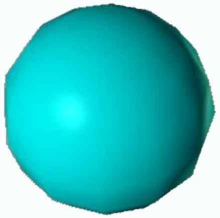
J. A. Sheikh et al., J. Phys. G48, 123001 (2021)

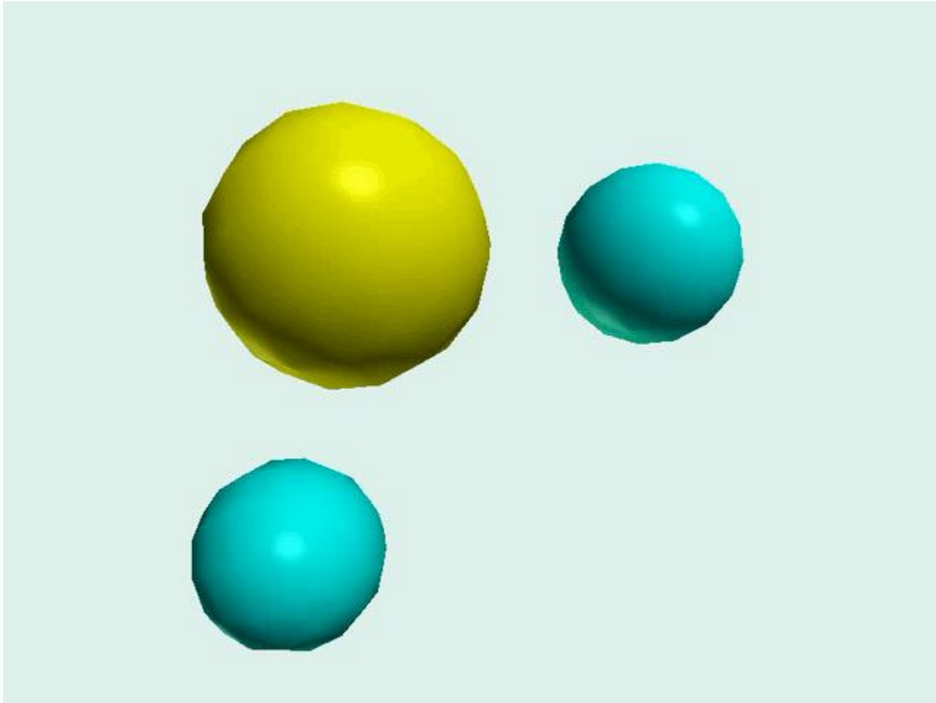
Ammonia molecule NH_3

Nitrogen atom

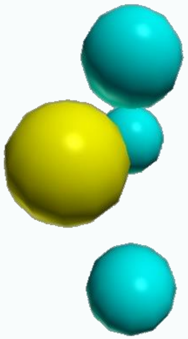


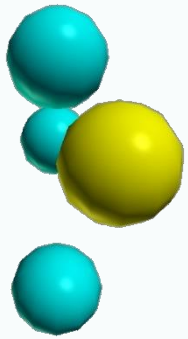
Hydrogen atom





$$|L\rangle =$$



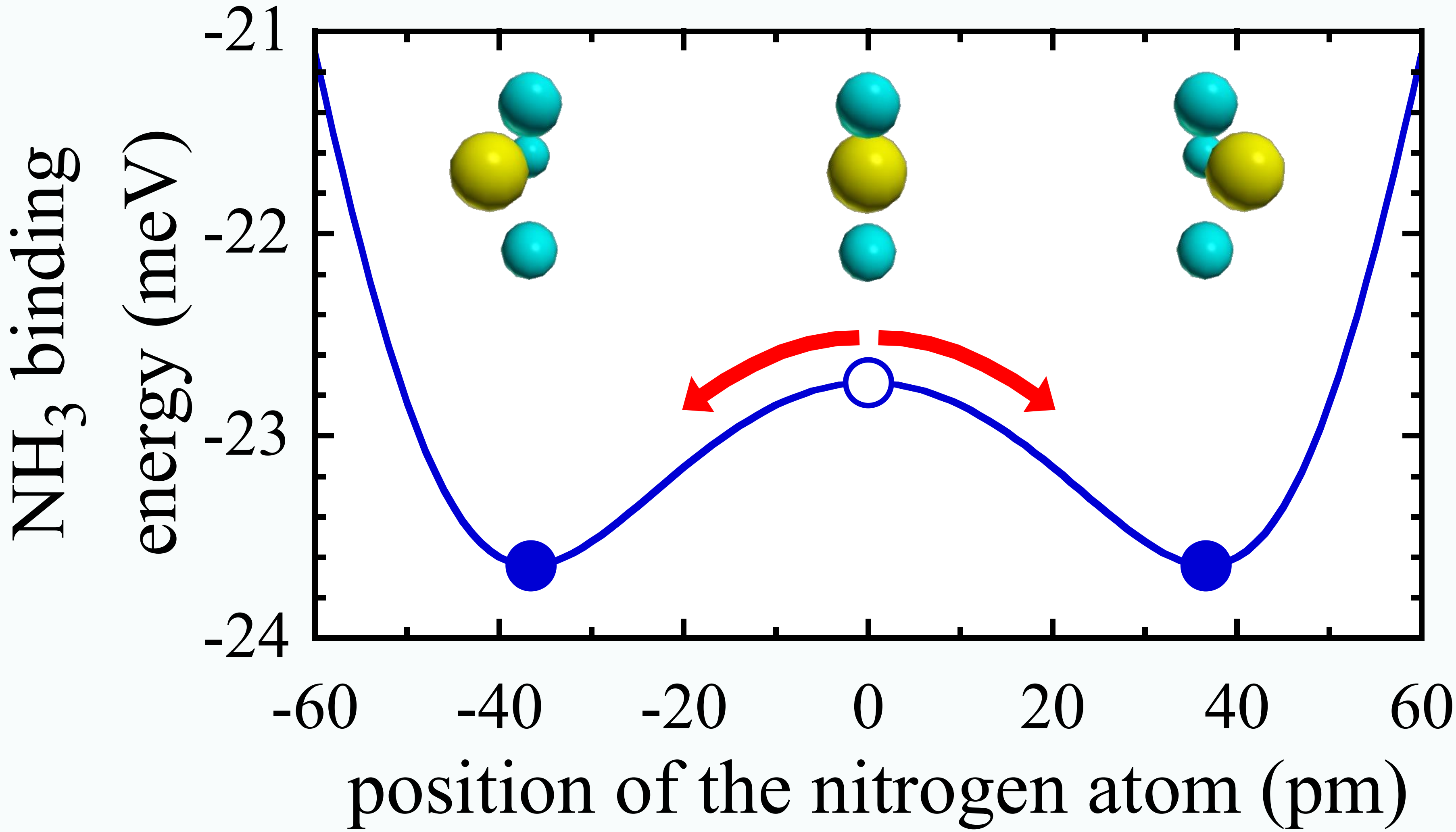


$$= |R\rangle$$

left state

right state

Ammonia molecule NH_3 - symmetry breaking



$$E_{\mathrm{NH_3}}(r_{\mathrm{NH}}, r_{\mathrm{HH}}) = 3\epsilon_{\mathrm{NH}}\left[\left(\frac{d_{\mathrm{NH}}}{r_{\mathrm{NH}}}\right)^{12} - 2\left(\frac{d_{\mathrm{NH}}}{r_{\mathrm{NH}}}\right)^{6}\right] + 3\epsilon_{\mathrm{HH}}\left[\left(\frac{d_{\mathrm{HH}}}{r_{\mathrm{HH}}}\right)^{12} - 2\left(\frac{d_{\mathrm{HH}}}{r_{\mathrm{HH}}}\right)^{6}\right]$$

Let P be the plane-reflection operator with respect to the H_3 plane, then

$$\begin{aligned} P|R\rangle &= |L\rangle \\ P|L\rangle &= |R\rangle \end{aligned}$$

Let us denote overlaps and matrix elements by

$$\begin{aligned} 1 &= \langle L|L\rangle = \langle R|R\rangle \\ \epsilon &= \langle L|R\rangle \\ E_0 &= \langle L|H|L\rangle = \langle R|H|R\rangle \\ \Delta &= \langle L|H|R\rangle \end{aligned}$$

In the non-orthogonal basis of $|L\rangle$, $|R\rangle$ the Hamiltonian matrix reads

$$H = \begin{pmatrix} E_0 & \Delta \\ \Delta & E_0 \end{pmatrix}$$

The eigenstates must correspond to the restored-symmetry states

$$|\pm\rangle = \frac{1}{\sqrt{2 \pm 2\epsilon}}\left(|L\rangle \pm R\rangle\right)$$

i.e.,

$$P|\pm\rangle = \pm|\pm\rangle$$

The eigenenergies read

$$E_\pm = \langle\pm|H|\pm\rangle = \frac{E_0 \pm \Delta}{1 \pm \epsilon}$$

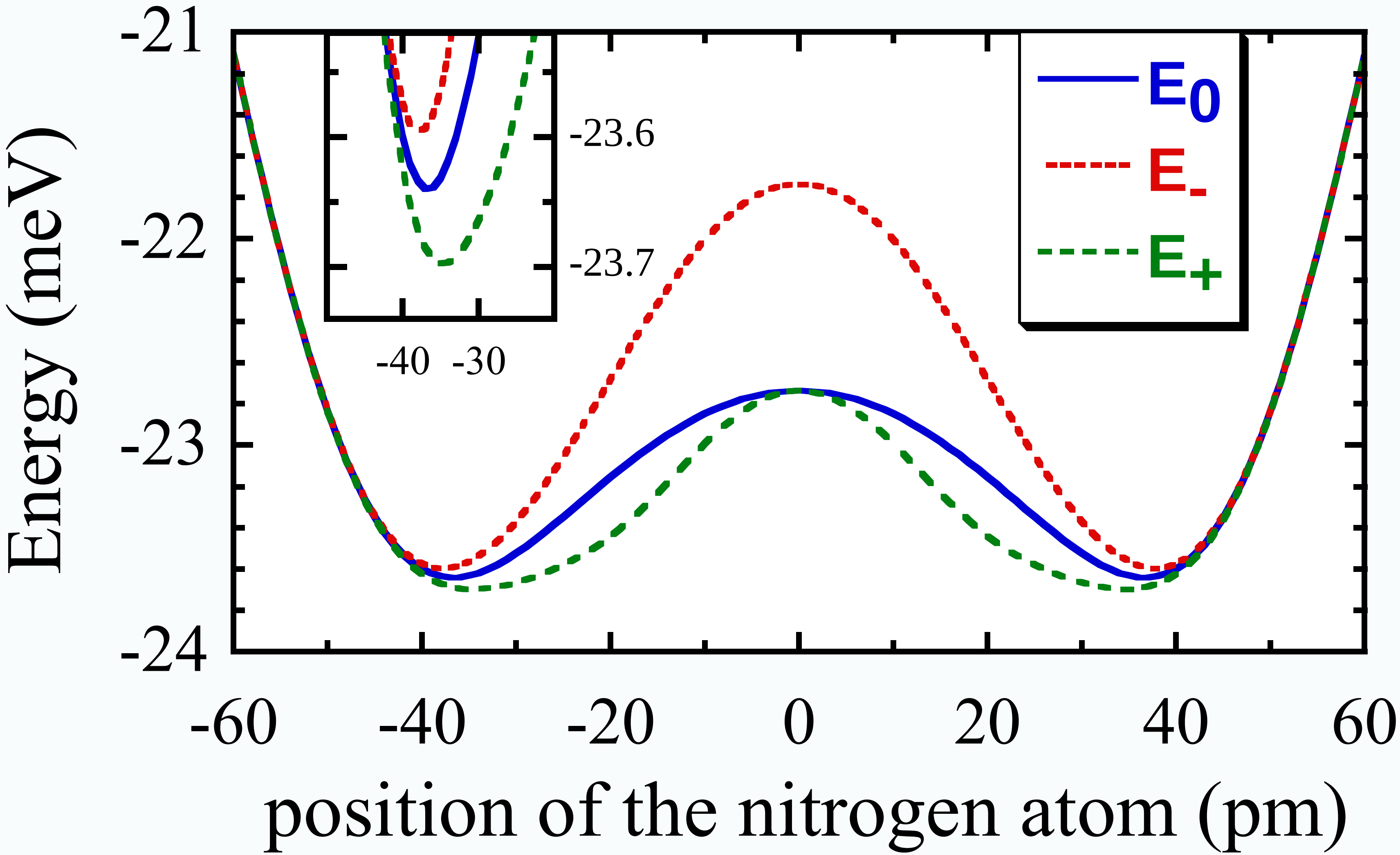
States $|L\rangle$ and $R\rangle$ are wave packets, e.g.,

$$|L\rangle = \frac{1}{2}\left(\sqrt{2+2\epsilon}|+\rangle + \sqrt{2-2\epsilon}|-\rangle\right)$$

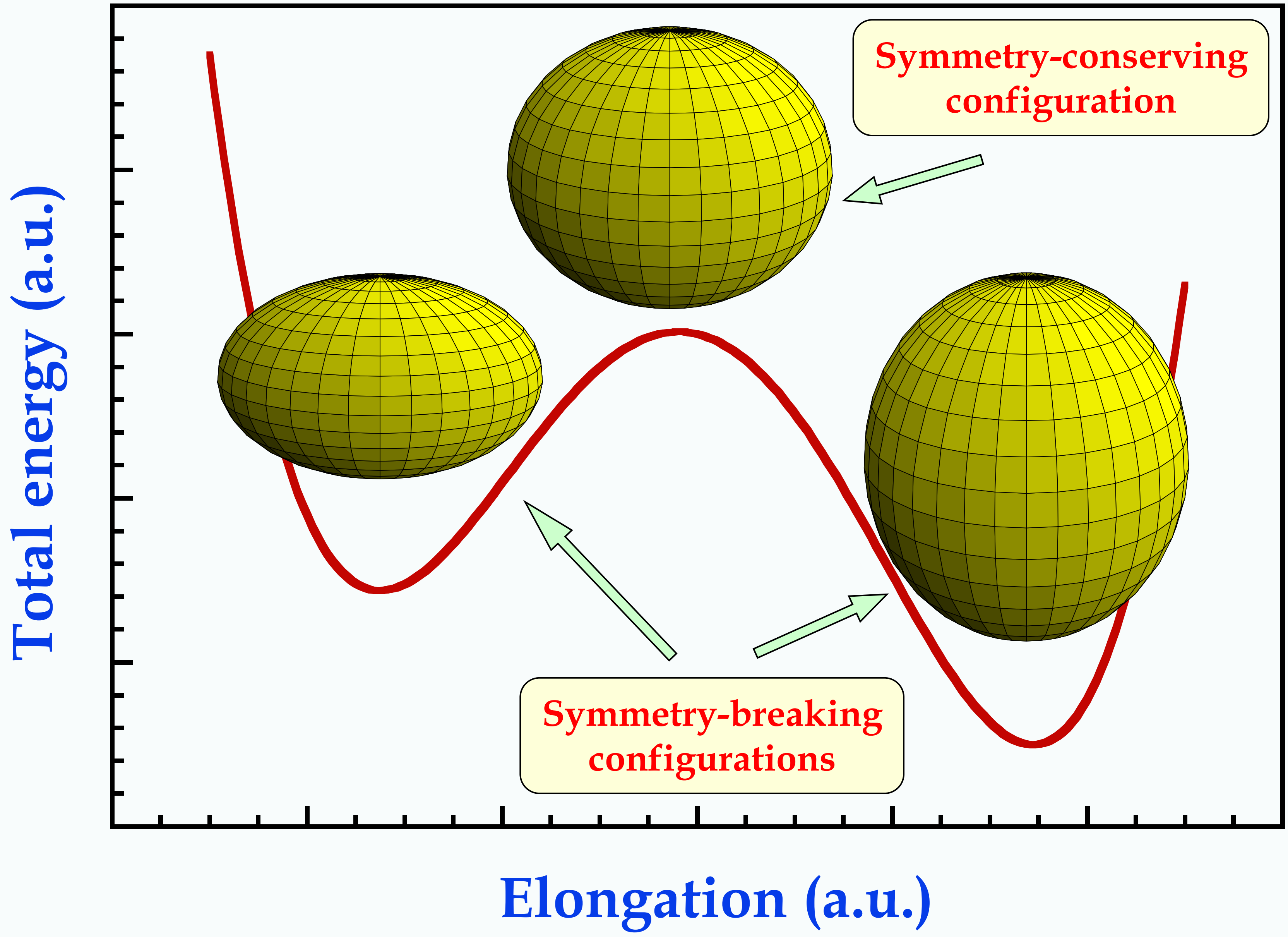
which evolve in time
($\epsilon << \Delta/E_0$ assumed) as:,

$$|L,t\rangle = e^{iE_0 t/\hbar}\left(\cos(\Delta t/\hbar)|L,0\rangle + i\sin(\Delta t/\hbar)|R,0\rangle\right)$$

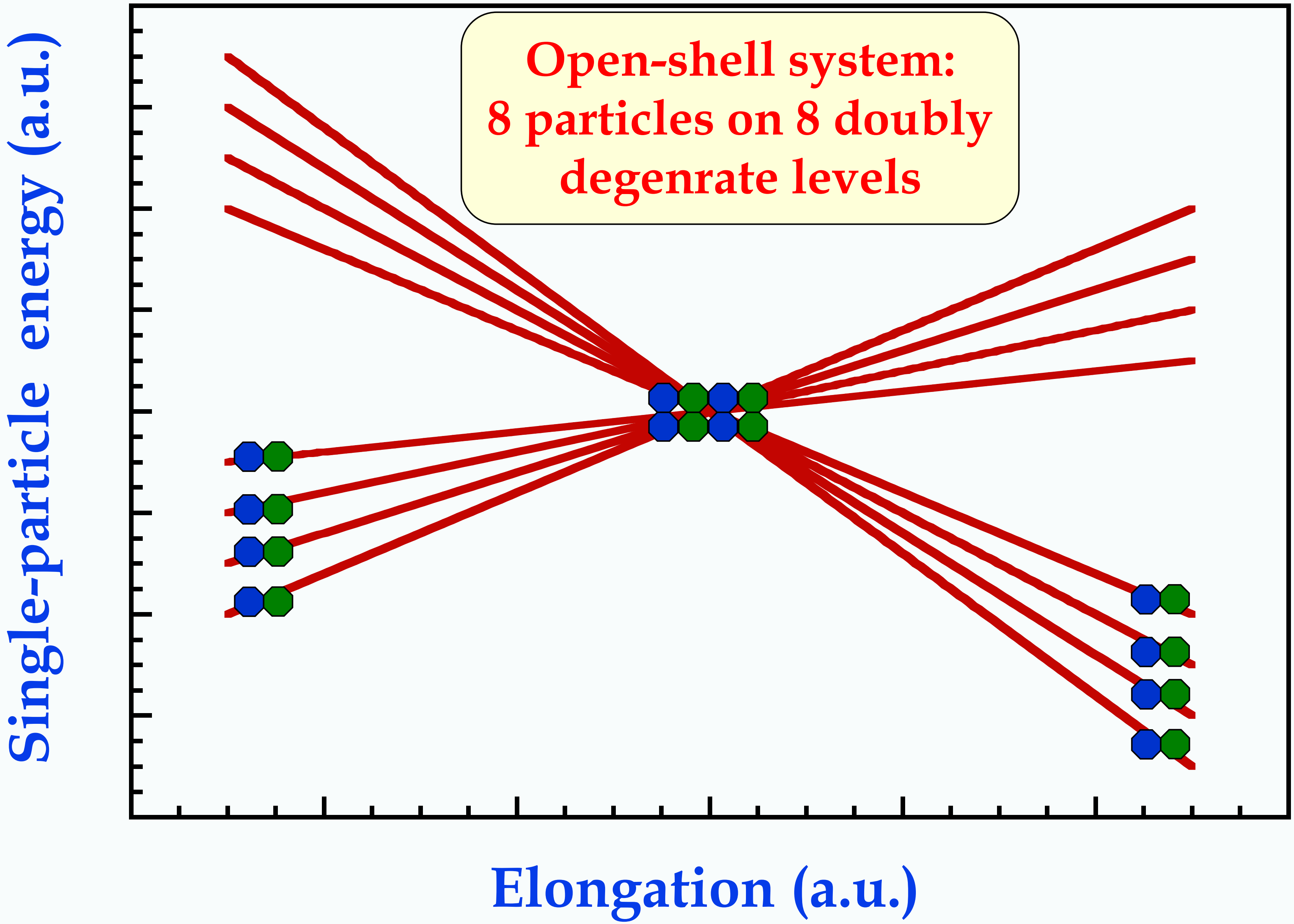
Ammonia molecule NH_3 - symmetry restoration



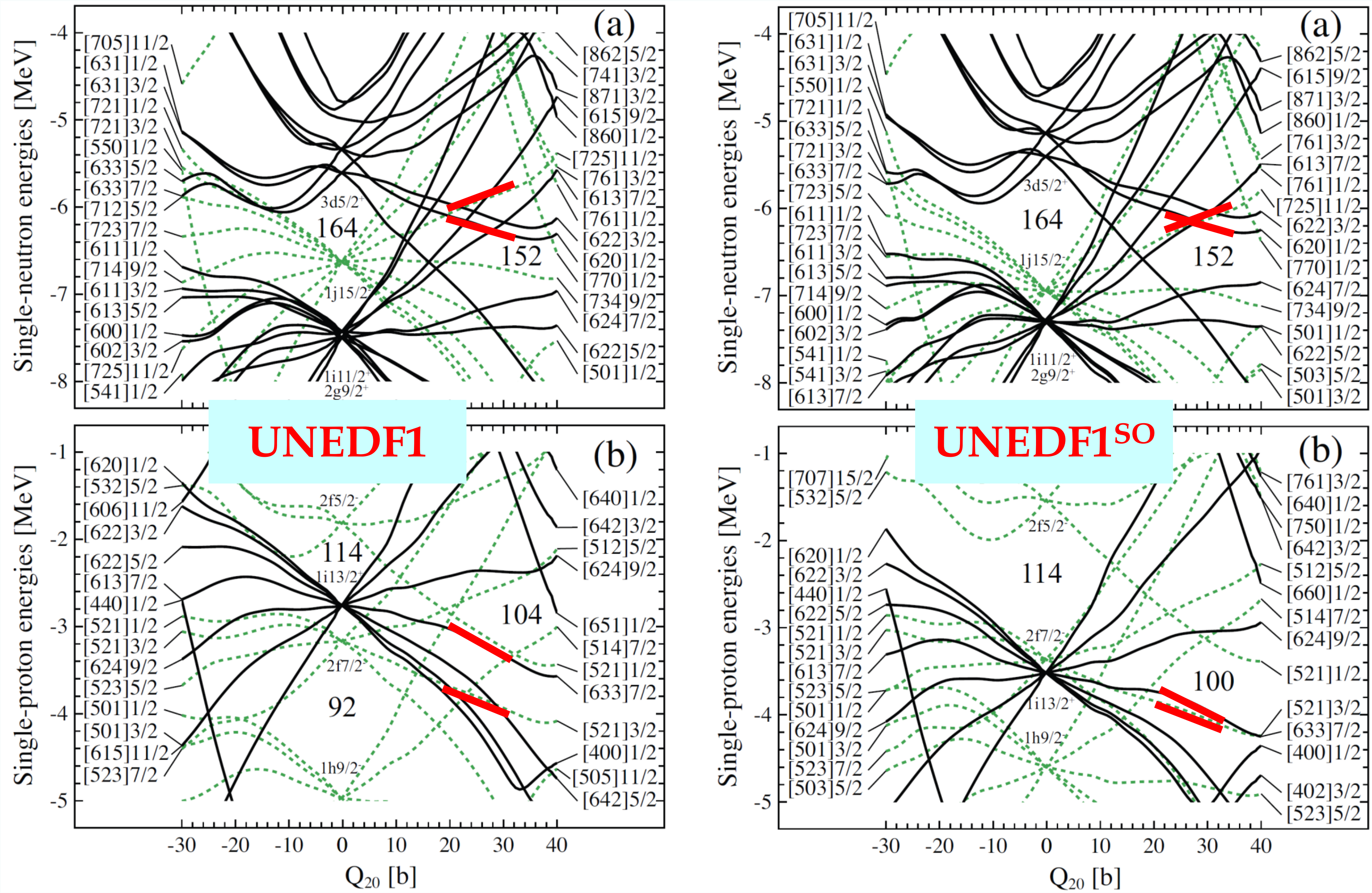
Nuclear deformation



Origins of nuclear deformation



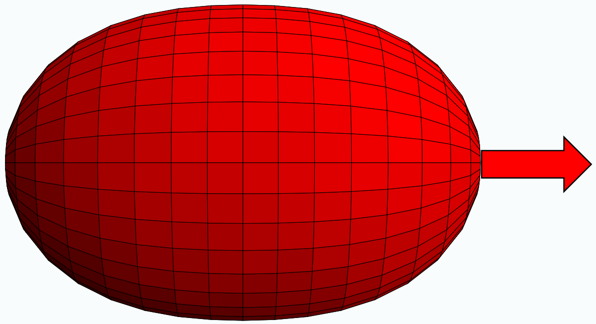
Nilsson diagrams in ^{254}No

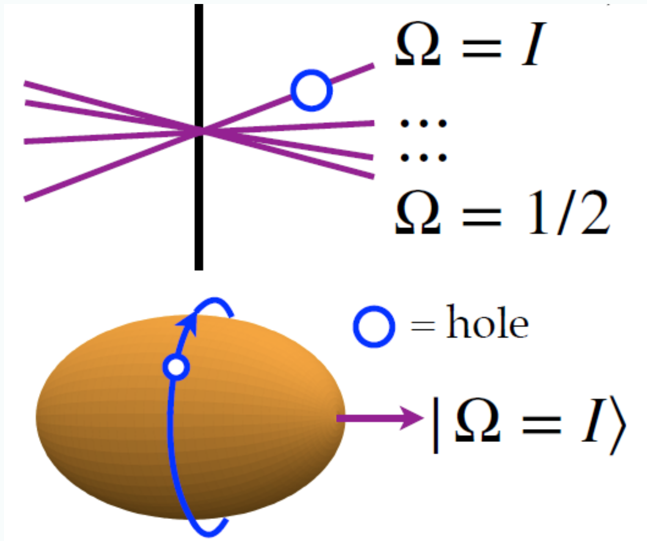


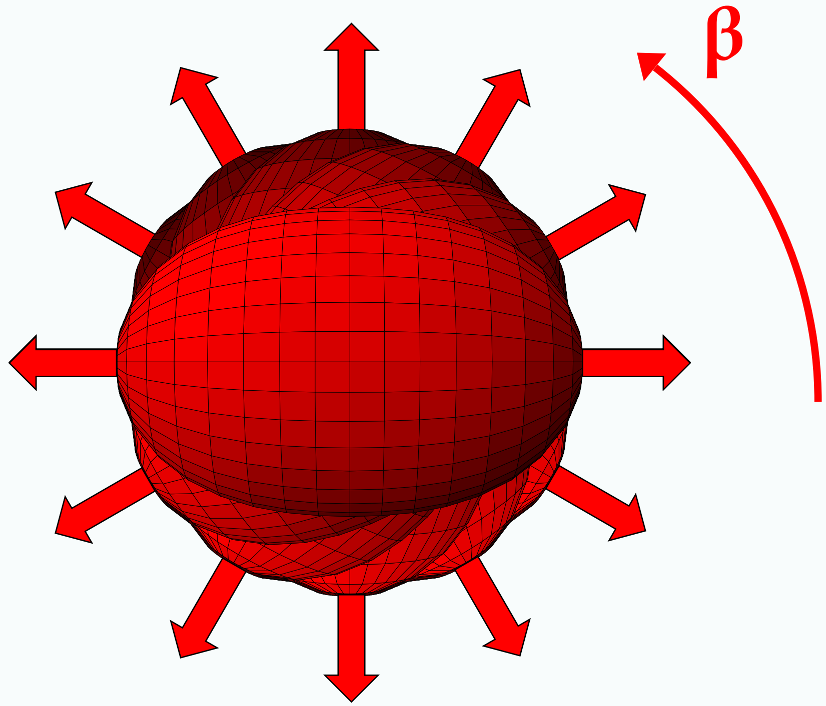
Yue Shi, *et al.*, Phys. Rev. C89, 034309 (2014)

Time-odd spin alignment & symmetry restoration

"Intrinsic"
Symmetry broken







"Laboratory"
Symmetry restored

$$|IM\rangle = \mathcal{N}_I \int_{\beta=0}^{\pi} \mathrm{d}\beta\, d^I_{M\Omega}(\beta)|\Omega,\beta\rangle$$

J. A. Sheikh et al., J. Phys. G48, 123001 (2021)

Spectroscopic moments are determined for symmetry-restored wave functions without using effective charges or effective g-factors and compared with experimental data.

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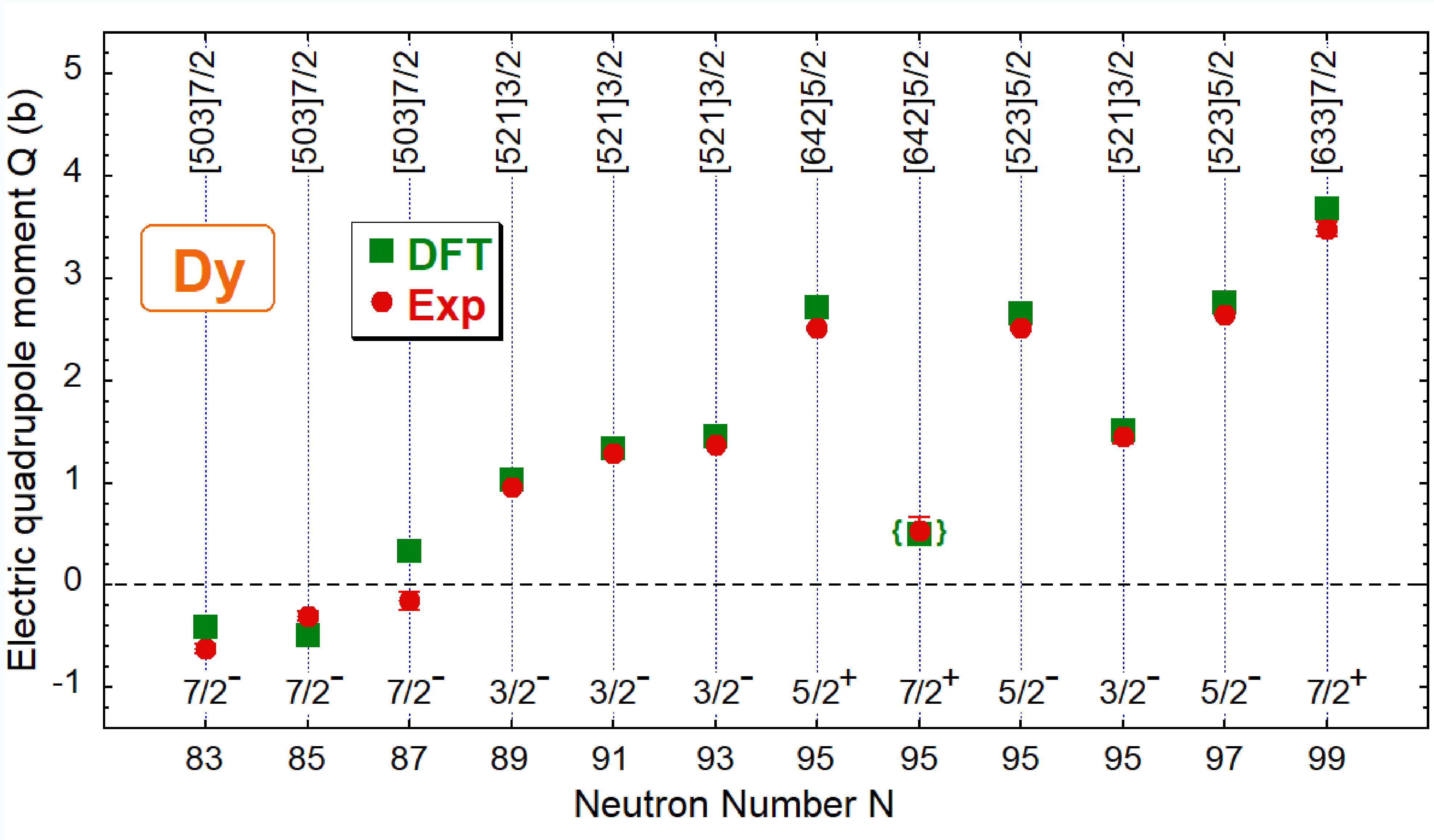
Deformations of odd dysprosium isotopes

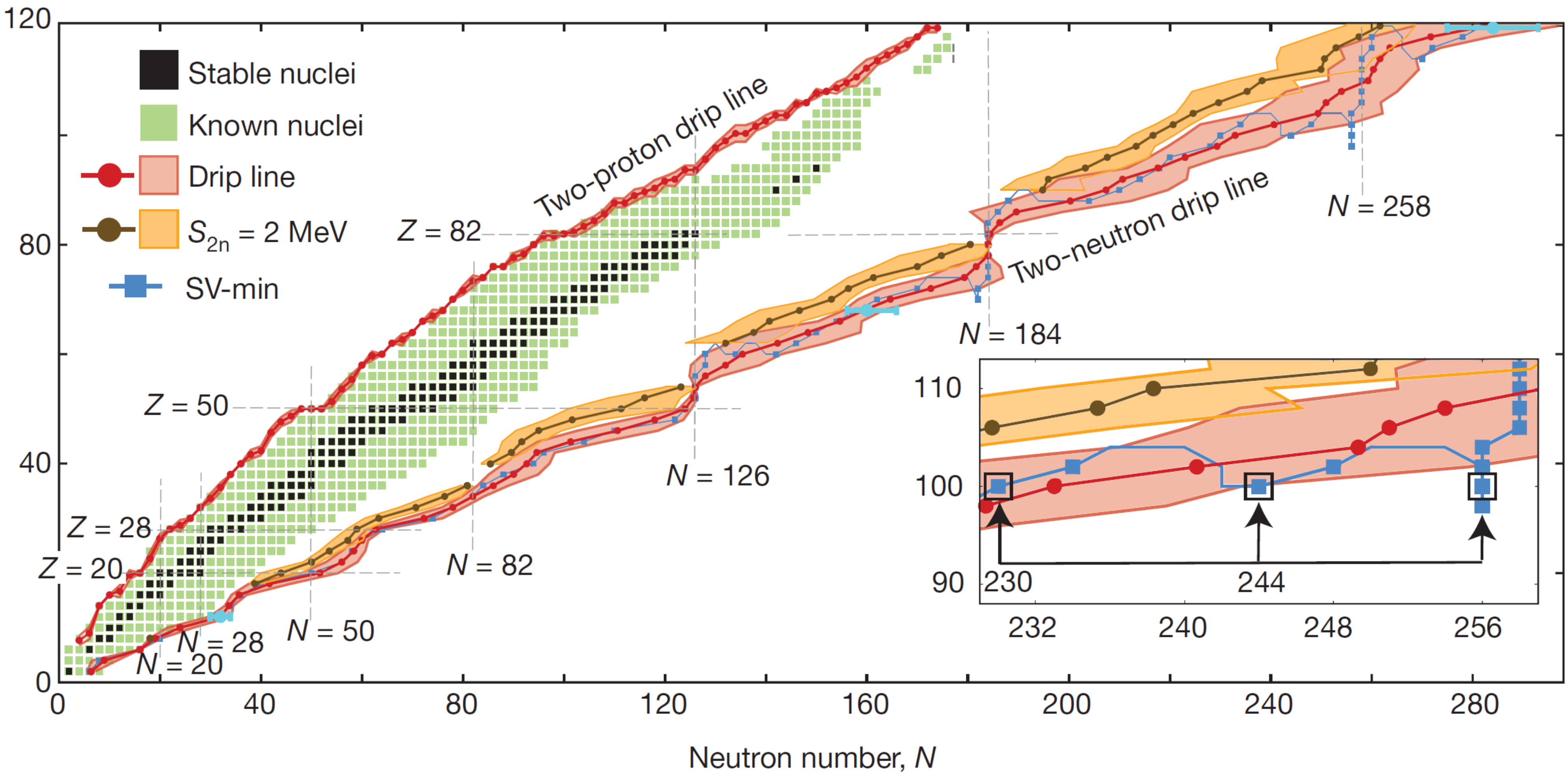


J.D., *et al.*, to be published (2025)

What do the energy density functionals give us?

1) **“Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful”**
G.E.P. Box and N.R. Draper
Empirical Model Building and Response Surfaces
(John Wiley & Sons, New York, 1987)

6900±500 bound nuclei



The limits of the nuclear landscape

J. Erler, N. Birge, M. Kortelainen, W. Nazarewicz, E. Olsen, A.M. Perhac, M. Stoitsov,

Nature 486, 509 (2012)

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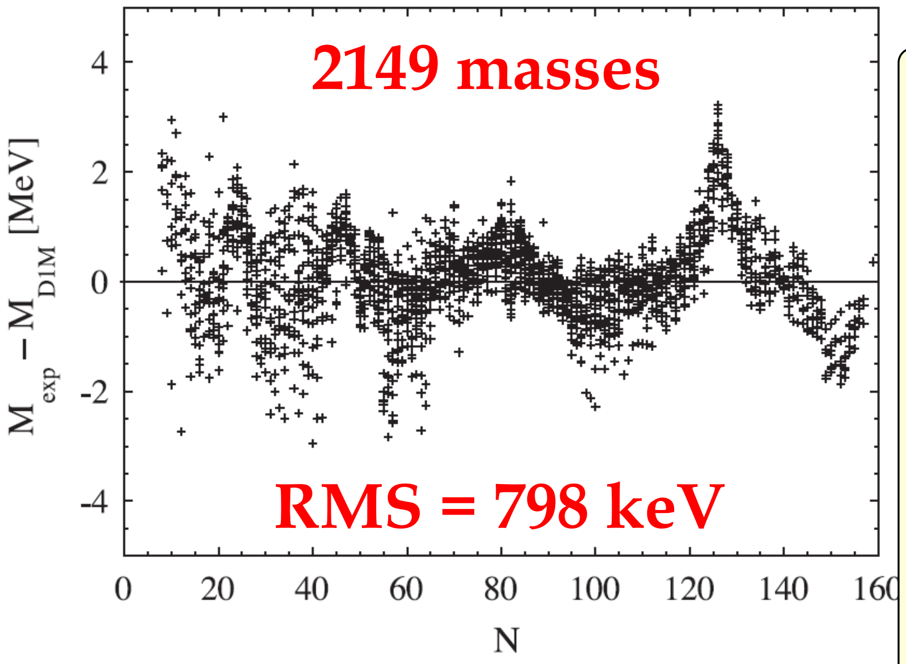
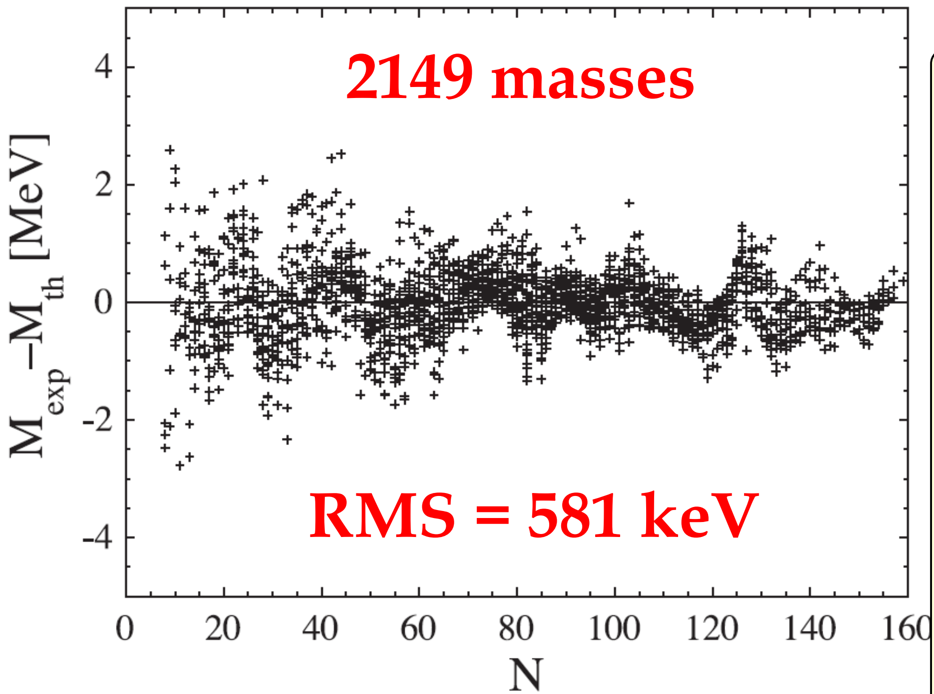
Nuclear binding energies (masses)



S. Goriely *et al.*, Phys. Rev. Lett. 102, 242501 (2009)

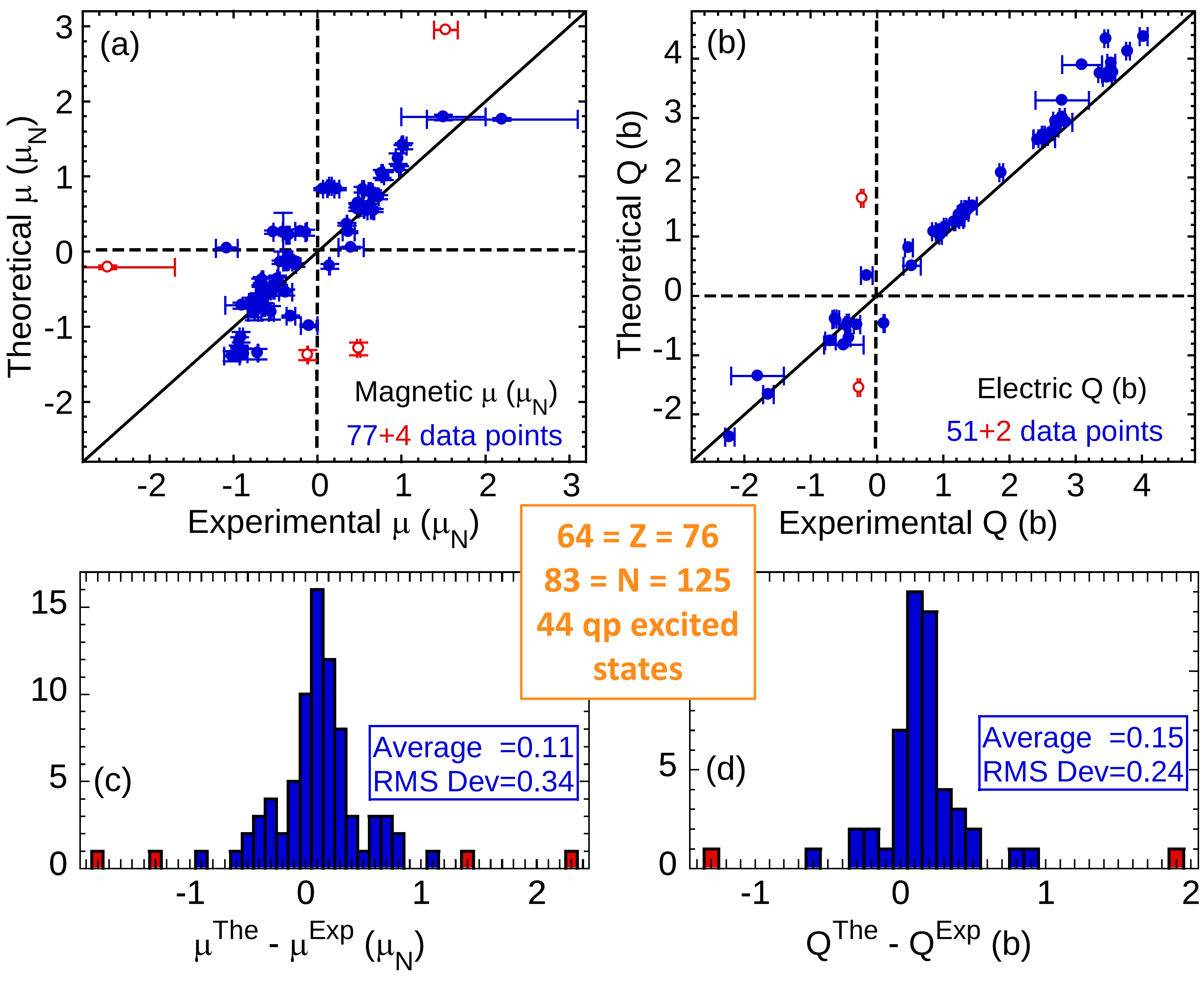
The first Gogny HFB mass model. An explicit and self-consistent account of all the quadrupole correlation energies are included within the 5D collective Hamiltonian approach.



S. Goriely *et al.*, Phys. Rev. Lett. 102, 152503 (2009)

The new Skyrme HFB nuclear-mass model, in which the contact-pairing force is constructed from microscopic pairing gaps of symmetric nuclear matter and neutron matter.

Summary of results obtained in the Gd – Os isotopes



64 = Z = 76
83 = N = 125
44 qp excited states

J.D., et al., to be published (2025)

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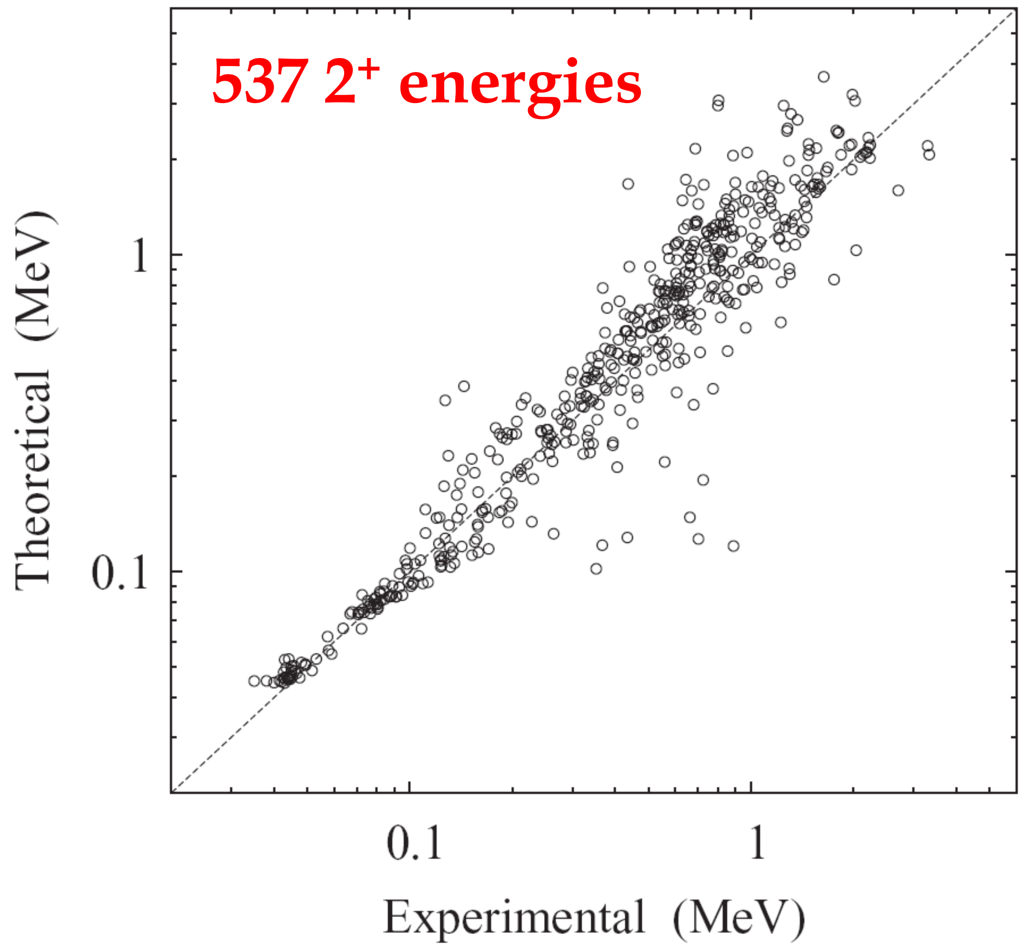
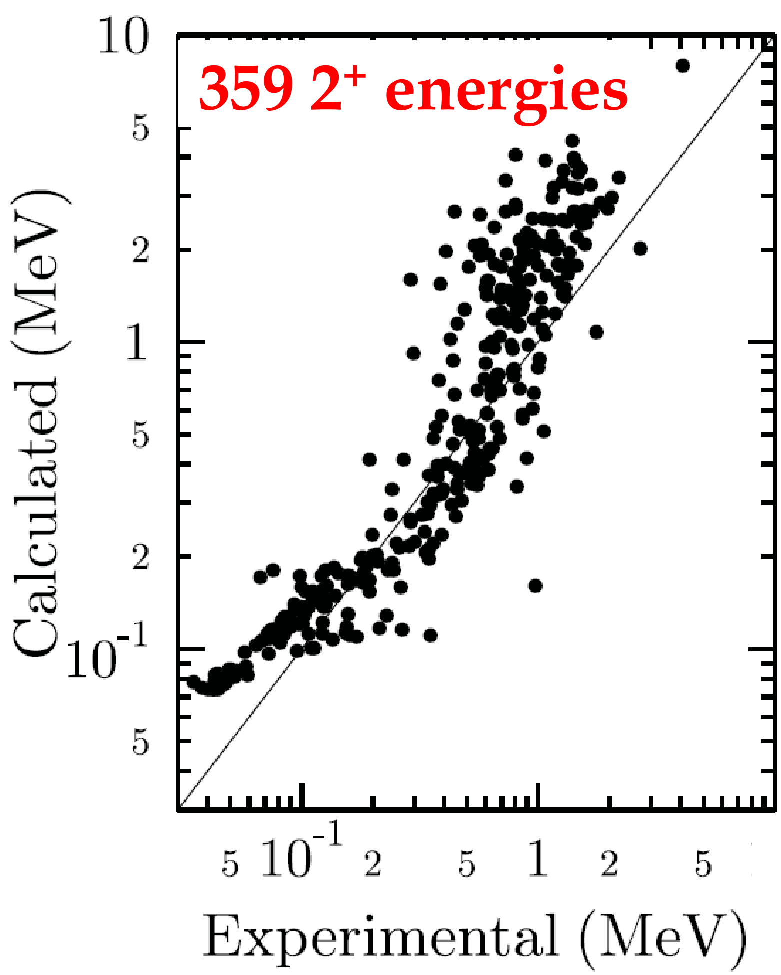
First 2^+ excitations of even-even nuclei



J.-P. Delaroche *et al.*, Phys. Rev. C81, 014303 (2010)



B. Sabbey *et al.*, Phys. Rev. C75, 044305 (2007)

Gogny HFB calculations plus the 5D collective Hamiltonian approach.

Skyrme HF+BCS calculations plus the particle-number and angular-momentum projection and shape mixing.

Thank you

Muon-nucleus coupling, a project

To determine the self-consistent deformed and polarised states of a muon moving around a deformed and polarised nucleus followed by the symmetry restoration.

PRECISION FRONTIER

Witek Nazarewicz & discussions with:

Edwin Kolbe (2001)

Krzysztof Pachucki (2018, NO!)

Kyle Godbey (2023)

Natalia Oreshkina & Konstantin Beyer (2023)

……..

Muon wave function in ^{185}Re

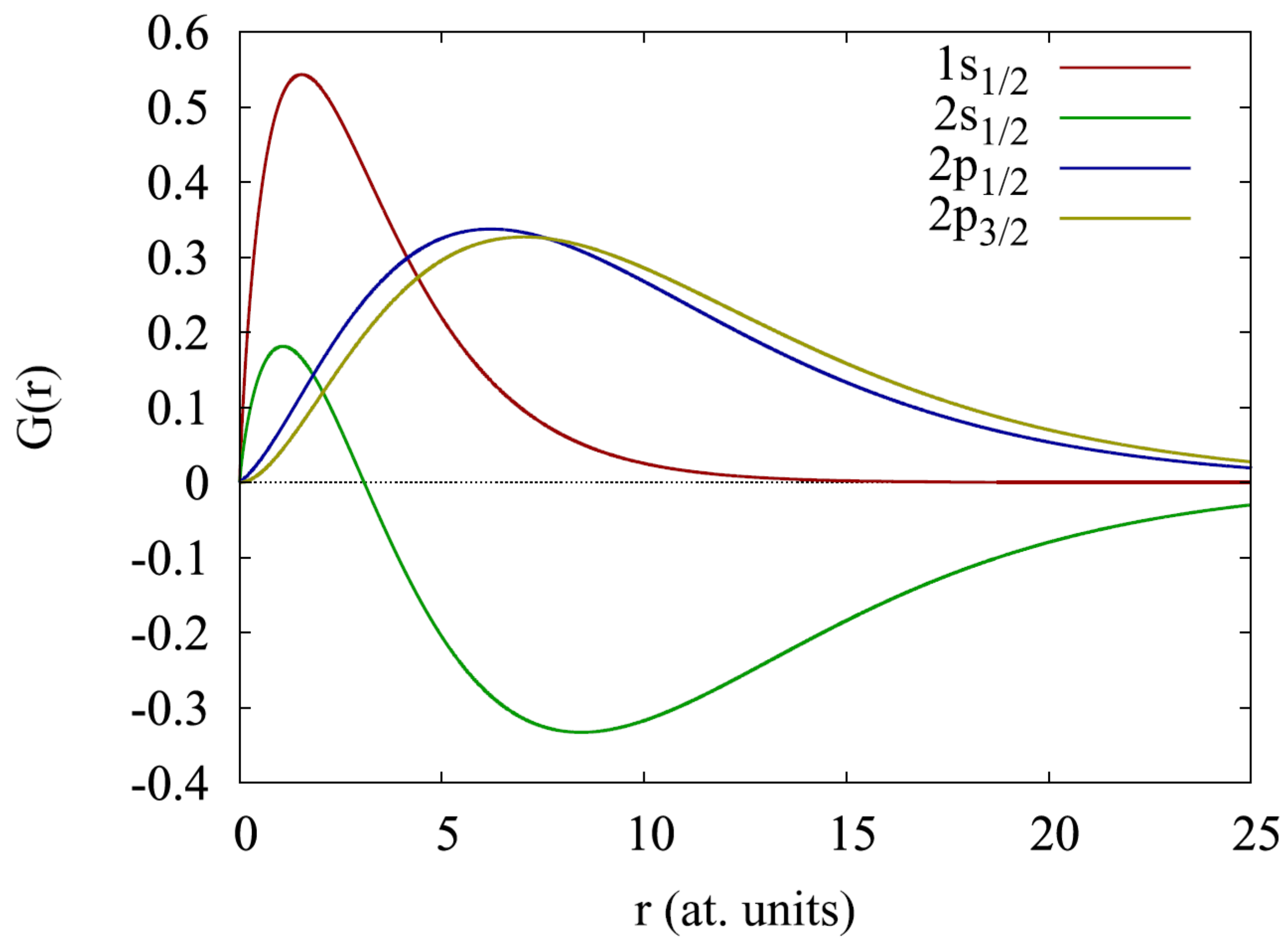


Fig. 1. The G component of electronic radial wave function (5) calculated with the homogeneously charged nuclear model is plotted for four lowest lying states for hydrogen-like $^{185}_{75}$Re.

B.S.M. Patoary and N.S. Oreshkina, Eur. Phys. J. D 72 (2018) 54

Muon wave function in ^{90}Zr, ^{120}Sn, and ^{208}Pb

PHYSICAL REVIEW LETTERS **128,** 203001 (2022)

Evidence Against Nuclear Polarization as Source of Fine-Structure Anomalies in Muonic Atoms

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[2]*Dipartimento di Fisica, Università degli Studi di Milano, via Celoria 16, I-20133 Milano, Italy*
[3]*INFN, Sezione di Milano, via Celoria 16, I-20133 Milano, Italy*

(Received 25 January 2022; revised 29 March 2022; accepted 18 April 2022; published 17 May 2022)

A long-standing problem of fine-structure anomalies in muonic atoms is revisited by considering the splittings $\Delta 2p = E_{2p_{3/2}} - E_{2p_{1/2}}$ in muonic ^{90}Zr, ^{120}Sn, and ^{208}Pb and $\Delta 3p = E_{3p_{3/2}} - E_{3p_{1/2}}$ in muonic ^{208}Pb. State-of-the-art techniques from both nuclear and atomic physics are brought together in order to perform the most comprehensive to date calculations of nuclear-polarization energy shifts. Barring the more subtle case of μ-^{208}Pb, the results suggest that the dominant calculation uncertainty is much smaller than the persisting discrepancies between theory and experiment. We conclude that the resolution to the anomalies is likely to be rooted in refined quantum-electrodynamics corrections or even some other previously unaccounted-for contributions.

Muon-nucleus coupling, a project

1. **Spherical nucleus and muon:** a self-consistent solution for a combined nucleus-muon system moving in the common Coulomb field.
2. **Spin-polarized nucleus and muon:** a self-consistent solution for a combined nucleus-muon system moving in the combined Coulomb and magnetic fields.
   (Bohr-Weisskopf effect: the influence of the nuclear magnetization distribution on electron hyperfine splitting; a few percent effect).
3. **Deformed nucleus and muon:** a self-consistent solution for a muon moving in the combined deformed Coulomb and magnetic fields.
4. **Symmetry restoration** of the combined deformed and polarised nucleus-muon wave function.
5. **Post-analysis** of the symmetry-restored nucleus-muon wave function in terms of the separately symmetry-restored nucleus and muon wave functions.

Thank you