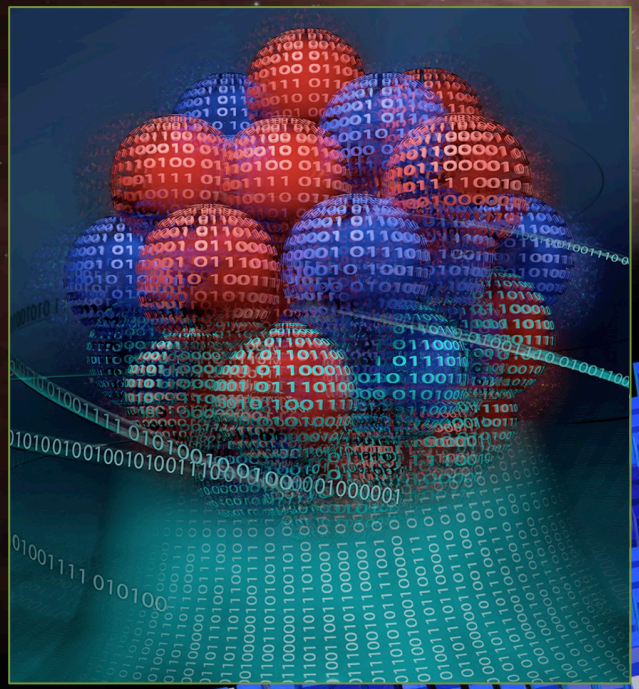
HFB-Gamow problem and supercritical Dirac regime

Witold Nazarewicz, FRIB@MSU

EMMI Workshop on Super-Heavy elements
Sorbonne Université, October 24-26, 2022



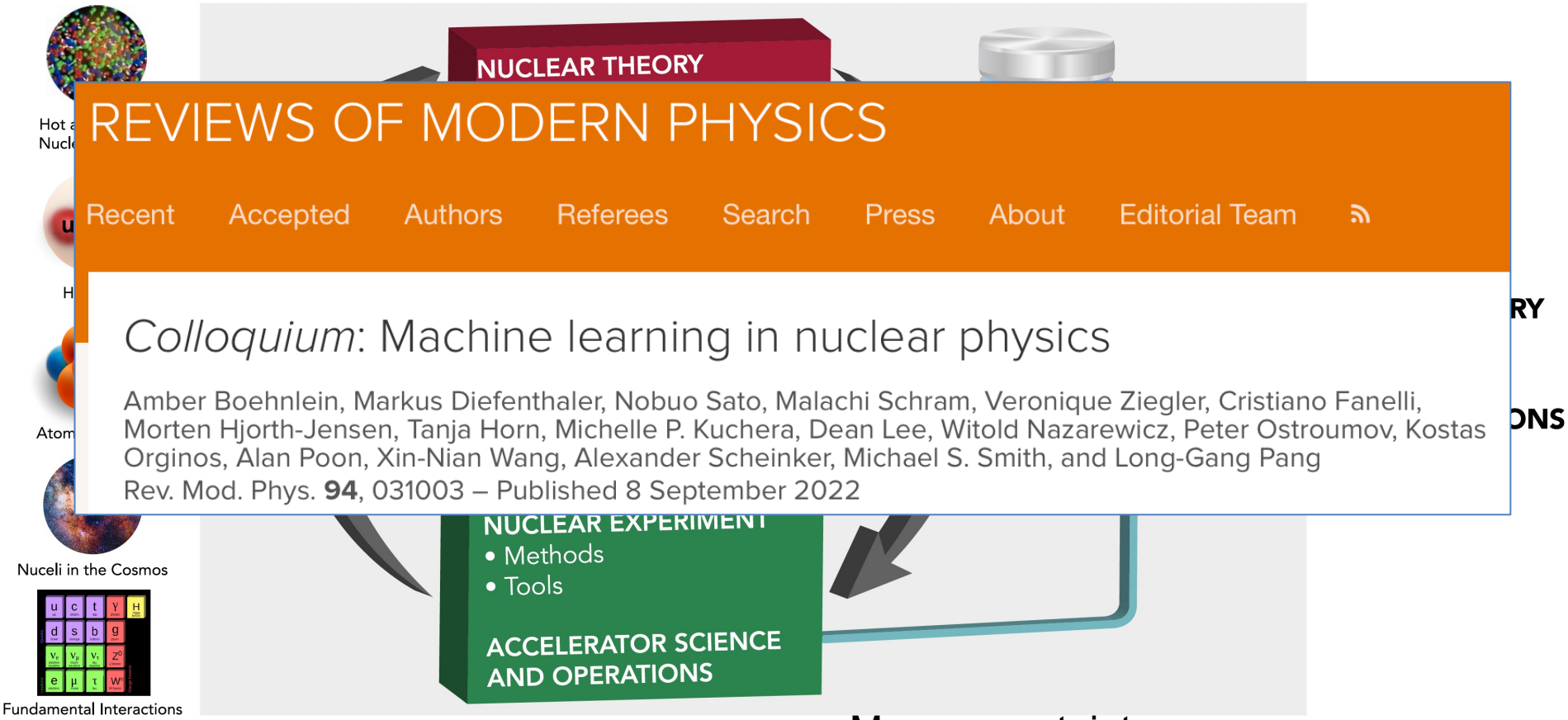
Pushing the Limits of the Periodic Table – A Review on Atomic Relativistic Electronic Structure Theory and Calculations for the Superheavy Elements*

O. R. Smits[c,3], P. Indelicato[a,1], W. Nazarewicz[b,2], M. Piibeleht[3], P. Schwerdtfeger[d,3]

Menu

- Prelude
- The problem
- Nuclear physics context
- HFB and Dirac spectra
- Gamow states and resonant-state expansions
- Perspectives

Speeding-up the cycle of the scientific method with machine learning



REVIEWS OF MODERN PHYSICS

Recent Accepted Authors Referees Search Press About Editorial Team

Colloquium: Machine learning in nuclear physics

Amber Boehnlein, Markus Diefenthaler, Nobuo Sato, Malachi Schram, Veronique Ziegler, Cristiano Fanelli, Morten Hjorth-Jensen, Tanja Horn, Michelle P. Kuchera, Dean Lee, Witold Nazarewicz, Peter Ostroumov, Kostas Orginos, Alan Poon, Xin-Nian Wang, Alexander Scheinker, Michael S. Smith, and Long-Gang Pang

Rev. Mod. Phys. **94**, 031003 – Published 8 September 2022

Many uncertainty sources:

- Hamiltonian/functional parameters
- Hilbert-space truncations
- Systematic errors
- Numerical approximations
- Extrapolations
- …

Nuclear charge density from nuclear DFT

Nuclear charge densities in spherical and deformed nuclei: Toward precise calculations of charge radii, P.G. Reinhard, WN, Phys. Rev. C 103, 054310 (2021)

$$\rho_c(\boldsymbol{r}) = \frac{1}{(2\pi)^3} \int d^3q e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} F_c(\boldsymbol{q})$$

nuclear charge density

nuclear charge form factor

$$F_c(\boldsymbol{q}) = \sum_{t\in\{p,n\}} \Big[G_{E,t}(\boldsymbol{q}) \left(1 - \tfrac{1}{2}\boldsymbol{q}^2\mathcal{D}\right) F_t(\boldsymbol{q}) - \mathcal{D}\left[2\mu_t G_{M,t}(\boldsymbol{q}) - G_{E,t}(\boldsymbol{q})\right] F_{\ell s,t}(\boldsymbol{q}) \Big].$$

$$\mathcal{D} = \frac{\hbar^2}{(2mc)^2}$$

G_E and G_M are the *intrinsic* proton and neutron electromagnetic form factors

$$F_t(\boldsymbol{q}) = \int d^3r\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \rho_t(\boldsymbol{r}),$$

$$F_{\ell s,t}(\boldsymbol{q}) = \int d^3r\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \boldsymbol{\nabla}\cdot\boldsymbol{J}_t(\boldsymbol{r})$$

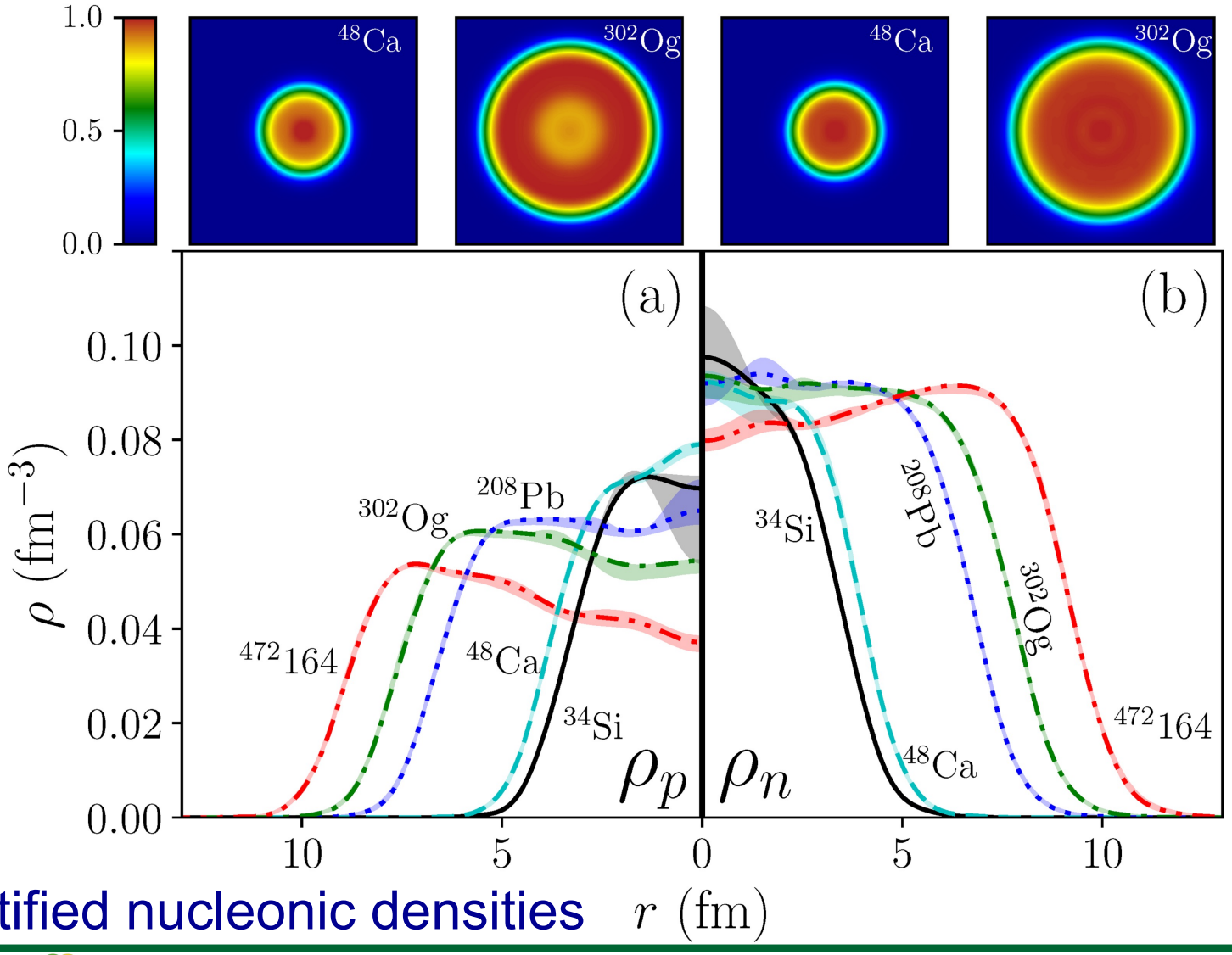
spin-orbit current

General expression. Valid for spherical and deformed nuclei

Nucleonic densities are NOT Sphere/Shell/Fermi distributions!

Central depression and Coulomb redistribution

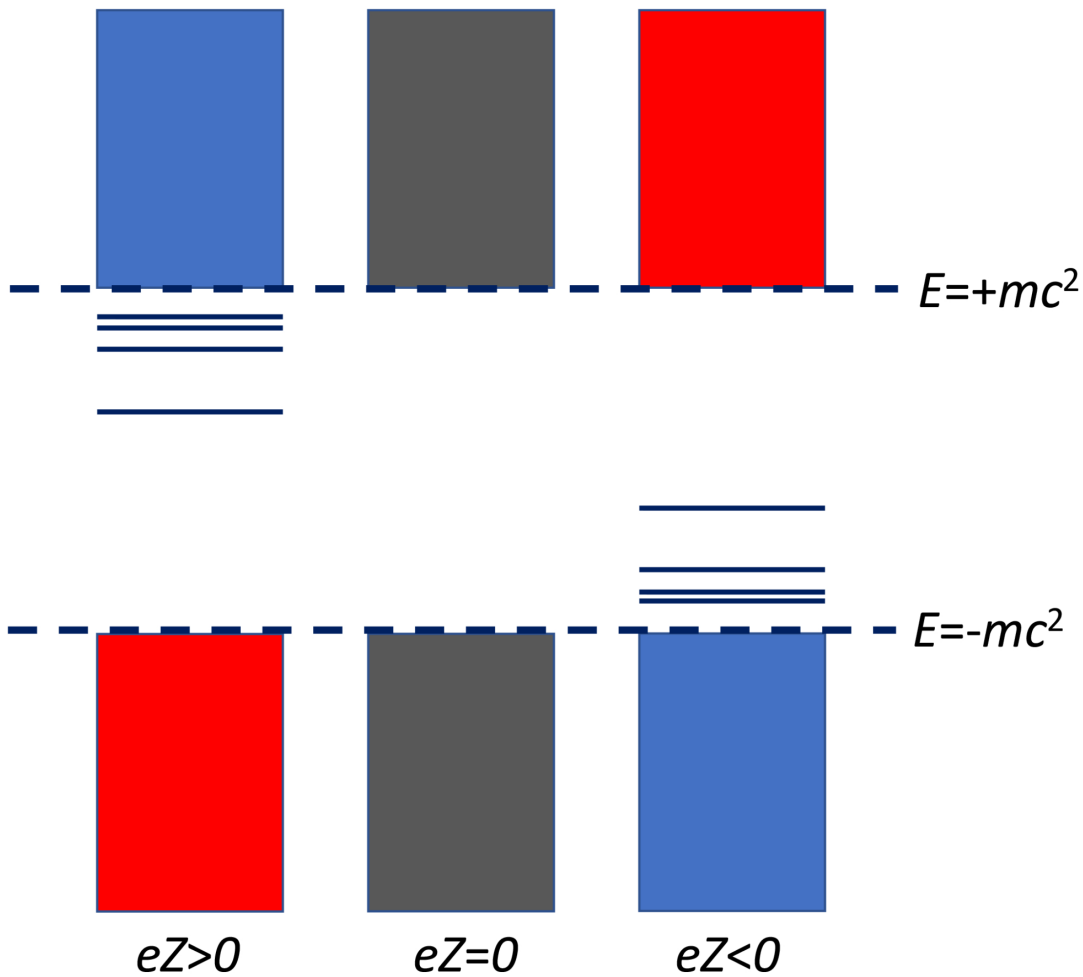
B. Schuetrumpf et al., Phys. Rev. C 96, 024306 (2017)

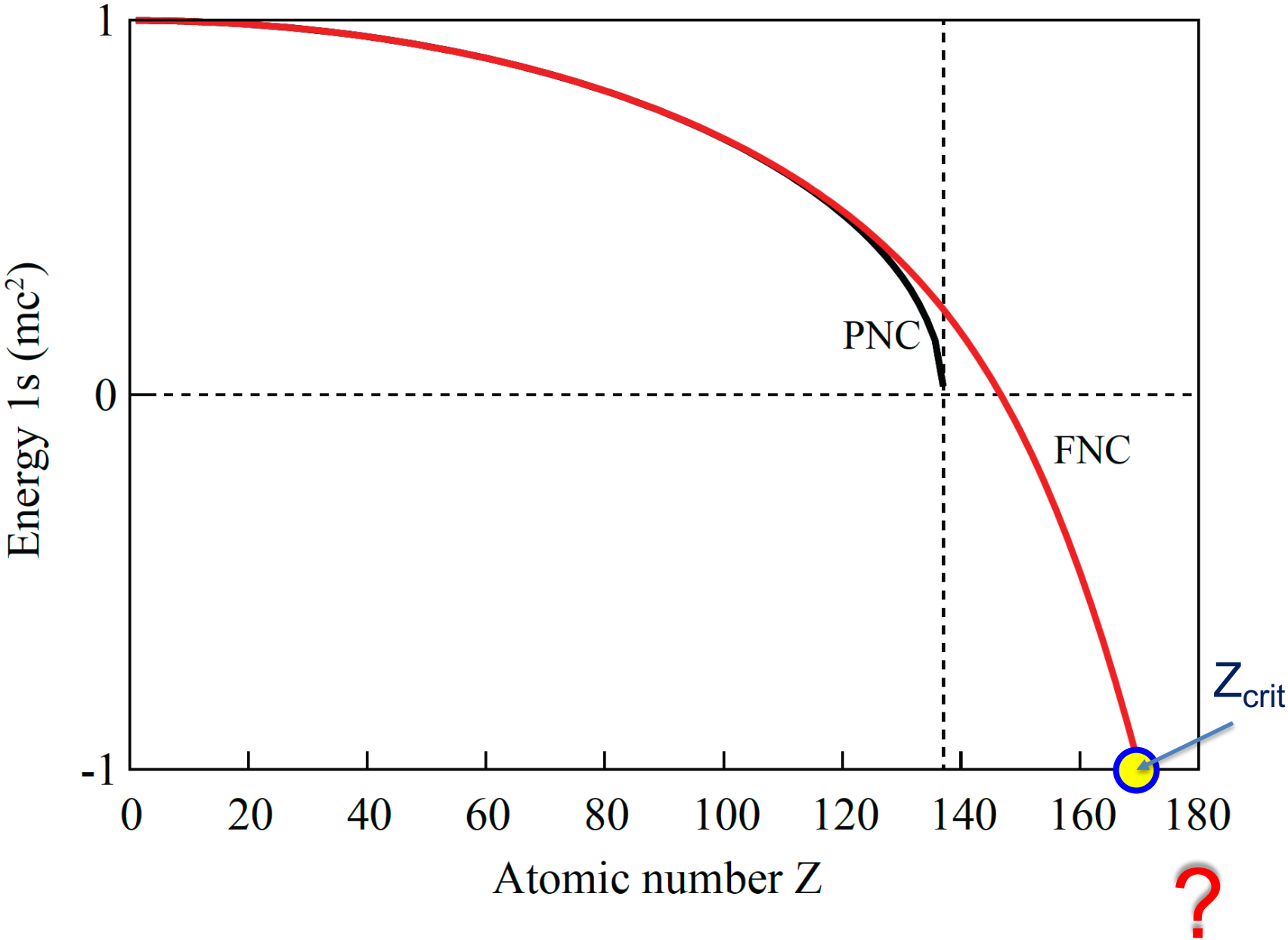


quantified nucleonic densities

One-body Dirac equation

$$\begin{pmatrix} mc^2 + V(r) - E_{n\kappa} & c\left(-\frac{d}{dr} + \frac{\kappa}{r}\right) \\ c\left(\frac{d}{dr} + \frac{\kappa}{r}\right) & -mc^2 + V(r) - E_{n\kappa} \end{pmatrix} \begin{pmatrix} P_{n\kappa}(r) \\ Q_{n\kappa}(r) \end{pmatrix} = 0,$$




1
0
-1
Energy 1s (mc²)
PNC
FNC
Z_crit
0
20
40
60
80
100
120
140
160
180
Atomic number Z
?

Hartree-Fock-Bogoliubov (HFB or Bogoliubov-de Gennes) method

$$\mathcal{R} = \mathcal{R}^+ = \mathcal{R}^2 = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}$$

Generalized density matrix

$$\mathcal{R}\begin{pmatrix} B_0^* \\ A_0^* \end{pmatrix} = \begin{pmatrix} B_0^* \\ A_0^* \end{pmatrix}$$

quasihole states

$$\mathcal{R}\begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = 0$$

quasiparticle states

HF potential

pairing potential

$$\mathcal{H}' := \begin{pmatrix} T+\Gamma-\lambda & \Delta \\ -\Delta^* & -T^*-\Gamma^*+\lambda \end{pmatrix}$$

HFB Hamiltonian

$$\mathcal{H}'\begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} E_0 \qquad \mathcal{H}'\begin{pmatrix} B_0^* \\ A_0^* \end{pmatrix} = -\begin{pmatrix} B_0^* \\ A_0^* \end{pmatrix} E_0,$$

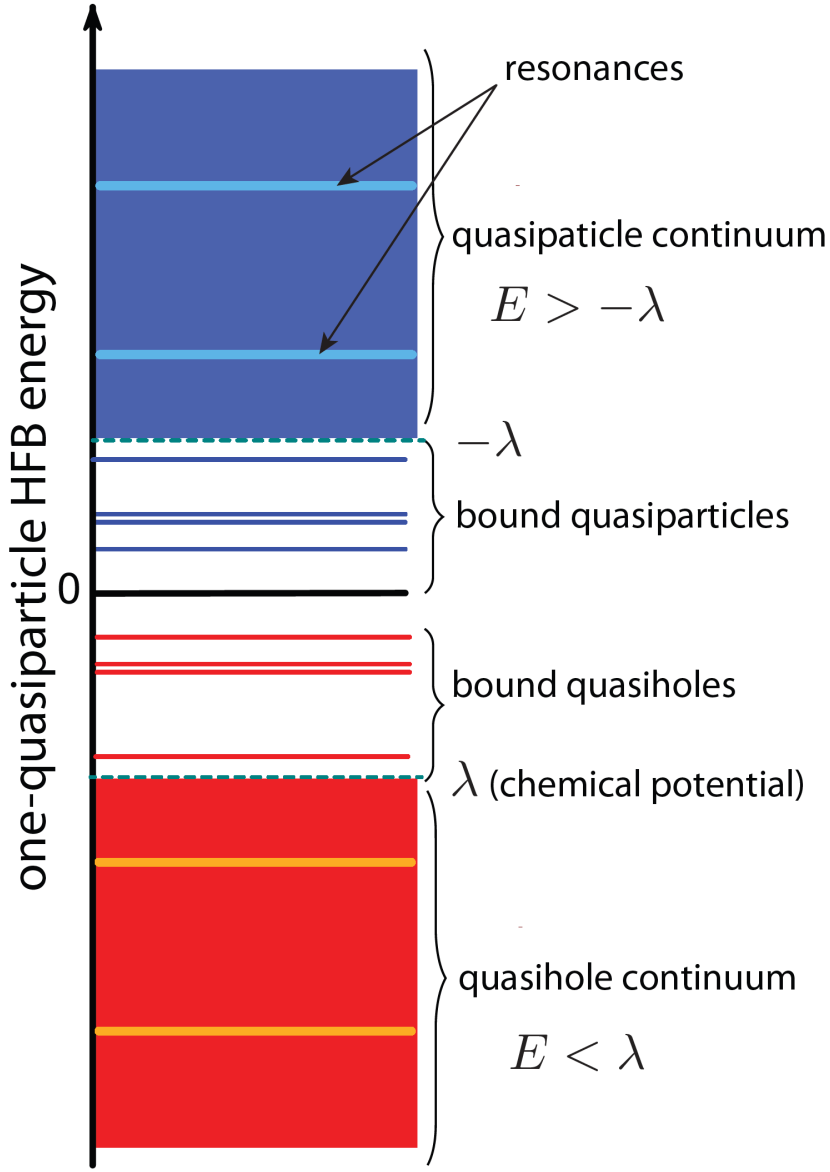
quasiparticle states

quasihole states

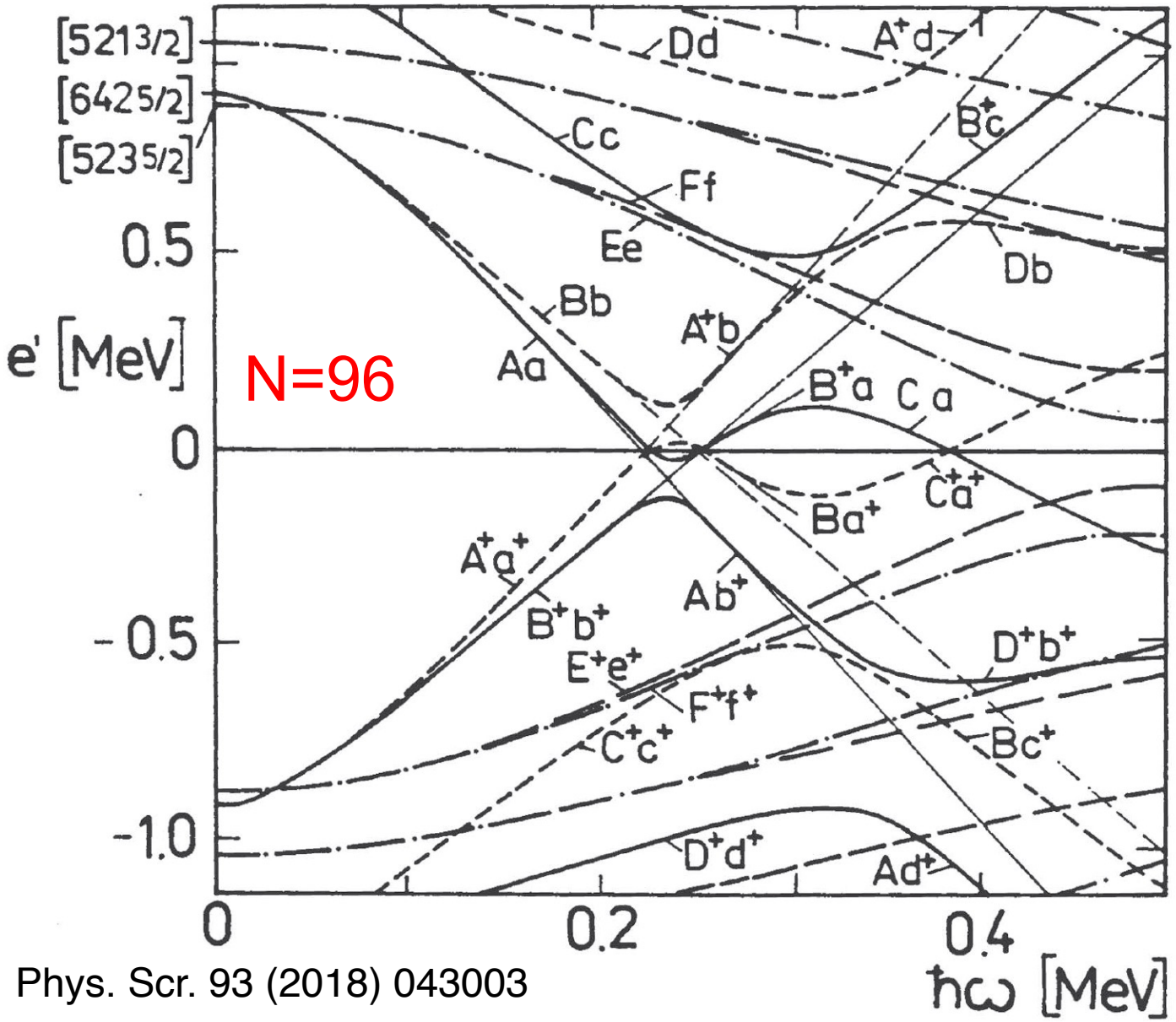
Quasiparticle spectrum of the HFB Hamiltonian

The bound states exist in the energy region $|E_i|<-\lambda$, where λ is the chemical potential (always negative for a particle-bound system).

- The spectrum is symmetric with respect to zero
- For $\lambda>0$ the entire spectrum is continuous.
- For $|E|<-\lambda$ both components are localized, and the spectrum is discrete



See, e.g., J. Dobaczewski et al., Phys. Rev. C 53, 2809 (1996)



Phys. Scr. 93 (2018) 043003

There are many formal similarities between the single-particle Dirac problem and one-quasiparticle HFB problem:

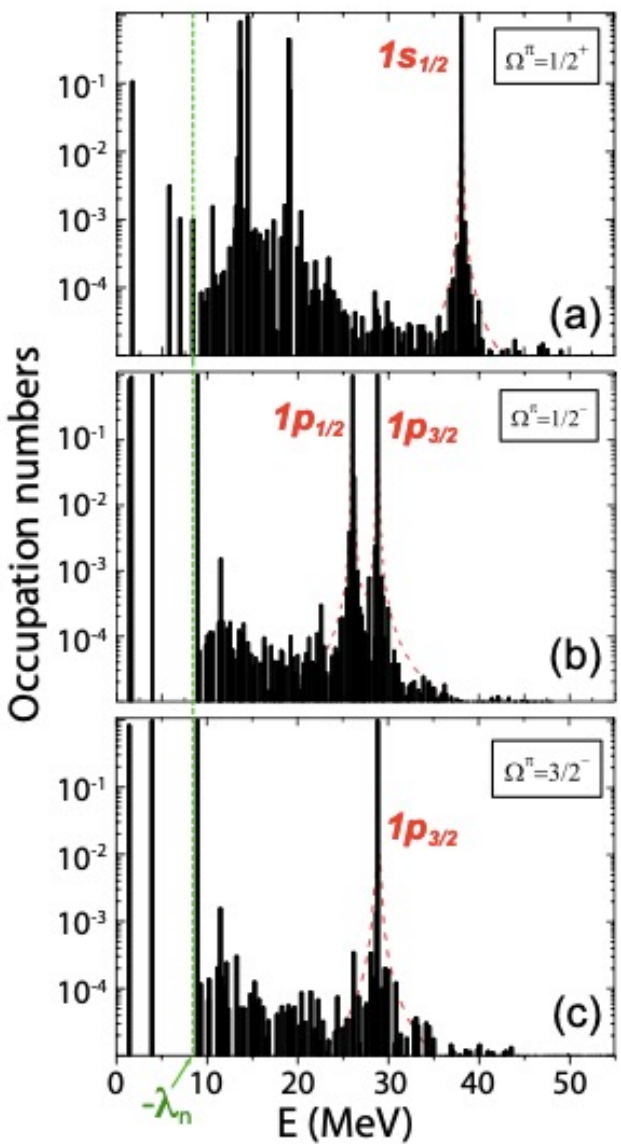
- The corresponding equations have a similar two-component form.
- In both cases, the energy spectra are symmetric with respect to zero energy. In the Dirac case, this is related to charge conjugation. In the HFB case, this is due to the quasiparticle-quasihole symmetry.
- In both cases, the resonances can be divided into particle resonances with the upper component dominating over the lower component and the hole resonances, for which the lower component dominates. At $Z > Z_{crit}$, the diving states resemble hole resonances of HFB.
- In both cases, one deals with spectra that are partly discrete and partly continuous. The continuum space contains metastable states (resonances) that are embedded in the non-resonant background.
- The Dirac and HFB spectra are bound neither from above nor from below. This leads to a variational collapse (Dirac) and difficulties with the use of the imaginary time method (for both Dirac and HFB).
- In both cases, one must face continuum-space truncations.

Those analogies can be helpful when tackling similar problems or interpreting similar phenomena with the Dirac equation.

Quasiparticle HFB continuum (box discretization)

J.C. Pei et al., Phys. Rev. C 84, 024311 (2011)

Neutrons, ^{70}Zn



the stabilization method

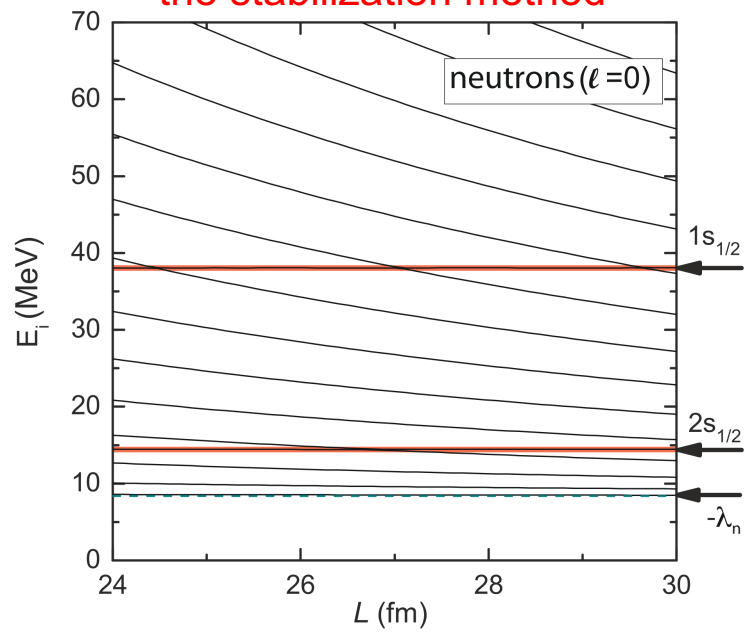


TABLE II. Energies (in MeV) and widths (in keV) of HFB neutron resonances in ^{90}Ni, calculated using the box stabilization (box) and smoothing-fitting (smf) methods. They are compared to the GHFB solutions of Ref. [8].

States	E_r	Γ_{box}	Γ_{smf}	Γ_{GHFB}
$1s_{1/2}$	51.419	–	$1.1e-3$	$1.09e-3$
$1p_{3/2}$	40.588	30.84	20.17	27.28
$1p_{1/2}$	38.770	32.26	34.67	27.14
$1d_{5/2}$	29.039	1.31	1.37	0.78
$1d_{3/2}$	25.017	25.44	23.08	22.57

Resonant (Gamow) states

A stationary approach to time-dependent process

$$\hat{H}\Psi = \left(E - i\frac{\Gamma}{2}\right)\Psi$$

outgoing solution

$$\Psi(0,k) = 0, \quad \Psi(\vec{r},k) \xrightarrow[r\to\infty]{} O_l(kr)$$

$$k_n = \sqrt{\frac{2m}{\hbar^2}\left(E_n - i\frac{\Gamma_n}{2}\right)}$$

complex pole of the S-matrix

- J.J. Thompson, 1884
- Gamow, Z. Phys. 51, 204 (1928)
- Siegert, Phys. Rev. **36**, 750 (1939)
- Humblet and Rosenfeld, Nucl. Phys. **26**, 529 (1961)

Outgoing flux and width of the Gamow state

Humblet and Rosenfeld: Nucl. Phys. 26, 529 (1961)

$$\left[\hat{T}+\hat{V}\right]\Psi=\left(e-i\frac{\Gamma}{2}\right)\Psi$$

$$\left[\hat{T}+\hat{V}\right]\Psi^{*}=\left(e+i\frac{\Gamma}{2}\right)\Psi^{*}$$

$$\hbar\int_{S}\vec{j}\,d\vec{S}=\Gamma\int_{V}\rho\,d^{3}r$$

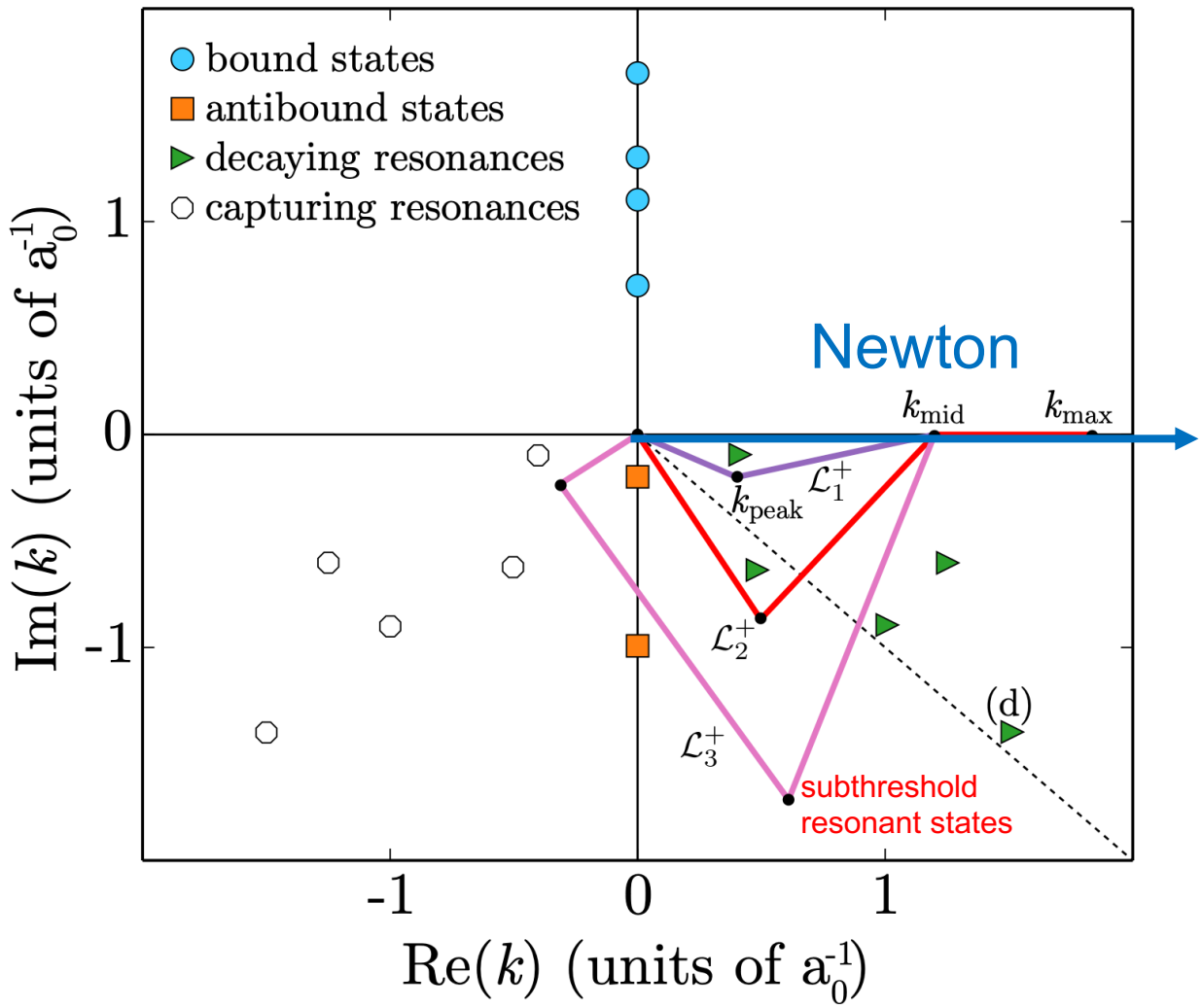
$$\vec{j}=\frac{\hbar}{2\mu i}\left(\Psi^{*}\vec{\nabla}\Psi-\Psi\vec{\nabla}\Psi^{*}\right),\quad \rho=\Psi^{*}\Psi \qquad \vec{\nabla}\vec{j}-\frac{\Gamma}{\hbar}\rho=0 \quad \left(\vec{\nabla}\vec{j}+\frac{\partial\rho}{\partial t}=0\right)$$

S can be taken as a sphere of radius *R:*

$$\Gamma=\frac{\hbar R^{2}\int j_{r}\,d\Omega}{\int_{V_R}\rho\,d^{3}r}$$

An extremely useful expression for narrow resonances!

Gamow states in the complex-k plane



- Resonant states with Re(E)>0 and small Γ can be associated with resonances.
- For antibound states Re(E) < 0 and Γ=0.
- For subthreshold resonant states Re(E) < 0 and Γ>0.
- Low-momentum antibound and threshold resonant states result in the low-energy cross-section enhancement.

$$\sum_{n\in(b,d)} |u_n\rangle\langle u_n| + \int_{L^+} |u(k)\rangle\langle u(k)| dk = 1.$$

One-body Gamow states and completeness relations

Berggren, Nucl. Phys. A109, 265 (1968); A389, 261 (1982)
Berggren and Lind, PRC 47, 768 (1993); Lind, Phys. Rev. C47, 1903 (1993)

$$\sum_{n\in(b,d)} |u_n\rangle\langle u_n| + \int_{L^+} |u(k)\rangle\langle u(k)| dk = 1.$$

Particular case: Newton completeness relation

$$\sum_{n\in(b)} |u_n\rangle\langle u_n| + \int_0^{+\infty} |u(k)\rangle\langle u(k)| dk = 1.$$

Gamow Shell Model: a CI approach for open quantum systems

One-body states must be normalized. Contour is discretized.

Many-body Slater determinants (SD) are built

$$|SD_i\rangle = |u_{i_1} \cdots u_{i_A}\rangle \qquad \sum_i |SD_i\rangle\langle\widetilde{SD_i}| \simeq 1$$

GSM Hamiltonian matrix is computed and diagonalized
(the matrix is complex symmetric!)

Many-body Gamow states must be identified

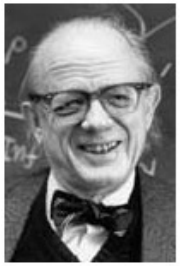
…By combining von Neumann's Hilbert space with the theory of distributions, Gel'fand and collaborators introduced the rigged Hilbert space (RHS). The rigged Hilbert space is the Hilbert space equipped with distribution theory — in Quantum Mechanics, to rig a Hilbert space means simply to equip that Hilbert space with distribution theory. Thus, the RHS is not a replacement but an enlargement of the Hilbert space.

Eur. J. Phys. 26 287 (2005)

Feshbach 1962: Q+P=1

Q – bound states

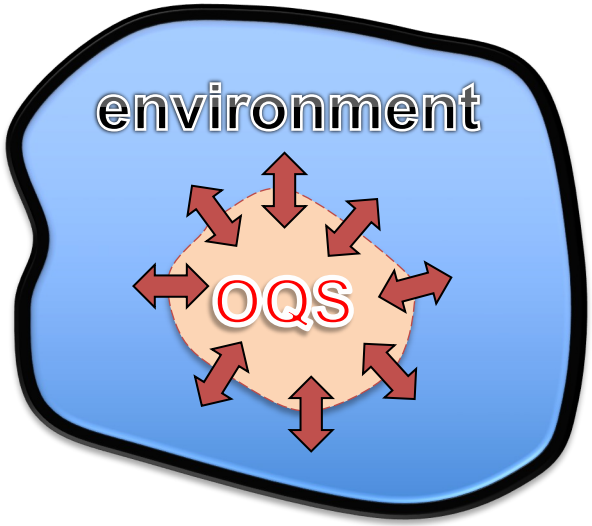
P – scattering states



Berggren 1968: Q+P=1

Q – resonant states

P – scattering states

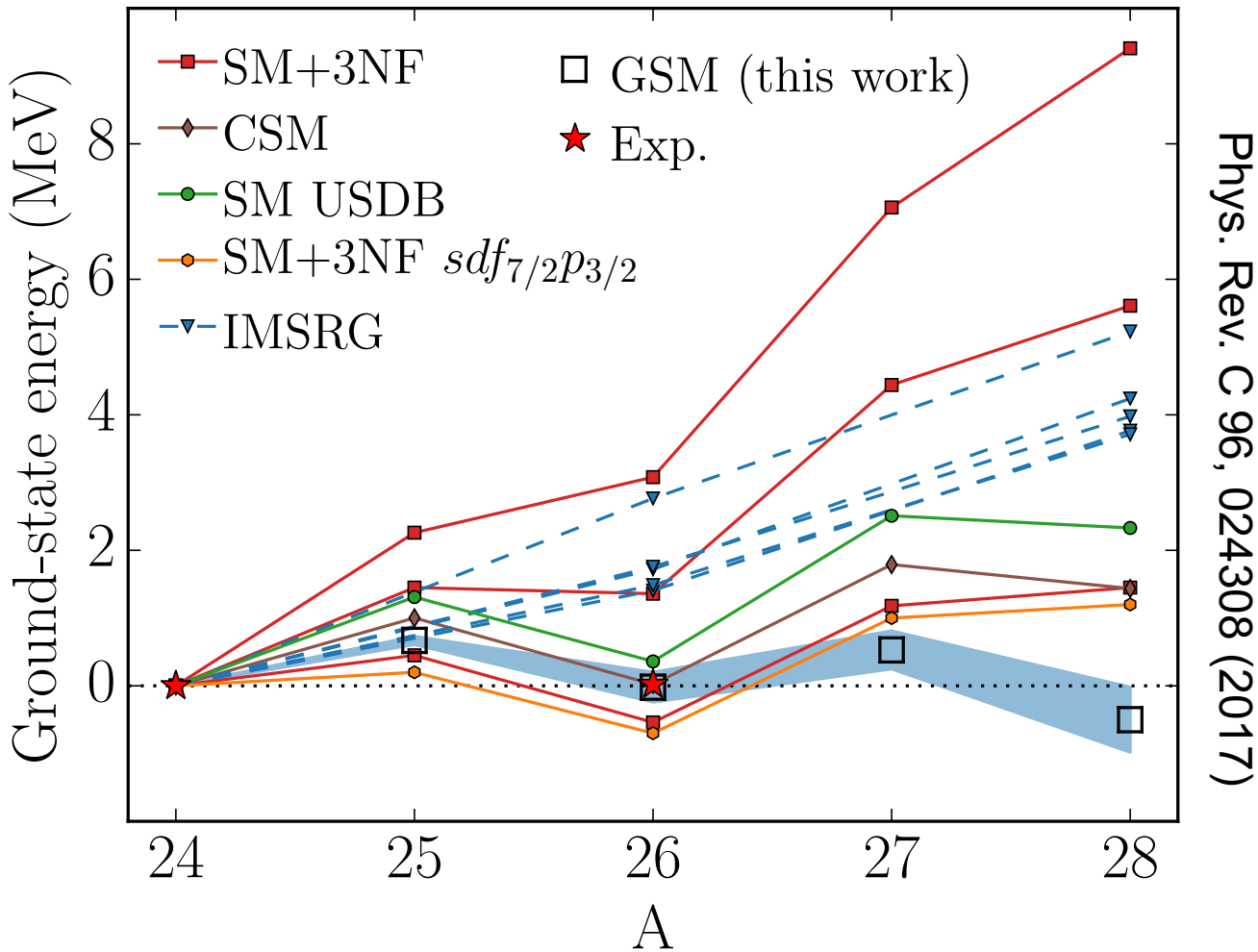


Gamow Shell Model (CI approach based on Berggren basis)

- 1998-1999: Concept (M. Płoszajczak & WN)
- 2001: Formulated
- 2002: first applications (N. Michel et al.)
  - Based on the Rigged Hilbert Space formulation of quantum mechanics
  - Biorthogonal basis; inner product defined; Gamow states normalized using external complex scaling
  - Scattering contour is identified and discretized for each partial wave
  - Many-body Slater determinants are built out of resonant and scattering states
  - GSM Hamiltonian matrix is computed (using external complex scaling) and diagonalized (the matrix is complex symmetric). The Hamiltonian matrix depends on the continuum structure!
  - Based on the generalized variational principle
  - The many-body Gamow states are identified
  - Expectation values of operators are computed
- 2006: Discretization/truncation optimized by means of the density matrix renormalization group (DMRG) (J. Rotureau)
- 2007: Gamow-Coupled-Cluster approach developed (G. Hagen)
- 2008: Gamow-HFB approach developed (N. Michel)
- 2012: GSM + Resonating Group Method extension for reactions
- 2013: No-core GSM
- 2014: Equivalence with complex scaling demonstrated
- 2017: CGSM; Equivalence of COSM and Jacobi-based formulations (S. Wang)

… and much much more. Numerous nuclear and atomic (molecular) applications

Nuclear example: the oxygen chain



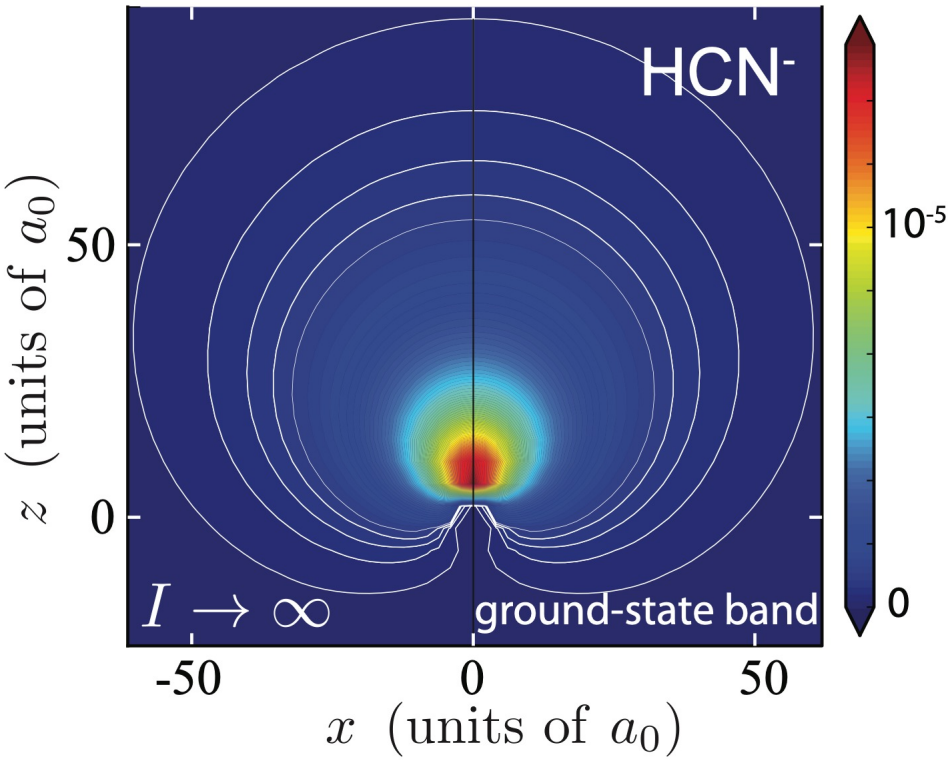
Phys. Rev. C 96, 024308 (2017)

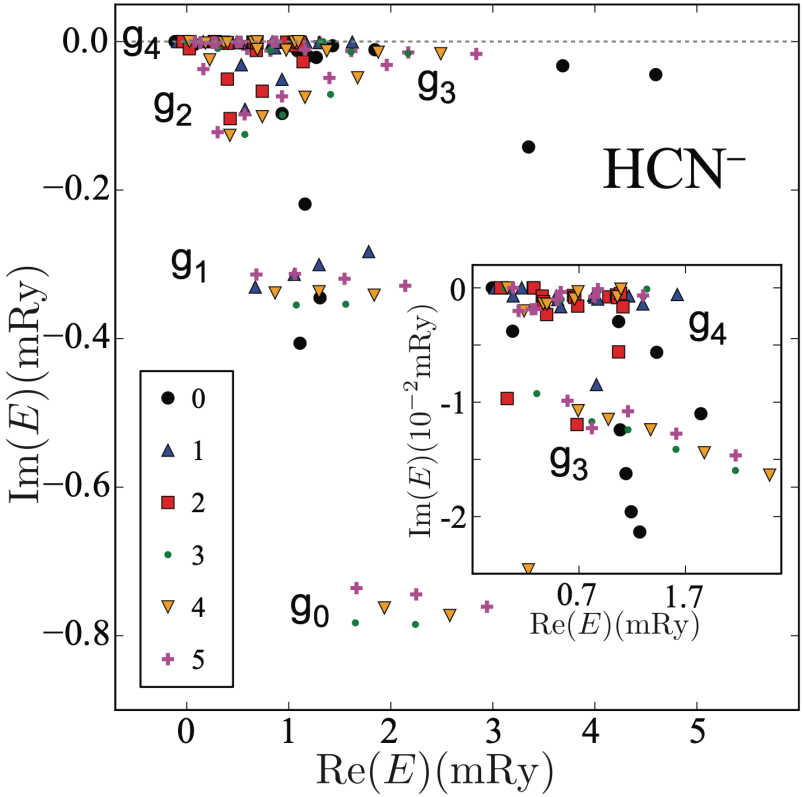
- *spdf* space essential for description of $^{26\text{-}28}$O
- ^{26,28}O predicted to be threshold systems
- *pf* continuum adds ~400keV to the binding energy of ^{28}O

Atomic example: multipole-bound anions

K. Fossez et al., Phys. Rev. A 91, 012503 (2015); X. Mao et al., Phys. Rev. A 98, 062515 (2018)

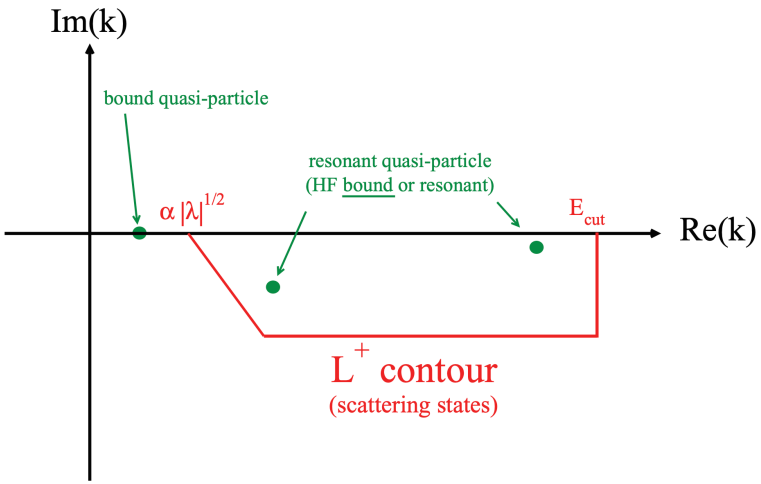
Bound and resonance states of the dipolar anion of hydrogen cyanide

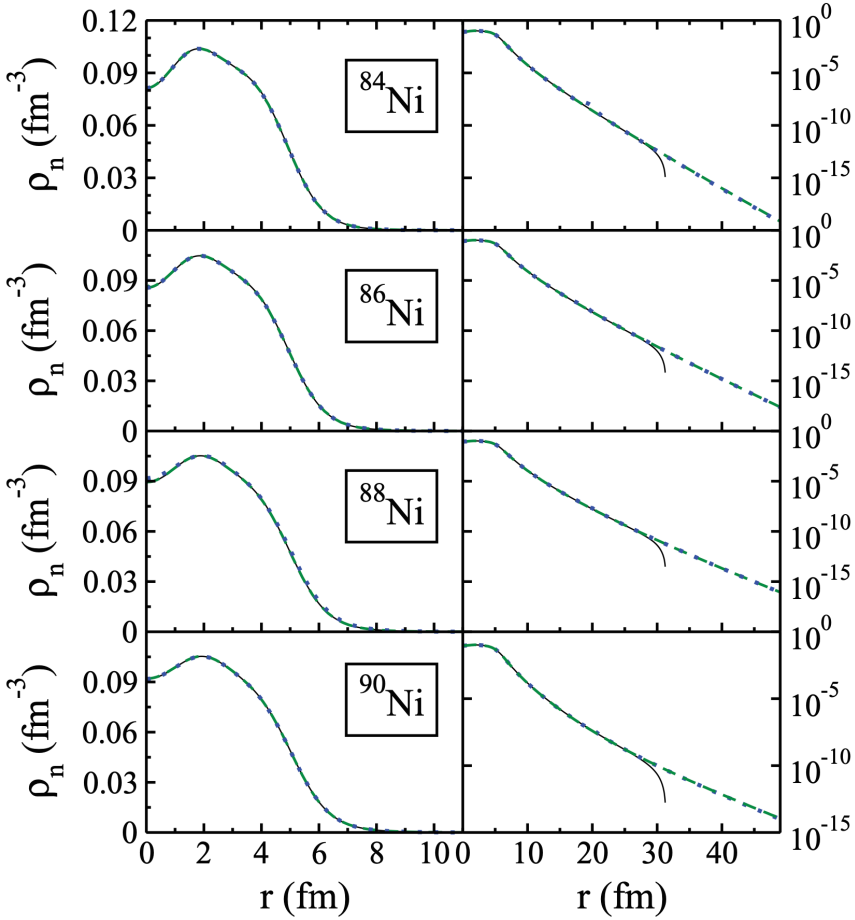




Gamow-HFB

N. Michel et al., Phys. Rev. C 78, 044319 (2008)



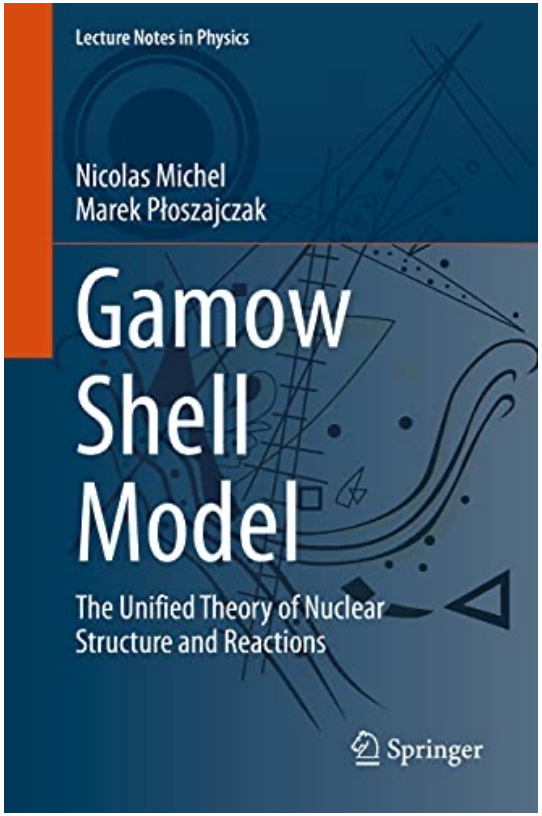


Dirac-Gamow states:

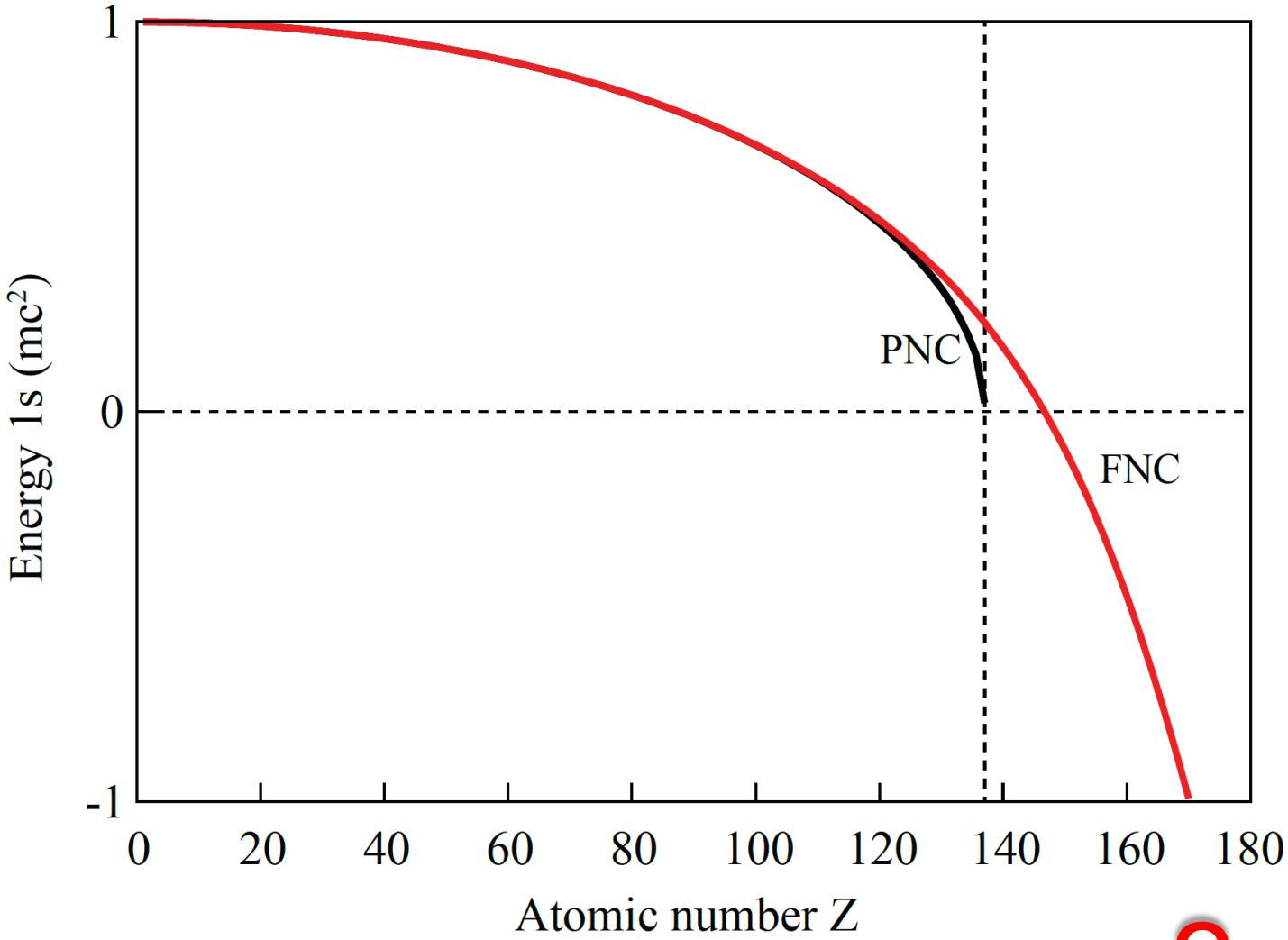
- Relativistic Hartree-Bogoliubov theory in continuum: Zhang et al., Phys. Rev. C 102 024314 (2020)
- Probing resonances in the Dirac equation with the complex momentum representation method: Fang et al., Phys. Rev. C 95 024311 (2017)

Open problems in the theory of nuclear open quantum systems

N. Michel et al., J. Phys. G **37**, 064042 (2010)



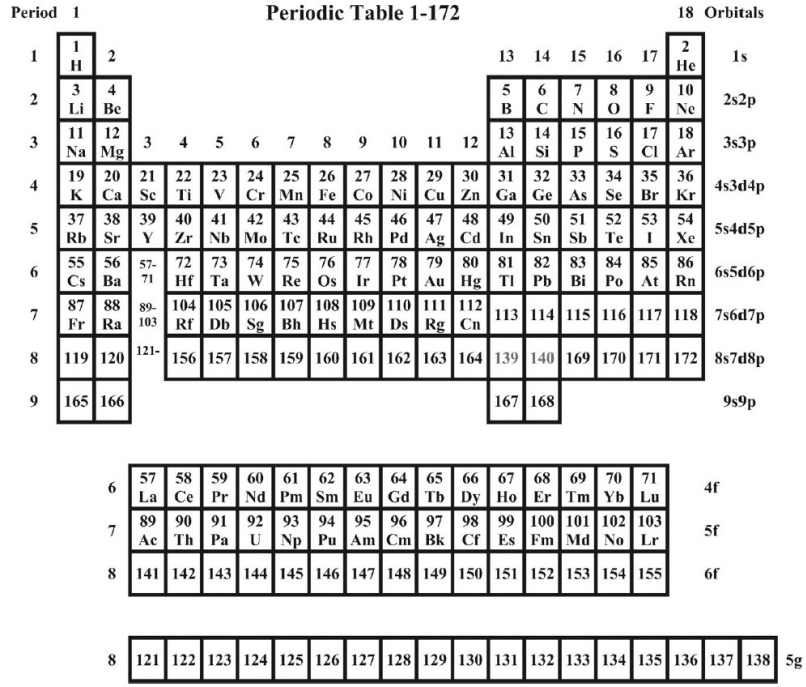
Gamow Shell Model: The Unified Theory of Nuclear Structure and Reactions (Lecture Notes in Physics Book 983)



?

diving states are Gamow resonances!

Where is the end of the Periodic Table?



A suggested Periodic Table up to Z ≤172

P Pyykkö, Phys. Chem. Chem. Phys. 13, 161 (2011)

"The chemical predictions quoted here are based on theoretical, relativistic quantum chemical calculations using established electronic Hamiltonians. The nuclei *are simply assumed to exist*, with a realistic, finite nuclear size.

A quantum chemist *can always assume a finite nucleus* of realistic size for any Z < 173 and do ab initio calculations for that theoretical model, whether or not such nuclei or their compounds are ever made."

"The discovery of a chemical element is the experimental demonstration, beyond reasonable doubt, of the existence of a nuclide with an atomic number *Z* not identified before, existing for at least 10^{-14} s". (IUPAC 1991)

Atoms cannot exist without atomic nuclei!

In order to define a nuclide, its lifetime should be longer than the single-particle time scale $3 \cdot 10^{-22}$ s that corresponds to the time scale needed to create the nuclear mean field.

- Superheavy nuclei with N>184 are expected to be short-lived because of fission.
- Because of the presence of exotic topologies (bubbles, tori) due to the Coulomb frustration, the stability of nuclei with Z>120 is difficult to access theoretically.
- It is possible that the periodic table will end well before reaching Z_{crit} for purely nuclear reasons.

No chemistry for nuclides with lifetimes between 10^{-14} and 10^{-22} s! The gaps in the periodic table?

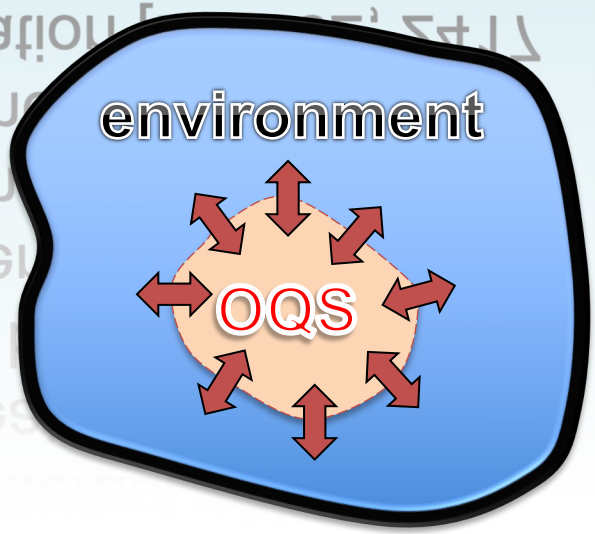
Conclusions

- Many similarities between HFB and Dirac problems
- Despite some work on resonances embedded in the continuum, a direct utilization of Dirac Gamow states in atomic many-body calculations for heavy atoms is practically nonexistent.
- The basic mathematical formulation rests on the rigged Hilbert space structure which comes with its own challenges. To be of use in atomic structure calculations of the superheavy elements, Dirac Gamow states need be studied within a multi-electron framework.
- Computing Dirac Berggren ensemble that can be used in a numerical atomic structure program packages will offer many exciting avenues.

Thank You

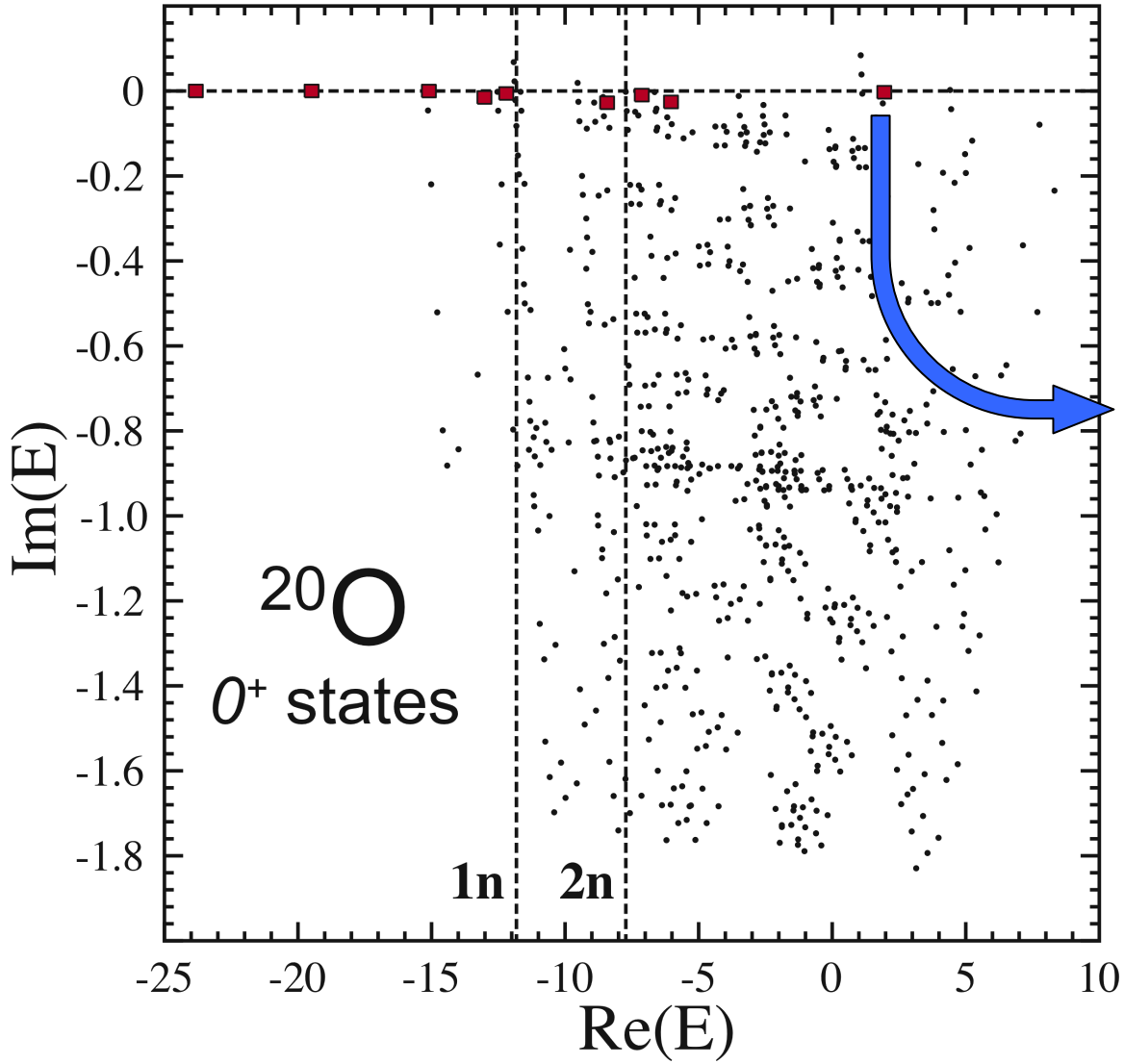
BACKUP

All real world quantum systems interact with their surrounding environment to a greater or lesser extent. Such systems are said to be open. No matter how weak the coupling that prevents the system from being isolated, the evolution of an open quantum system is eventually plagued by nonunitary features such as decoherence and dissipation [PRL 82, 2417 (1999)]



Selection of the many-body poles

N. Michel et al., Phys. Rev. Lett. 89, 042502 (2002); Phys. Rev. C 70, 064313 (2004)

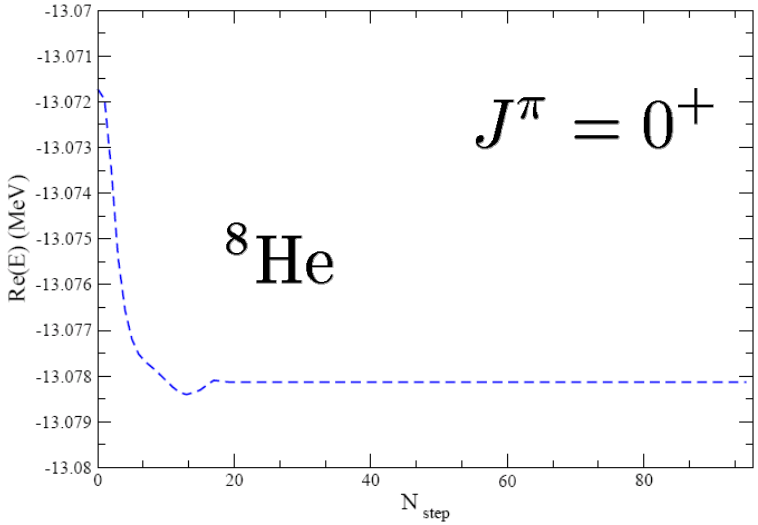


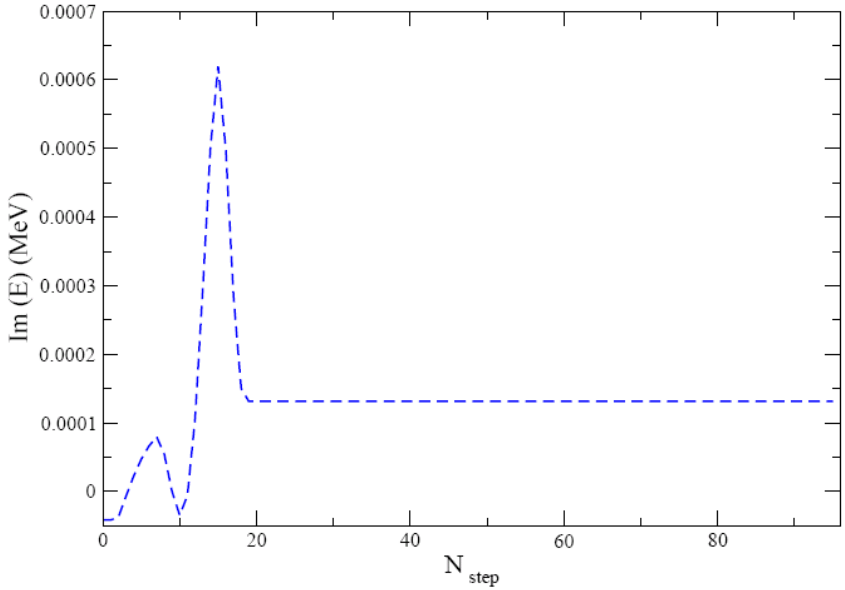
Resonances do not depend on the contour

4 neutrons in sd shell

DMRG: Density Matrix Renormalization Group

treatment of the non-resonant continuum





DMRG: S. R. White, Phys. Rev. Lett. 69, 2863 (1992)
U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005)

The many-body states constructed from the s.p. poles form a *reference* subspace, and the remaining states containing contributions from nonresonant shells form a *complementary* subspace

Warm-up phase followed by sweeping phase

total dimension=481250
largest matrix in DMRG=2061

J. Rotureau et al., PRL 97, 110603 (2006); PRC 79, 014304 (2009)

Complex scaling

Introduced in the early 1970s in atomic physics to guarantee that wave functions and resonances are square integrable.

$$\boldsymbol{r} \to e^{i\theta}\boldsymbol{r}$$

$$\hat{U}(\theta)\psi(\boldsymbol{r}) = e^{i\frac{3}{2}\theta}\psi(e^{i\theta}\boldsymbol{r})$$

Uniform complex scaling

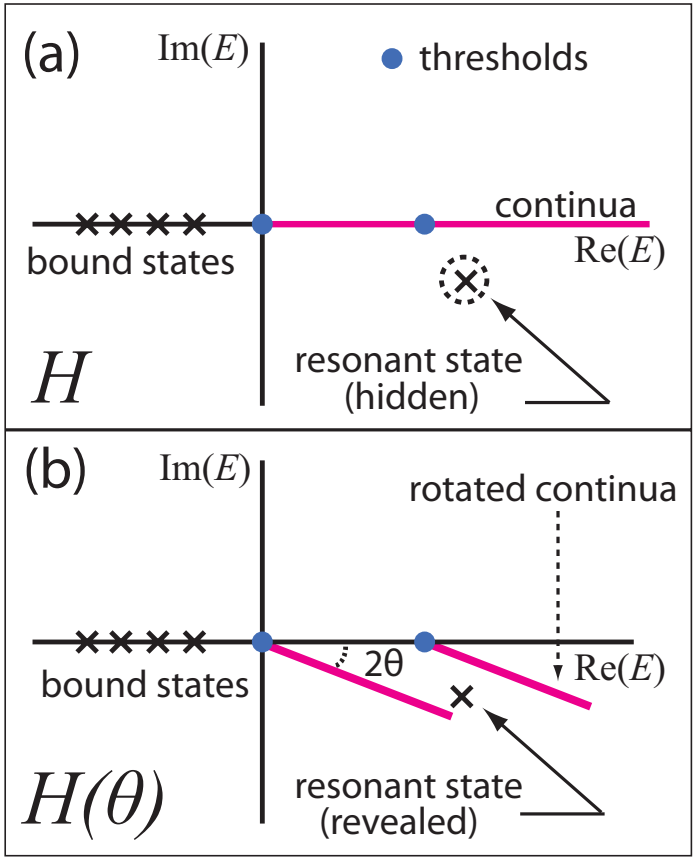
The transformed Hamiltonian is no longer hermitian as it acquires a complex potential. However, for a wide class of local and nonlocal potentials, called *dilation-analytic potentials*, the so-called ABC (Aguilar-Balslev-Combes) theorem is valid:

- The bound states of h and h_θ are the same;
- The positive-energy spectrum of the original Hamiltonian h is rotated down by an angle of 2θ into the complex-energy plane;
- The resonant states of h with eigenvalues E_n satisfying the condition $|\arg(E_n)|<2\theta$ are also eigenvalues h_θ and their wave functions are square integrable.
- To obtain densities, etc., back-rotation+regularization needed

$$\boldsymbol{r} \to \boldsymbol{r}_0 + e^{i\theta}\boldsymbol{r}$$

External complex scaling

Complex scaling (2)



Myo et al., PRC C76, 054309 (2007)