MQP excitations in nuclei: a theoretical perspective

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October 28th, 2024

The microscopic modelling of odd-mass and odd-odd nuclei.

Saclay, October 2022

Purpose of the talk

Introduce and discuss **microscopic** methods in order to study multi-quasiparticle excitation with a focus in **odd nuclei**.
So far, little (if any) attention has usually been paid by the theory community to odd nuclei (and MQP excitations)

The outline of the presentation is as follows

- Introduction
  Main differences between odd and even systems
  Some phenomenological models
- Mean field (HF and HFB): blocking
  shell model view
  Hartree-Fock
  HFB + blocking
- Beyond mean field
  Symmetry restoration
  Fluctuations

Odd and even

What makes and odd system different from an even one ?

- Pairing interaction: in even systems all nucleons form **Cooper pairs** whereas in odd systems there is always a **"single" nucleon**
  In addition to typical odd-even effect in binding energies, etc the **"single" nucleon has the tendency to quench pairing correlations**
- Time reversal invariance: Cooper pair wave function is invariant under time-reversal. The "single" nucleon one is not
  In even systems time-reversal invariance is broken for generic multiquasiparticle excitations
- **Core - "single" nucleon**: Given the above, it is customary to consider the whole nucleus as made of an even core plus the single nucleon.

Models

Based on the core + single particle paradigm

- Particle plus rotor: Based on the $I = R + j$ decomposition
  - Strong coupling limit (deformed)

$$E_{IK} = E_K + \frac{\hbar^2}{2\mathcal{J}}[I(I+1) - K^2 + \delta_{K,1/2}a(-1)^{I+1/2}(I+1/2)]$$

  - Weak coupling limit (spherical)
  - Aligned limit (spherical+high j orbital)
- Particle + vibration coupling: More microscopic, based on QRPA and fermionic extensions

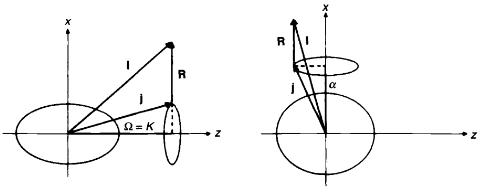
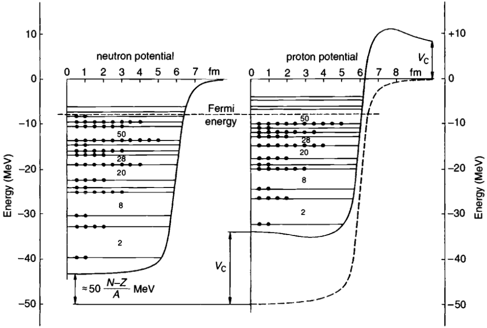


Fig. 11.3. Schematic illustration of the two extreme coupling schemes; deformation alignment (left figure) and rotation alignment (right figure) (from R.M. Lieder and H. Ryde, *Adv. in Nucl. Phys.*, eds. M. Baranger and E. Vogt (Plenum Publ. Corp., New York) vol. 10 (1978) p. 1).

Mean field

The mean field approach is the starting point for any microscopic treatment of nuclear dynamics

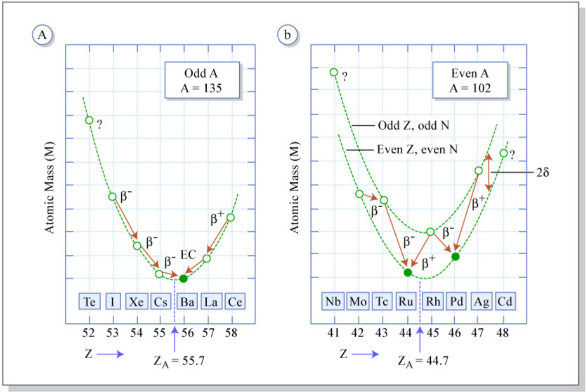
Mean field generates orbits where one places protons and neutrons respecting Pauli exclusion principle



Slater determinants

Pairing

- Strong experimental evidence supporting the existence of a short range attractive interaction: **Pairing**
  Mass parabolas



e-e 163, e-o: 51, o-e: 50, o-o:4

Pairing

PHYSICAL REVIEW VOLUME 110, NUMBER 4 MAY 15, 1958

Possible Analogy between the Excitation Spectra of Nuclei and Those of the Superconducting Metallic State

A. Bohr, B. R. Mottelson, and D. Pines*
Institute for Theoretical Physics, University of Copenhagen, Copenhagen, Denmark, and Nordisk Institut for Teoretisk Atomfysik, Copenhagen, Denmark

(Received January 7, 1958)

The evidence for an energy gap in the intrinsic excitation spectrum of nuclei is reviewed. A possible analogy between this effect and the energy gap observed in the electronic excitation of a superconducting metal is suggested.

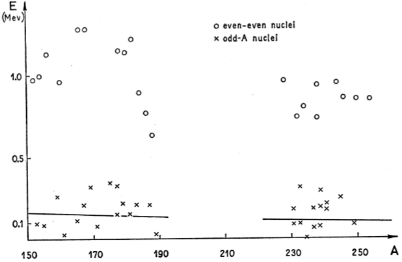


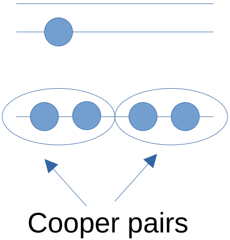
Fig. 1. Energies of first excited intrinsic states in deformed nuclei, as a function of the mass number. The experimental data may be found in *Nuclear Data Cards* [National Research Council, Washington, D. C.] and detailed references will be contained in reference 1 above. The solid line gives the energy $\delta/2$ given by Eq. (1), and represents the average distance between intrinsic levels in the odd-A nuclei (see reference 1).

The figure contains all the available data for nuclei with $150<A<190$ and $228<A$. In these regions the nuclei are known to possess nonspherical equilibrium shapes, as evidenced especially by the occurrence of rotational spectra (see, e.g., reference 2). One other such region has also been identified around $A=25$; in this latter region the available data on odd-A nuclei is still represented by Eq. (1), while the intrinsic excitations in the even-even nuclei in this region do not occur below 4 Mev.

We have not included in the figure the low lying $K=0$ states found in even-even nuclei around Ra and Th. These states appear to represent a collective odd-parity oscillation.

Pairing

- Pairing leads to correlated structures: **Cooper pairs** of protons and neutrons coupled to $J = 0^+$ ($k, \bar{k}$ scheme: time reversal invariance !)



- BCS theory of superconductivity

$$|BCS\rangle = \mathcal{N} \prod_{k>0} (u_k + v_k c^+_k c^+_{\bar{k}})|\rangle$$

$$\alpha^+_k = u_k a^+_k - v_k a_{\bar{k}} \qquad \alpha^+_{\bar{k}} = u_k a^+_{\bar{k}} + v_k a_k$$

Focused on "pairs" , breaks particle number symmetry

Framework

- The interplay between Cooper pairs and the “single nucleon” in odd nuclei require the introduction of the Hartree-Fock-Bogoliubov (HFB) method
- The same holds if one is dealing with two-quasiparticle excitations, etc
- The concept of “blocked” HFB wave function appears naturally. Fortunatelly, an addapted version of Wick’s theorem also applies in this case
- Time reversal symmetry is broken because one is dealing with Cooper pairs $J = 0$ and a single nucleon with angular momentum j
- Due to polarization effects, many **“blocking configurations”** have to be explored

Multi-quasiparticles

Mean field plus pairing (Hartree Fock Bogoliubov, HFB) based on the Bogoliubov transformation to quasi-particles

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^+ & V^+ \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} \equiv W^+ \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$$

The c^+ and c creation and annihilation operators in a convenient fermion single particle basis (harmonic oscillator, ...)

- **HFB ground state** defined by $\beta_\mu|\Phi\rangle = 0$.
- Wick's theorem to compute mean values $\langle\Phi|c_k^+ c_l^+ c_m c_n|\Phi\rangle$
- U and V determined by the variational principle on $\langle\Phi|\hat{H}|\Phi\rangle$
- HFB solution: $\hat{H} = H_0 + \sum_\mu E_\mu \beta_\mu^+ \beta_\mu + \cdots$ Quasiparticle energies E_μ

Multi-quasiparticles

If $|\Phi\rangle$ is a fully paired state corresponding to an even nucleus and with number parity even then, in the canonical basis

$$|HFB\rangle = \mathcal{N} \prod_{k>0} (u_k + v_k a_k^+ a_{\bar{k}}^+)|\rangle$$

- $\beta_\mu^+|\Phi\rangle$ corresponds to an odd system (number parity changes)
  In the canonical basis $\mathcal{N} a_{k_0}^+ \prod_{k>0,\neq k_0}(u_k + v_k a_k^+ a_{\bar{k}}^+)|\rangle$
  k_0 is the **blocked** level
- $\beta_\mu^+ \beta_\nu^+|\Phi\rangle$ is an elementary excitation of $|\Phi\rangle$
  In the canonical basis $\mathcal{N} a_{k_0}^+ a_{k_1}^+ \prod_{k>0,\neq k_0,\neq k_1}(u_k + v_k a_k^+ a_{\bar{k}}^+)|\rangle$
- $\beta_\mu^+ \beta_\nu^+ \beta_\rho^+|\Phi\rangle$ is an elementary excitation of the odd system
- $\beta_\mu^+ \beta_\nu^+ \beta_\rho^+ \beta_\sigma^+|\Phi\rangle \dots$ four-QP states
- $\vdots$

Multi-quasiparticles (MQP)

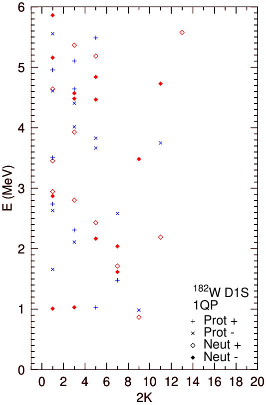
- **MQP perturbative:** U, V obtained once for all (from g.s. $|\Phi_0\rangle$). Excitation energy: sum of the quasiparticle energy of each blocked level $E_{\mu\nu} = E_\mu + E_\nu + \cdots$ for $\beta_\nu^+ \beta_\mu^+ |\Phi_0\rangle$
- **MQP selfconsistent:** Each mqp excitation has its own U and V amplitudes obtained by invoking the variational principle. For instance, minimizing 2qp energies

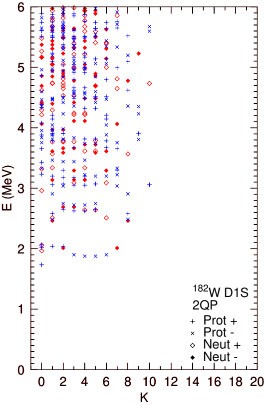
$$\delta E_{\mu\nu} = \delta \langle \Phi | \beta_\mu \beta_\nu \hat{H} \beta_\nu^+ \beta_\mu^+ | \Phi \rangle = 0 \Longrightarrow U^{(\mu\nu)} \, V^{(\mu\nu)}$$

$$E_{\mu\nu} = \langle \Phi | \beta_\mu \beta_\nu \hat{H} \beta_\nu^+ \beta_\mu^+ | \Phi \rangle - \langle \Phi_0 | \hat{H} | \Phi_0 \rangle$$

- **Selfconsistency**: each excitation has its own multipole deformation parameters, pairing properties, etc
- MQP excitations treated with the **blocking** method
- **Axial symmetry:** K good quantum number
- **Constrains** on collective variables provide specific PES for each MQP. Crucial for a proper treatment of fluctuations.

One and two qp excitations

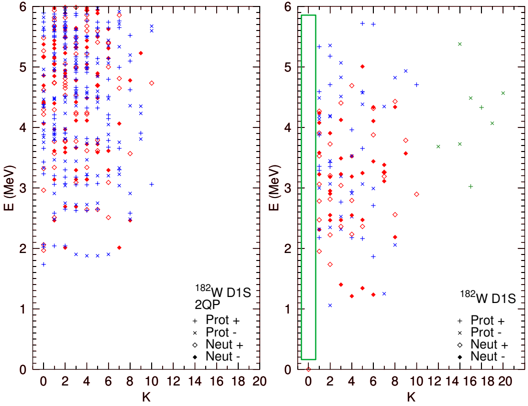




Symbol code inverted in 2QP energies

- ^{182}W
- Axial calculation
- Gogny force
- K is a good quantum number
- 1QP excitation energies E_μ
- 2QP excitation energies $E_\mu + E_\nu$

Selfconsistency

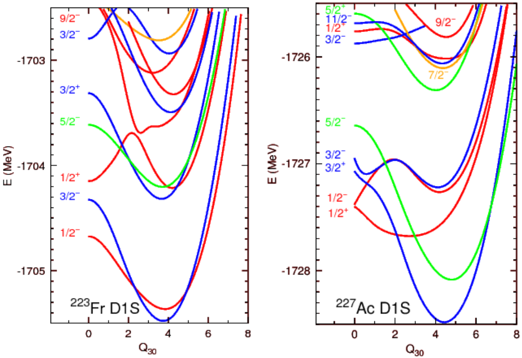


- Axial calculation
- Gogny force
- K is a good quantum number
- Factor of two reduction excitation energies
- Green symbols, 4QP excitation

Symbol code inverted in 2QP energies

Note: Many blocked configurations converge to the same state. This explains the smaller number of blocked states as compared to perturbative 2QP excitations of the ground state and the absence of $K = 0$ states. **Orthogonality constraint!**

Selfconsistency



- Axial calculation
- Gogny force D1S
- K is a good quantum number
- Shape of PES depend on blocked level. Relevant for fluctuations on collective coordinates

Selfconsistency shifts the octupole moment of blocked configurations to non-zero values and each configuration has its own value of Q_{30}

The blocking method

Common wisdom: to treat quasiparticle excitations just exchange corresponding columns of U and V amplitude
To get an easy understanding of this rule let us consider the quasiparticle density for the fully paired HFB gs vacuum

$$\mathbb{R} = \begin{pmatrix} \langle\Phi|\beta^\dagger_\mu\beta_\nu|\Phi\rangle & \langle\Phi|\beta^\dagger_\mu\beta^\dagger_\nu|\Phi\rangle \\ \langle\Phi|\beta_\mu\beta_\nu|\Phi\rangle & \langle\Phi|\beta_\mu\beta^\dagger_\nu|\Phi\rangle \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{I} \end{pmatrix}$$

where I is the identity matrix.
From $\mathbb{R}$ one gets the single particle generalized density

$$\mathcal{R} = \begin{pmatrix} \langle\Phi|c^\dagger_k c_l|\Phi\rangle & \langle\Phi|c^\dagger_k c^\dagger_l|\Phi\rangle \\ \langle\Phi|c_k c_l|\Phi\rangle & \langle\Phi|c_k c^\dagger_l|\Phi\rangle \end{pmatrix} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix} = W\mathbb{R}W^\dagger\,.$$

used to compute observables (Wick's theorem).

The blocking method

For $|\tilde{\Phi}_\mu\rangle = \beta^+_{\mu_1} \cdots \beta^+_{\mu_M}|\Phi\rangle$ one gets

$$\mathbb{R}_\mu = \begin{pmatrix} \mathbb{I}_\mu & 0 \\ 0 & \mathbb{I} - \mathbb{I}_\mu \end{pmatrix} \quad (\mathbb{I}_\mu)_{\sigma\rho} = 1 \quad \text{if} \quad \mu = \sigma = \rho\,; \quad 0 \text{ otherwise}\,,$$

The following decomposition holds

$$\mathbb{R}_\mu = \mathbb{S}_\mu \mathbb{R} \mathbb{S}^\dagger_\mu\,, \quad \mathbb{S}_\mu = \begin{pmatrix} \mathbb{I} - \mathbb{I}_\mu & \mathbb{I}_\mu \\ \mathbb{I}_\mu & \mathbb{I} - \mathbb{I}_\mu \end{pmatrix}$$

Where the "swap" matrix $\mathbb{S}$ acting on W gives $W_\mu = W\mathbb{S}_\mu$, where **the μ columns of U and V are exchanged**. Then

$$\begin{aligned} \mathcal{R}_\mu &= \begin{pmatrix} \langle\tilde{\Phi}|c^\dagger_k c_l|\tilde{\Phi}\rangle & \langle\tilde{\Phi}|c^\dagger_k c^\dagger_l|\tilde{\Phi}\rangle \\ \langle\tilde{\Phi}|c_k c_l|\tilde{\Phi}\rangle & \langle\tilde{\Phi}|c_k c^\dagger_l|\tilde{\Phi}\rangle \end{pmatrix} \\ &= W\mathbb{R}_\mu W^\dagger = W\mathbb{S}_\mu \mathbb{R} \mathbb{S}^\dagger_\mu W^\dagger = W_\mu \mathbb{R}\, W^+_\mu \end{aligned} \qquad (1)$$

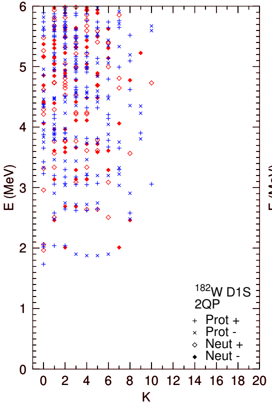
Self-consistent

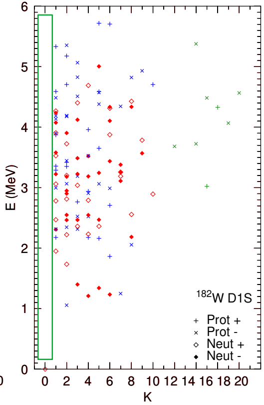
- U and V amplitudes are determined by the variational principle for each MQP configuration

$$\delta\langle\Phi|\beta_{\mu_N}\ldots\beta_{\mu_1}\hat{H}\beta^+_{\mu_1}\ldots\beta^+_{\mu_N}|\Phi\rangle = 0$$

- Iterative solution (Gradient, iterative diagonalization, etc)
- **If no orthogonality constraint imposed, it is very likely to converge always to the same minimum with the same quantum numbers irrespective of initial configuration**
- Orthogonality can be enforced by using symmetry quantum numbers, like K or π, i.e. $\mu \rightarrow \Omega_\mu, \pi_\mu, \ldots$
- For those states with the same quantum numbers, a constraint on the overlap $\langle\Phi|\Phi_m\rangle$ is required ($|\Phi_m\rangle$ target state to be orthogonal to). Easy to handle with the **gradient method** used to solve HFB and some linear algebra stuff.

Selfconsistency





- Axial calculation
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Symbol code inverted in 2QP energies

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Orthogonality constraint

- The overlap $\langle \Phi_1 | \Phi_0 \rangle$ is proportional to $\det A$ with

$$A = U_1^+ U_0 + V_1^+ V_0$$

- The gradient of the constraint is easy to compute, and turns out to be proportional to

$$A^{-1} \det A$$

- This is a indeterminacy as $\det A \to 0$ implies a non invertible A. The conundrum is solved using the Singular Value Decomposition (SVD) of A.
- The situation is simpler if a constraint on $\langle \Phi_1 | \Phi_0 \rangle \approx 1$ is required as in recent publications on fission

Density dependent forces

- Density dependent forces depend upon the mean field solution $|\Phi\rangle$ through the spatial density $\rho(\vec{r}) = \langle\Phi|\hat{\rho}(\vec{r})|\Phi\rangle$
- The quasiparticle energies E_{μ_i} are obtained from the $|\Phi\rangle$ solution through **generalized Brillouin** and contain the rearrangement term
- MQP excitations should satisfy $E_{\mu_1} + \cdots + E_{\mu_M} = \langle\Phi|\beta_{\mu_M}\cdots\beta_{\mu_1}\Delta\hat{H}\beta^+_{\mu_1}\cdots\beta^+_{\mu_M}|\Phi\rangle + \cdots$
- This requires the density

$$\rho(\vec{r})_{\mu_1,\ldots,\mu_M} = \langle\Phi|\beta_{\mu_M}\cdots\beta_{\mu_1}\hat{\rho}\beta^+_{\mu_1}\cdots\beta^+_{\mu_M}|\Phi\rangle$$

in the density dependent part of the interaction [1]

[1] Using $\rho(\vec{r})_{\mu_1,\ldots,\mu_M} = \rho_0(\vec{r}) + \sum_{\mu=\mu_1}^{\mu_M} \rho^{11}_{\mu,\mu}(\vec{r})$ and expanding the ρ^α term to first order in $\rho^{11}_{\mu,\mu}$ the energy $E_{\mu_1,\ldots,\mu_M}$ can be written as the sum of the HFB energy of the reference state plus the sum of quasiparticle energies E_{μ_i} plus an interaction term

Equal Filling Approx

- The Equal Filling Approx (EFA) represents a good alternative if time-odd components of the force are not relevant (or not under control)
- Typical example: BCPM functional
- **Odd nuclei:** both the blocked quasiparticle K_i and its time reversed partner have **statistical** occupancy one-half.
- Justified by using quantum statistical admixtures with fixed probabilities
- For two (four, etc) quasiparticle both the blocked quasiparticles K_i, K_j and their time reversed partners have **statistical** occupancy 0.5

EFA

- The EFA can be viewed as a quantum statistical system where both $\beta^+_{\mu_B}|\phi\rangle$ and $\beta^+_{\bar{\mu}_B}|\phi\rangle$ are present with equal probability $1/2$.
- Introduce a quantum density operator $\mathcal{D}$ ($\hat{\mathcal{D}}\beta^\dagger_\mu = p_\mu \beta^\dagger_\mu \hat{\mathcal{D}}$) and mean values are replaced by traces over multiquasiparticle excitations
- Thanks to Gaudin's theorem (Wick's theorem for statistical averages) every mean value takes the standard form in terms of density and pairing tensor, but as a function of the statistical density and pairing tensor.
- The statistical density and pairing tensor are nothing but the EFA quantities
- The formalism of finite temperature can be borrowed
- As a consequence, EFA is a variational theory and gradient methods can be used to derive and solve the EFA-HFB equation.

EFA

In the EFA, the time-reversal-breaking term is "averaged" in the density

$$\rho^{EFA}_{kk'} = \left(V^* V^T \right)_{kk'} \tag{2}$$

$$+ \frac{1}{2} \left(U_{k'\mu_B} U^*_{k\mu_B} - V^*_{k'\mu_B} V_{k\mu_B} + U_{k'\overline{\mu}_B} U^*_{k\overline{\mu}_B} - V^*_{k'\overline{\mu}_B} V_{k\overline{\mu}_B} \right) \tag{3}$$

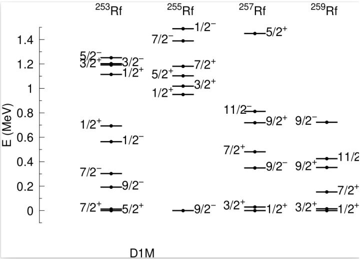
and pairing tensor

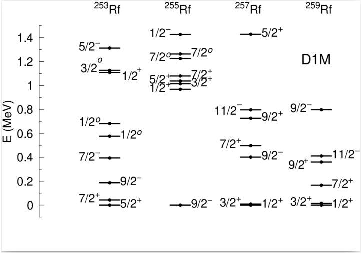
$$\kappa^{EFA}_{kk'} = \left(V^* U^T \right)_{kk'} \tag{4}$$

$$+ \frac{1}{2} \left(U_{k\mu_B} V^*_{k'\mu_B} - U_{k'\mu_B} V^*_{k\mu_B} + U_{k\overline{\mu}_B} V^*_{k'\overline{\mu}_B} - U_{k'\overline{\mu}_B} V^*_{k\overline{\mu}_B} \right) \tag{5}$$

Every mean value is written replacing the "blocked" density and pairing tensor by the EFA ones.

Examples

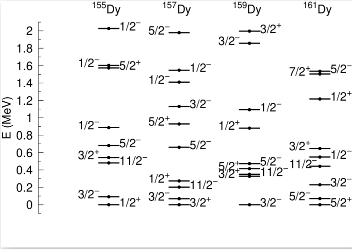


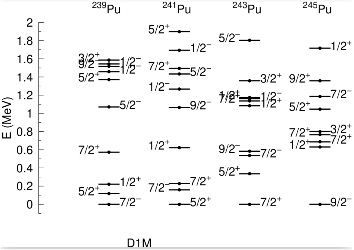


A comparison D1M (EFA) and D1M (fulll blocking)

- The two spectrum are similar and therefore one can conclude that **time-odd fields are not relevant**
- The same happens all over the nuclear chart
- The relevant factor for the reduction of excitation energies is the **quenching of pairing correlations** . Pairing correlations measured by $\langle \Delta N^2 \rangle$. Dynamic pairing !

Examples



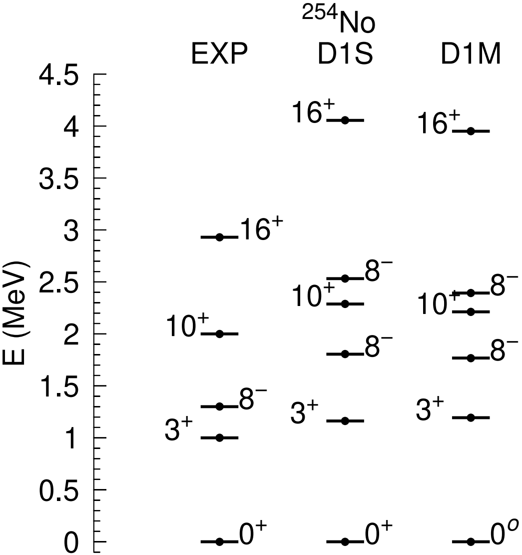


More examples of blocking calculations in the rare earth and actinide region

Note that there are just a few duplicated quantum numbers: no orthogonality constraint in this calculation

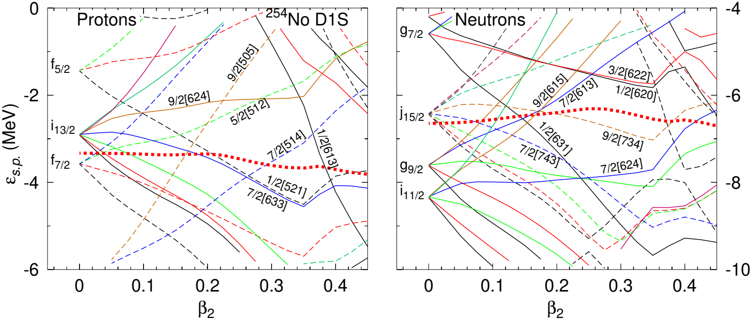
States with duplicated quantum numbers correspond to different deformation parameters (i.e. different local minima)

^{254}No (High-K isomers)



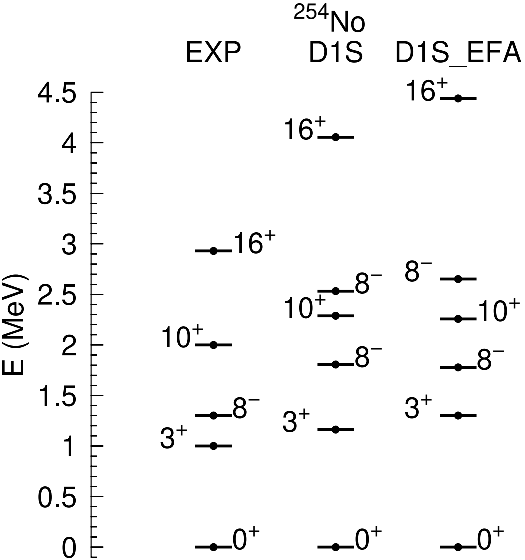
- ^{254}No
- Exp vs D1S and D1M
- 4QP isomers (2 prot - 2 neut)
- Perturbative 2QP energies typically twice as high
- Strong reduction of $\langle \Delta N^2 \rangle$.
- **Quenched pairing calls for dynamic pairing treatment**
- Dominant Nilsson components of the QP operators coincide with empirical assignments

^{254}No



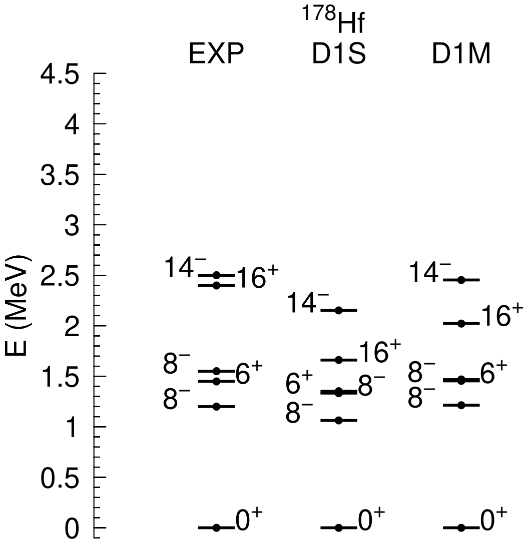
- ^{254}No with Gogny D1S
- Proton and neutron single particle energies
- $\beta_2 \approx 0.28$
- 3^+ 2QP proton $7/2^-$, $1/2^-$
- 8^- 2QP neutron $9/2^-$, $7/2^+$
- 10^+ 2QP neutron $7/2^-$, $11/2^+$
- 8^- 2QP proton $7/2^-$, $9/2^+$
- 16^+ 2QP-p $7/2^-$, $9/2^+$ 2QP-n $9/2^-$, $7/2^+$

^{254}No EFA



- ^{254}No
- D1S and D1S (EFA))
- Reasonable agreement between full blocking and EFA
- **Time-odd fields not relevant**
- Strong reduction of $\langle \Delta N^2 \rangle$.
- Quenching of pairing correlations is the main mechanism to explain the reduction of excitation energies .

^{178}Hf



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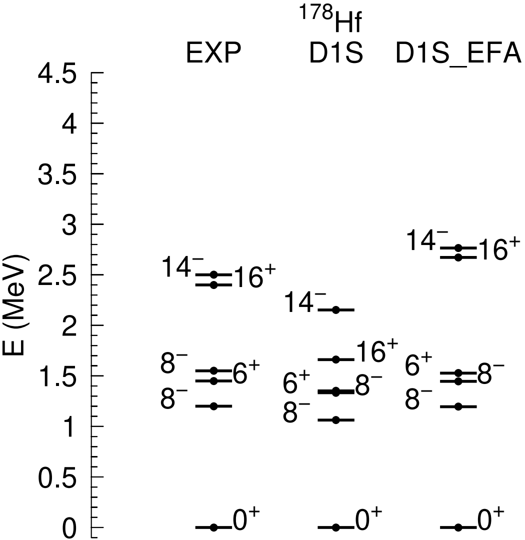
^{178}Hf EFA



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Odd-odd systems

The formalism described above can be easily extended to odd-odd systems by locking at the same time protons and neutrons

In the EFA, no Gallaguer-Mozkowski splitting

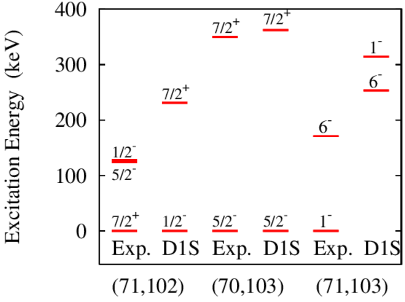


Figure 1: Low-lying band heads in the spectra of the nucleus ^{174}Lu and odd-A neighbors: ^{173}Lu (left); ^{173}Yb (center) ^{174}Lu (right). Due to the inversion of the lowest proton quasi-

- Reproducing experimental data not so easy
- GM splitting depends on spin-spin interaction
- Not well under control in Gogny D1S
- Density dependent channel seems to be responsible

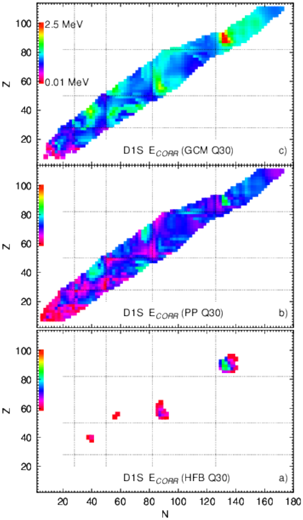
Beyond mean field

The spectra obtained are expected to be sensitive to interaction details and beyond mean field effects

- EDF contain very few parameters to fit single particle properties. Universal, no local fitting
- Pairing correlations severely quenched: **Dynamic pairing and particle number projection important**
- Non uniform response to collective parameters imply that symmetry restoration has to be implemented using the **Variation After Projection (VAP)** instead of Projection After Variation (PAV)
- Non uniform response to fluctuations in collective variables (Particle-Vibration coupling ?)

Beyond mean field effects may have a strong impact on the ordering of levels

Importance of VAP and fluctuations



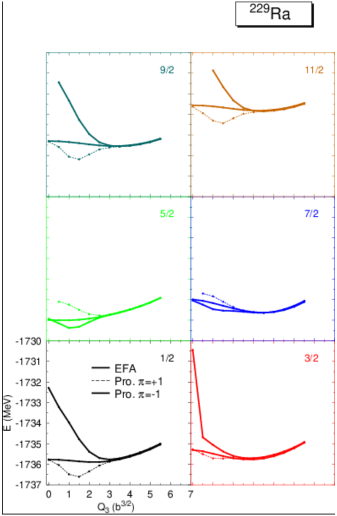
Octupole collectivity in even-even systems

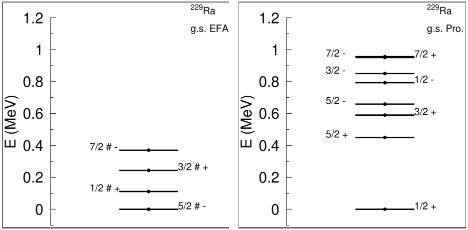
- a) Mean field octupole correlation energy
- b) VAP parity projection
- c) Fluctuations in the octupole moment

VAP and fluctuations important in the whole nuclear chart

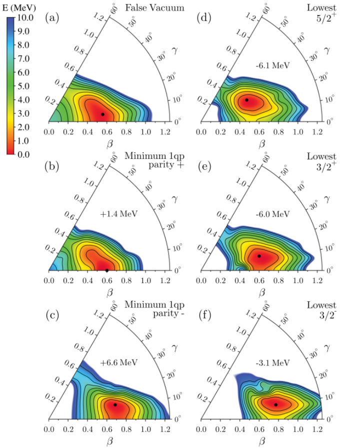
Non-trivial Z and N dependence

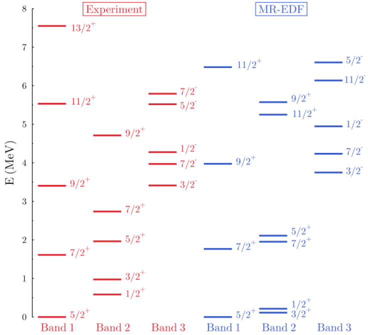
Beyond mean field, Parity projection





Symmetry restoration (AMP+PNP)

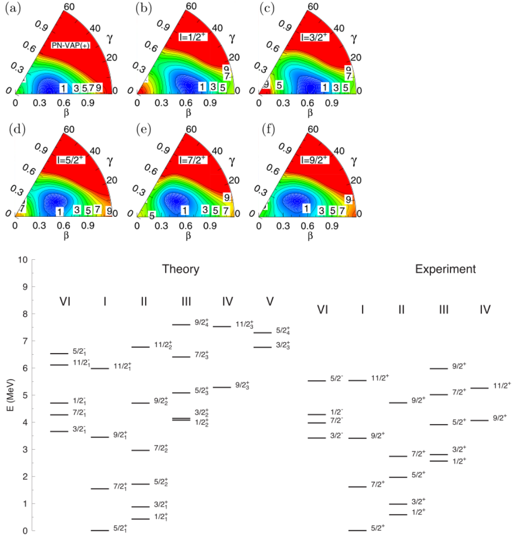




RVAP (Deformation) Lipkin Nogami (PNP)

SLyMR0
B. Bally, PhysRevLett.113.162501

Symmetry restoration (AMP+PNP)



Gogny D1S
RVAP (Deformation)
(VAP-PNP)
M. Borrajo,
PhysRevC.98.044317