Finite-size Spin Instabilities in Odd-Mass Nuclei

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Outline

- Introduction
  - Nuclear Energy Density Functional Theory
  - Warnings, disclaimers and the likes
- On blocking calculations in odd mass nuclei
  - What everybody knows
  - What not everybody knows
  - What few people know
- Spin instabilities
  - Manifestation of spin instabilities
  - Discussion on causes and consequences
- Conclusions and Outlook

INTRODUCTION

Nuclear Energy Density Functional Theory

- Start with ensemble of independent quasi-particles (= elementary excitations of the system) characterized by a density matrix ρ and a pairing tensor κ
- Construct scalar, vector and tensor fields by taking derivatives of densities ρ and κ up to second order and re-coupling spin and isospin degrees of freedom
- Couple fields to create a scalar, iso-scalar and time-even energy density that depends only on ρ and κ = Functional Theory
- Apply Variational Principle and solve the resulting equations of motion (HFB)
- Allow full spontaneous symmetry breaking for success: space-time symmetries, internal symmetries (particle number, time reversal invariance, etc.)

Skyrme EDF

- Originates from the local, zero-range Skyrme pseudo-potential (or effective interaction)
- Only applies to the p.h. channel, p.p. channel is modeled differently

$$\mathcal{H}_t^{\mathrm{even}}(\boldsymbol{r}) = C_t^{\rho}\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}\rho_t\tau_t + C_t^{J}\mathbb{J}_t^2 + C_t^{\nabla J}\rho_t\boldsymbol{\nabla}\cdot\boldsymbol{J}_t$$

$$\mathcal{H}_t^{\mathrm{odd}}(\boldsymbol{r}) = C_t^{s}\boldsymbol{s}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t\Delta\boldsymbol{s}_t + C_t^{T}\boldsymbol{s}_t\boldsymbol{T}_t + C_t^{j}\boldsymbol{j}_t^2 + C_t^{\nabla j}\boldsymbol{s}_t\cdot\boldsymbol{\nabla}\times\boldsymbol{j}_t$$

- Coupling constants C are related to parameters of the Skyrme force
- In general coupling constants dependent on the isoscalar local density break the one-to-one correspondence between the pseudo-potential and the functional

Warnings, Disclaimers and the likes

- The fundamental differences between the self-consistent mean-field (SCMF) theory and the EDF approach and their consequences on practical applications

  $\Rightarrow$ Stay at deformed HFB level, even if HFB approximation is poor
- The difficult problem of relating either the pseudo-potential or the functional to some realistic nuclear potential as .e.g. derived from EFT

  $\Rightarrow$ Consider only Skyrme forces
- The conundrum of the p.p. channel which needs to be treated on the same footing as the p.h. channel, yet remains somewhat "perturbative" with respect to it

  $\Rightarrow$ Consider only very simple pairing force (density-dependent delta)

BLOCKING IN ODD-MASS NUCLEI

Blocking approximation

- HFB vacuum = superposition of wave-functions with different N
- Lowest energy for fully paired state (even particle number only)
- Blocking approximation: assume the g.s. of the odd-mass nucleus is a 1 q.p. excitation of a fully-paired vacuum

$$\rho_{mn}^{(\mu)} = \rho_{mn} - V_{n\mu} V_{m\mu}^{*} + U_{n\mu}^{*} U_{m\mu}$$

- Equal Filling Approximation (EFA):
  - "average" of two q.p. connected by application of time-reversal operator:

$$\rho_{mn}^{\mathrm{EFA}} = \rho_{mn} \quad -\frac{1}{2}\left(V_{n\mu} V_{m\mu}^{*} - U_{n\mu}^{*} U_{m\mu}\right) -\frac{1}{2}\left(V_{n\bar{\mu}} V_{m\bar{\mu}}^{*} - U_{n\bar{\mu}}^{*} U_{m\bar{\mu}}\right)$$

  - Does not break time-reversal symmetry (in the intrinsic frame) by construction

Equal Filling Approximation

One quasi-particle energies in ^{163}Tb

Comparison between the EFA approximation (HFBTHO) and exact result (HFODD)

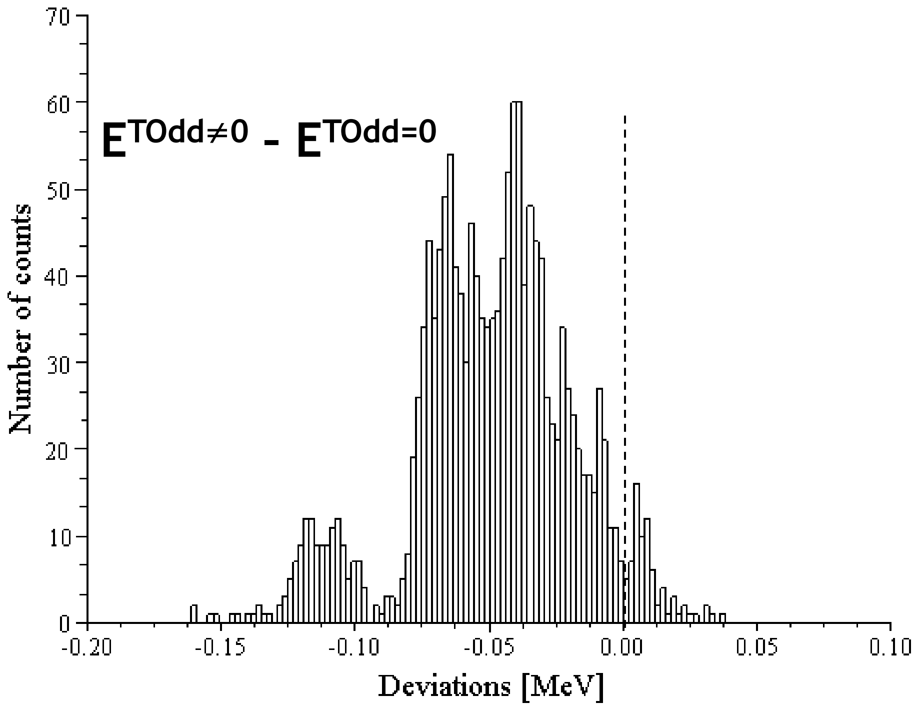
Blocked State	EFA	Exact ($T^{odd} = 0$)	Exact ($T^{odd} \neq 0$)
[4, 2, 0]1/2+	-1320.090	-1320.090	-1319.963
[4, 1, 3]5/2+	-1322.151	-1322.151	-1322.103
[4, 1, 1]3/2+	-1323.490	-1323.495	-1323.420
[4, 1, 1]1/2+	-1322.322	-1322.322	-1322.279
[4, 0, 4]9/2+	-1319.851	-1319.851	-1319.730
[5, 4, 1]3/2-	-1321.357	-1321.357	-1321.310
[5, 4, 1]1/2-	-1321.771	-1321.773	-1321.766
[5, 2, 3]7/2-	-1322.415	-1322.410	-1322.350
[5, 3, 2]5/2-	-1322.648	-1322.647	-1322.595
[5, 3, 0]1/2-	-1320.762	-1320.762	-1320.725

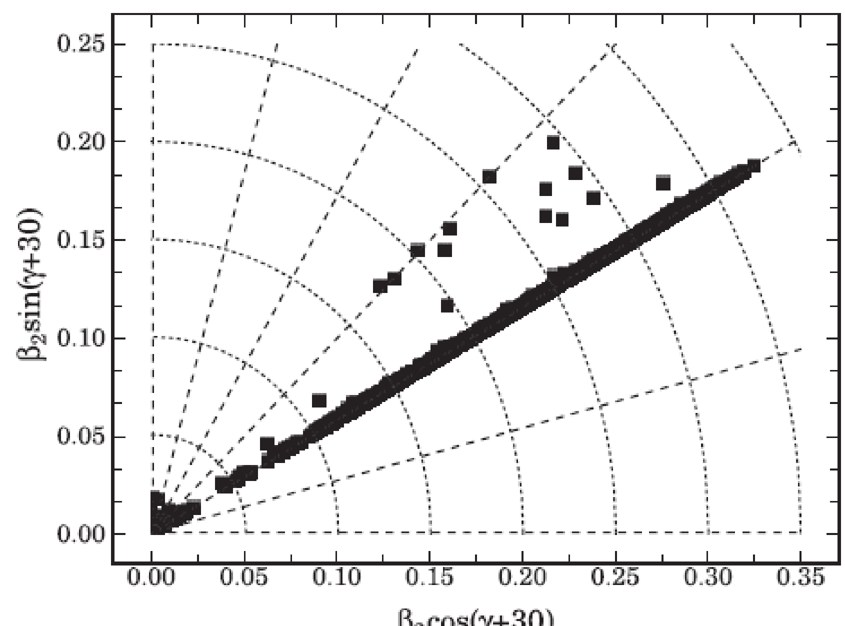
Equal-filling approximation is strictly equivalent to full blocking if time-odd terms are forced to zero

[SIII Interaction, 14 full spherical HO shells, spherical basis, surface-volume pairing]

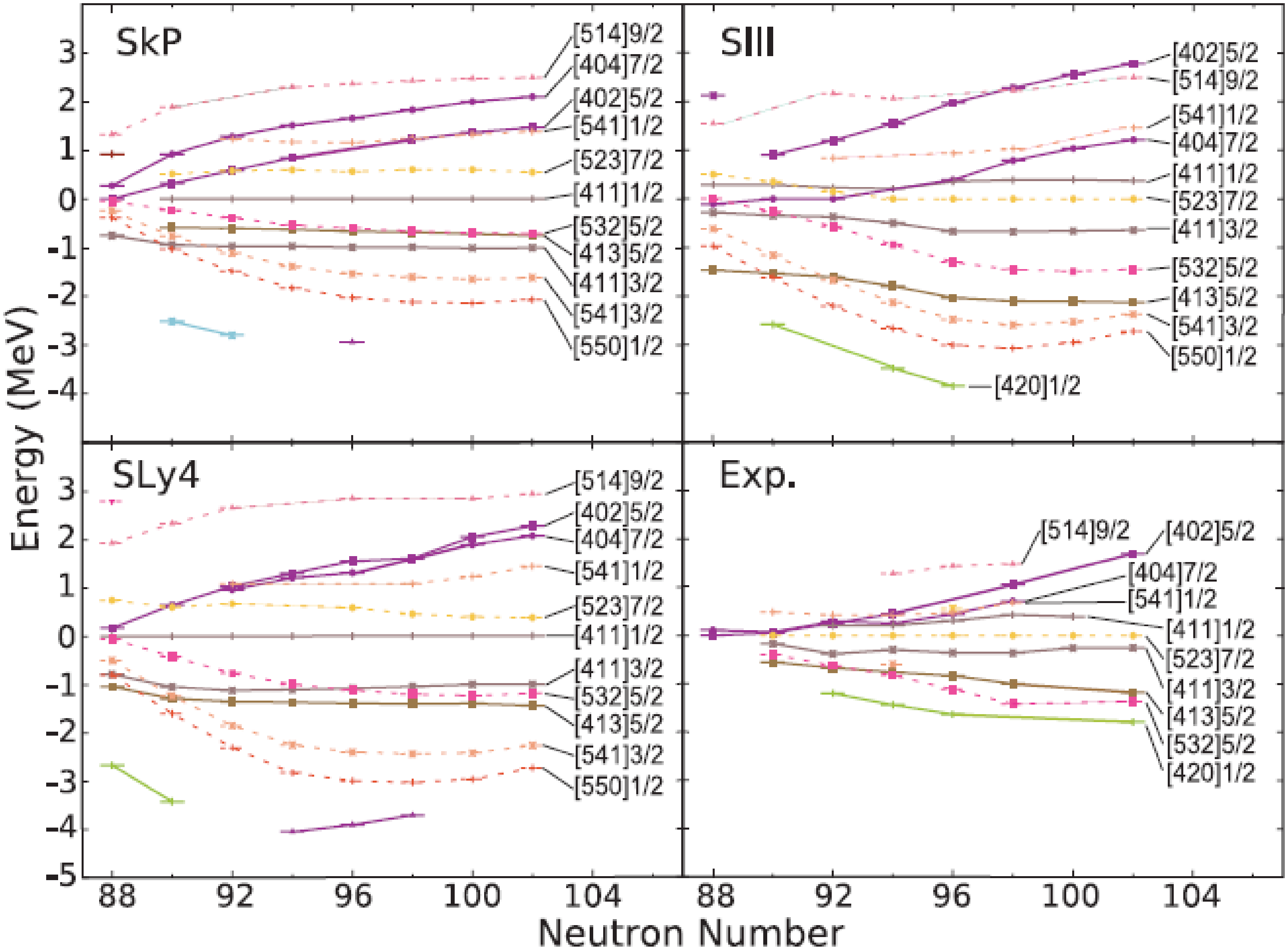
Effect of time-odd terms

- Effect of time-odd terms limited to about 50 keV on q.p. energies
- Maximum effect (150 keV) for highly-excited configurations (2-3 MeV energy)
- Polarization induced by deformation, nature and parameterizations of both p.h. and p.p. channels much more relevant
- Indirect effects of blocking calculations:
  - Triaxiality: weak overall, only for highly-excited configurations
  - Odd-Even Mass (OEM) filters: maximum 10 %





Comparison with experiment



Introducing the alispin

- Introduce alivector as linear combination of time-reversed states

$$|v_\mu\rangle = a|\mu\rangle + b|\bar{\mu}\rangle \quad \leftrightarrow \quad \begin{pmatrix} a \\ b \end{pmatrix} \in \mathrm{SU}(2)$$

- Introduce creation/anihilation operators $\xi_v^\dagger, \xi_v$ for alivectors, and define the density matrix as

$$\rho_{mn}^{(a,b)} = \langle v_\mu | c_n^\dagger c_m | v_\mu \rangle = \langle 0 | \xi_v c_n^\dagger c_m \xi_v^\dagger | 0 \rangle$$

- Explicitly

$$\begin{aligned} \rho_{mn}^{(a,b)} \quad = \rho_{mn} \quad &- \left(|a|^2 V_{n\mu} V_{m\mu}^* + |b|^2 V_{n\bar{\mu}} V_{m\bar{\mu}}^* - |a|^2 U_{n\mu}^* U_{m\mu} + |b|^2 U_{n\bar{\mu}}^* U_{m\bar{\mu}} \right) \\ &- \left(a^* b V_{n\bar{\mu}} V_{m\mu}^* + a b^* V_{n\mu} V_{m\bar{\mu}}^* - a^* b U_{n\bar{\mu}} U_{m\mu} + a b^* U_{n\mu}^* U_{m\bar{\mu}} \right) \end{aligned}$$

- Remarks
  - Analog of isoscalar/isovector versus proton/neutron, or (more accurate) flavor eigenstates versus mass eigenstates in neutrino physics
  - Quantity $\rho_{mn}^{(a,b)}$ can be defined whether time-reversal symmetry is conserved or not

Consequences (1/2)

- Special case 1: (a,b)=(0,1) or (a,b)=(1,0), the density matrix becomes

$$\rho_{mn}^{(1,0)} = \rho_{mn} - \left(V_{n\mu}V_{m\mu}^{*} - U_{n\mu}^{*}U_{m\mu}\right)$$
$$\rho_{mn}^{(0,1)} = \rho_{mn} - \left(V_{n\bar{\mu}}V_{m\bar{\mu}}^{*} - U_{n\bar{\mu}}^{*}U_{m\bar{\mu}}\right)$$

$$\rho_{mn}^{\mathrm{EFA}} = \frac{1}{2}\left(\rho_{mn}^{(1,0)} + \rho_{mn}^{(0,1)}\right)$$

- Special case 2: time-reversal symmetry is conserved $\Rightarrow$ number of relations between elements of the Boboliubov transformation such as

$$-V_{\bar{n}\mu}^{*} = V_{n\bar{\mu}} \qquad V_{n\mu}^{*} = V_{\bar{n}\bar{\mu}}$$

- Introducing alirotations

$$\mathfrak{R} : \begin{pmatrix} a' \\ b' \end{pmatrix} = e^{i\boldsymbol{\phi}\cdot\boldsymbol{\sigma}} \begin{pmatrix} a \\ b \end{pmatrix}$$

- Without proof

$$\mathfrak{R}\rho_{mn}^{(a,b)} \stackrel{T}{=} \rho_{mn}^{(a,b)} (= \rho_{mn}^{(1,0)} = \rho_{mn}^{(0,1)} = \rho_{mn}^{\mathrm{EFA}})$$

Consequences (2/2)

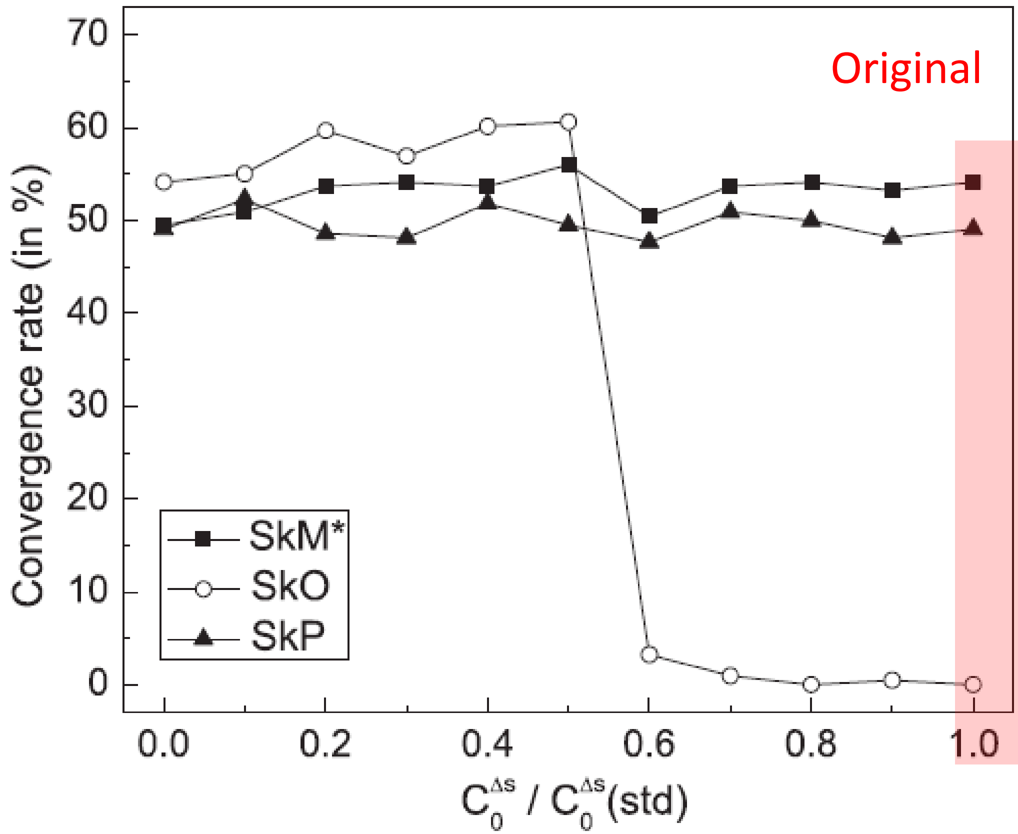
- If time-reversal symmetry is not conserved, the density-matrix is not an aliscalar but an alivector $\Rightarrow$ not invariant under alirotations
- Since E = E[ρ], the total energy of the system is also not invariant under alirotations
- In practice, $\mu \equiv$ (quantum numbers of some symmetry operators)
- Euler rotations of the intrinsic reference frame by (α, β, γ) induce a change of these conserved symmetries, hence $(\mu, \bar{\mu}) \rightarrow (\mu', \bar{\mu}')$.

  Ex.: for conserved y-signature (x$\rightarrow$+x, y$\rightarrow$-y, z$\rightarrow$+z), rotation by (0, π/2, 0) leads to conserved z-signature
- Consequence: changes in nucleus orientation in space (Euler rotation) induce alirotations
- Conclusion: total energy for a blocked state must depend on the orientation of the nucleus with respect to the intrinsic reference frame

SPIN INSTABILITIES

How it started

- Complete collapse of convergence rate in blocking calculations for some Skyrme forces
- Difference between energy computed directly and in the HF basis varies by less than 1 keV
- $C_0^{\Delta s}$(std) is the spin-isoscalar coupling constant for each functional
- Changing the criterion of convergence does not change the result



24 different one-quasiproton states in nine odd-A Ho isotopes with $88 \leq N \leq 104$ (216 “points”)

Linear Response Theory

- Compute response function (in momentum space) for a finite-size perturbation of nuclear matter

$$\mathcal{Q}^{(\alpha)} = e^{-i\omega t} \sum_a e^{i\boldsymbol{q}\cdot\boldsymbol{r}_a} \Theta_a^{(\alpha)}$$

- Simplifying case (no kinetic, spin-orbit, tensor term, isospin perturbation only), response function is

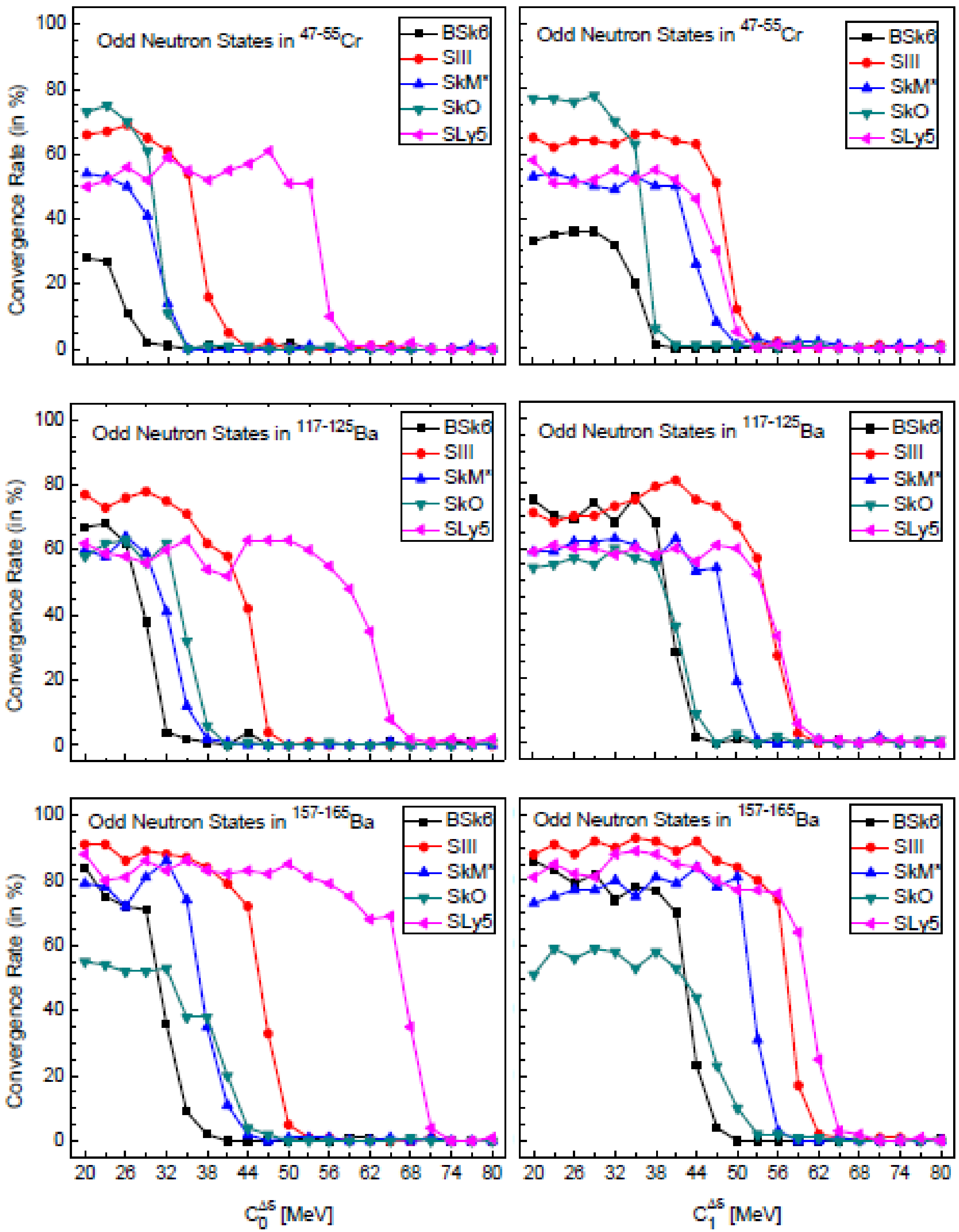
$$\Pi(\omega, \boldsymbol{q}) \sim \frac{\Pi_0(\omega, \boldsymbol{q})}{1 - 8[C_1^s - C_1^{\Delta s} \boldsymbol{q}^2] \Pi_0(\omega, \boldsymbol{q})}$$

- Suggest coupling constants C_1^s and $C_1^{\Delta s}$ drive the instabilities (create poles in the response function)
- Compatible with “experimental” observations

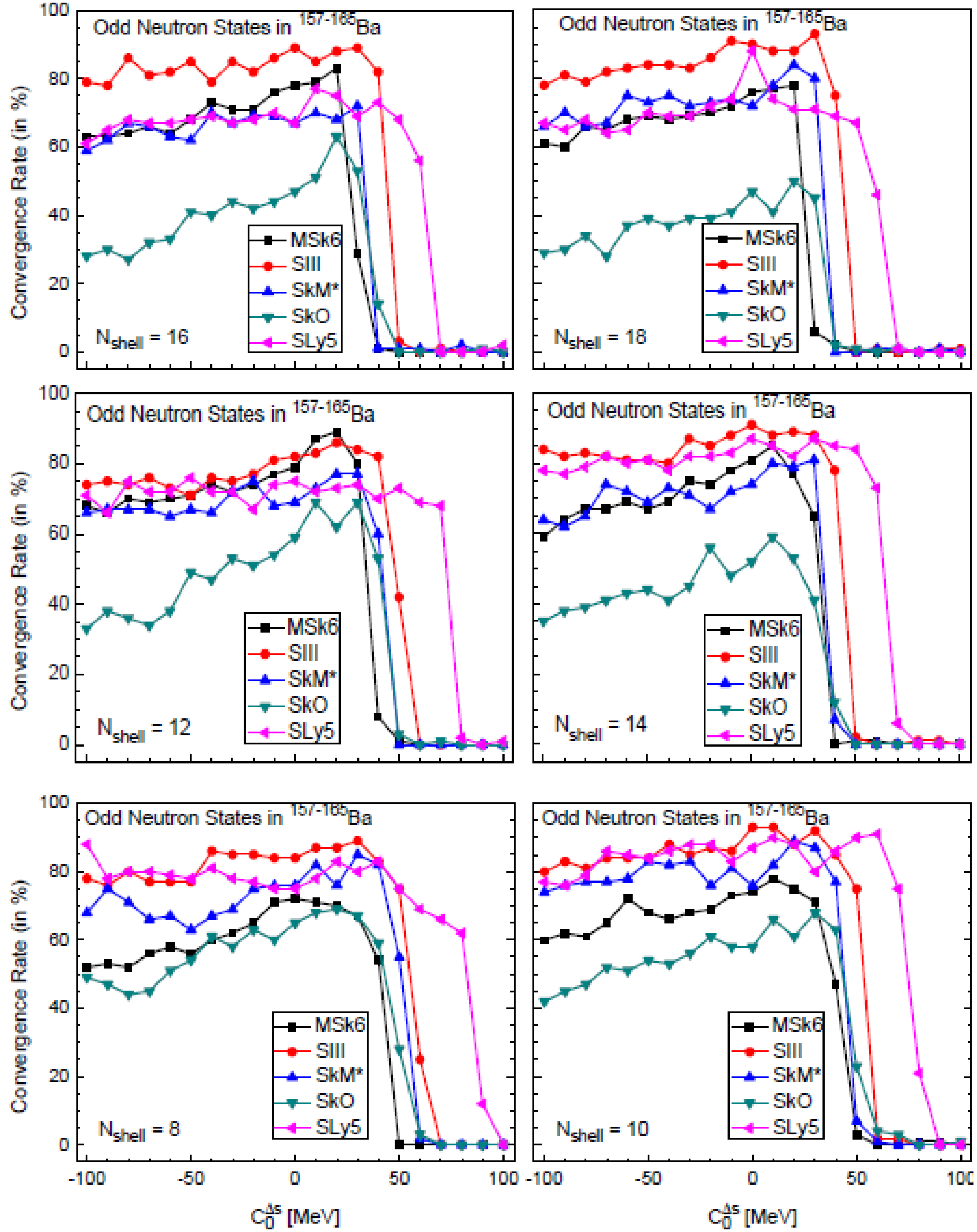
Procedure

- 3 different regions of the nuclear chart: $A \approx 50$, $A \approx 110$, $A \approx 160$
  - Well-deformed nuclei where most q.p. excitations have similar deformation, where shape coexistence is not important and where pairing collapse is limited
  - Sample include light, medium-mass and (moderately) heavy nuclei
  - Experimental information is irrelevant
- Five different parameterizations of the Skyrme force: SLy5, SkM*, SIII, SkO, MSk6

	m*	ρ	K	a_{sym}
SLy5	0.70	0.1596	230.1	32.01
SkM*	0.76	0.1450	356.0	-
SIII	0.79	0.1603	218.0	30.06
SkO	0.90	0.1605	223.5	31.98
MSk6	1.05	0.1575	231.1	28.00

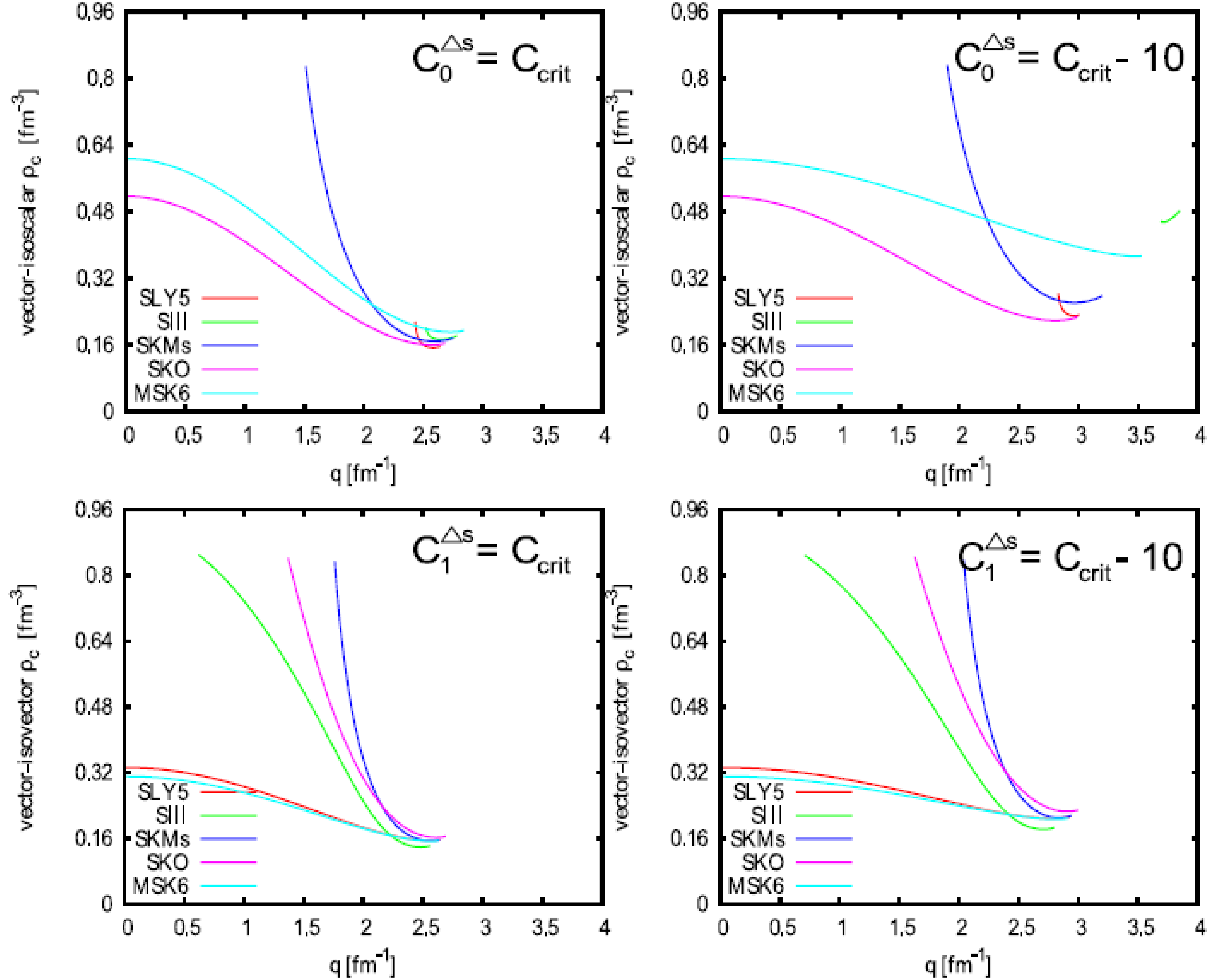


- All functionals show the same collapse of the convergence rate for large-enough values of $C_0^{\Delta s}/C_1^{\Delta s}$
- Effect occurs irrespective
  - Of the mass region
  - Of the iso-scalar/iso-vector nature of the channel
  - Of the type of particle (not shown here)
- The value of $C_0^{\Delta s}$ where the collapse occurs
  - changes with the interaction
  - changes with the mass region



- Effect clearly visible in very small bases of N=8 shells
- Small shift towards larger values for smaller bases than larger bases

Linear Response Theory



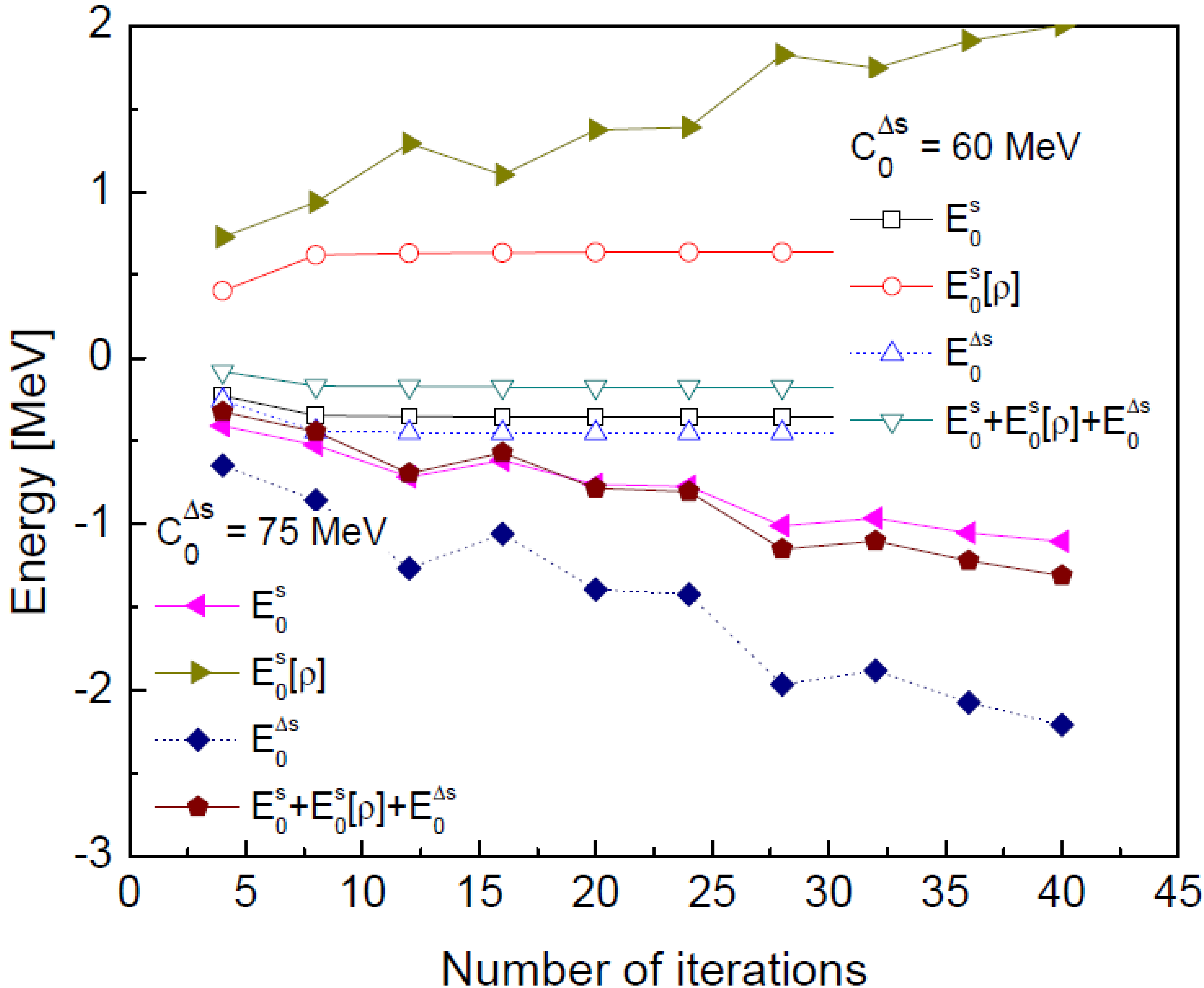
Looking closer

- Focus on one q.p. excitation, one nucleus, one interaction only
  - Study [521]3/2 in ^{157}Ba for the SLy5 interaction
  - All calculations done with 14 full spherical HO shells
  - Critical region somewhere between 70 < $C_0^{\Delta s}$ < 75
- Look at behavior of all components of total energy as function of number of iterations
- Recall: energy density made of time-odd fields reads

$$\mathcal{H}_t^{\mathrm{odd}}(\boldsymbol{r}) = C_t^s \boldsymbol{s}_t^2 + C_t^{\Delta s} \boldsymbol{s}_t \Delta \boldsymbol{s}_t + C_t^T \boldsymbol{s}_t \boldsymbol{T}_t + C_t^j \boldsymbol{j}_t^2 + C_t^{\nabla j} \boldsymbol{s}_t \cdot \boldsymbol{\nabla} \times \boldsymbol{j}_t$$

- Focus is on the first two terms: how do they evolve as function of the number of iterations for different values of the coupling constant $C_0^{\Delta s}$

Microscopic Origin of Instabilities



One last effort

$$s_z(\boldsymbol{r}) = \frac{1}{2}\sum_{\mu>0} v_\mu^2 \left(|\phi_\mu(\boldsymbol{r}\uparrow)|^2 - |\phi_\mu(\boldsymbol{r}\downarrow)|^2\right) + \frac{1}{2}\sum_{\mu\neq\mu_0>0} v_{\bar\mu}^2 \left(|\phi_{\bar\mu}(\boldsymbol{r}\uparrow)|^2 - |\phi_{\bar\mu}(\boldsymbol{r}\downarrow)|^2\right)$$

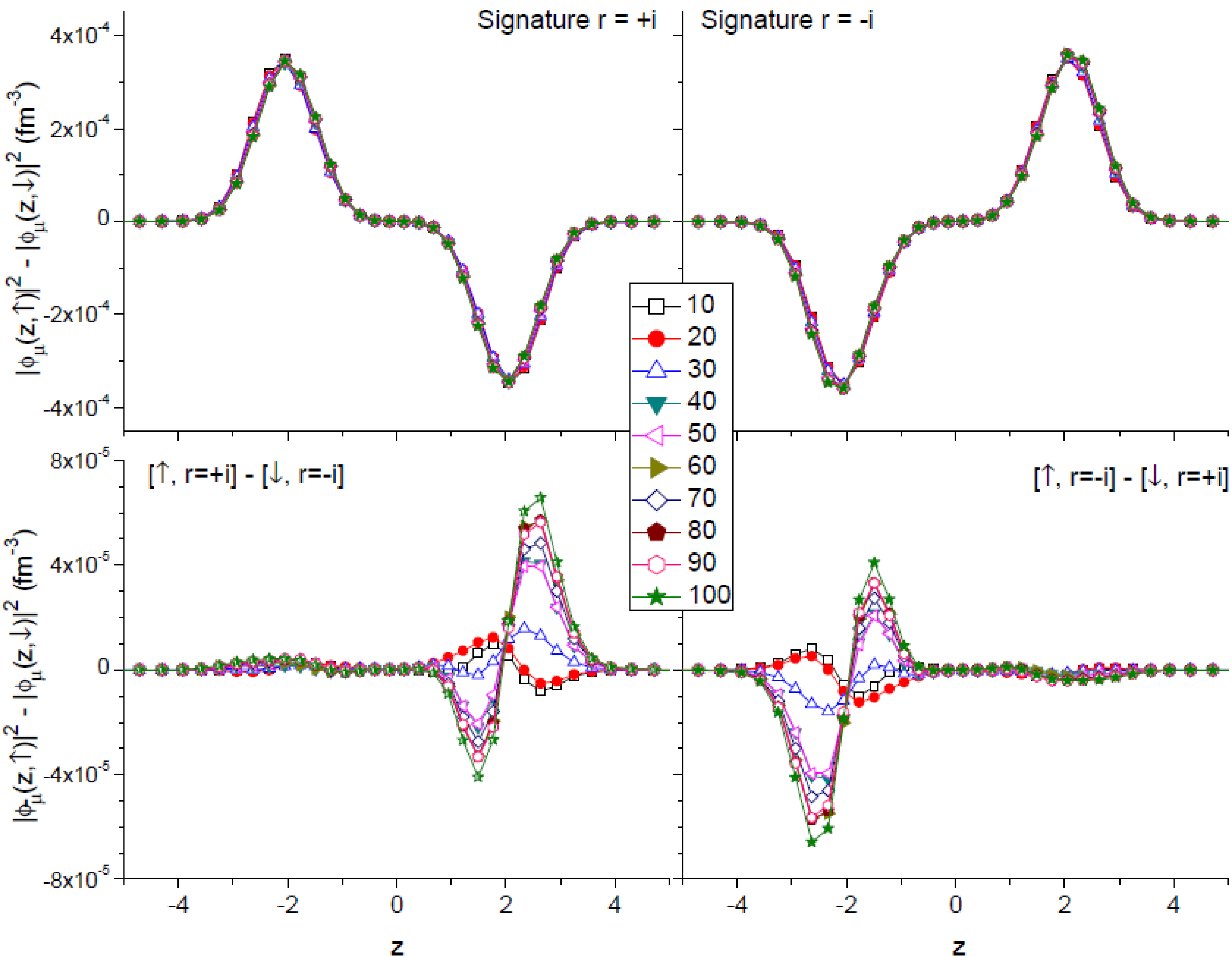
Spin density as difference between spin-up and spin-down components

$$s_z(\boldsymbol{r}) = \frac{1}{2}\sum_{\mu\neq\mu_0>0} \left(v_\mu^2|\phi_\mu(\boldsymbol{r}\uparrow)|^2 - v_{\bar\mu}^2|\phi_{\bar\mu}(\boldsymbol{r}\downarrow)|^2\right) + \frac{1}{2}\sum_{\mu\neq\mu_0>0} \left(v_{\bar\mu}^2|\phi_{\bar\mu}(\boldsymbol{r}\uparrow)|^2 - v_\mu^2|\phi_\mu(\boldsymbol{r}\downarrow)|^2\right) + \frac{1}{2}|\phi_{\mu_0}(\boldsymbol{r}\uparrow)|^2 - \frac{1}{2}|\phi_{\mu_0}(\boldsymbol{r}\downarrow)|^2$$

Spin density as difference between y-signature partners

- Why is spin density non-zero?
  - Spin-up and spin-down states do not have the same probability amplitude
  - Signature partners do not have the same probability amplitude/occupation
- Y-signature symmetry is related to time-reversal but it not the same!

Spin or signature effect?



Conclusions

- Spin instabilities in odd-mass nuclei seem to be caused by diverging spatial properties of signature partners…
  - … which causes a divergence of the spin density…
  - … which leads to an explosion of the $C_0^{\Delta s}$ term…
  - … which is only partially compensated by the density-dependent term of the time-odd channel.
- Spin instabilities observed in blocking calculations neatly correspond to finite-size instabilities of the corresponding interactions as predicted by linear response theory
- Advantage of the time-odd channel: Interaction/functional can be tuned without affecting basic properties such as mass, radius, etc.
- Attention: similar instabilities also occur in the time-even channel

Outlook

- Linear Response Theory should be taken into account in fits of new interactions/functionals
- Procedure
  - With preferred optimization algorithm, find new set of parameters for interaction/functional $\{x_i\}$
  - Compute linear response:
    - If pole for $\rho \in [\rho_{\mathrm{min}}, \rho_{\mathrm{max}}]$ in any *(S,T)* channel, reject new point
    - If no pole, accept and proceed
- Advantages
  - Linear response theory is very fast and results can be automatized
  - Whole class of instabilities can be avoided
- Need to publish a (open source) code for the linear response theory…!

Resources

- Collaborators: T.Duguet, A. Pastore, T. Lesinski
- Literature on blocking, alispin concept
  - N. Schunck et al., Phys. Rev. C **81**, 024316 (2010)
  - S. Perez-Martin et al., Phys. Rev. C **78**, 014304, (2008)
  - P. Olbratowski et al., Phys. Rev. C **73,** 054308 (2006)
  - T. Duguet et al., Phys. Rev. C **65**, 014310 (2001)
- Literature on linear response, its application in finite nuclei
  - A. Pastore et al., Phys. Rev. C **85**, 054317 (2012)
  - D. Davesne et al.Phys. Rev. C **80**, 024314 (2009)
  - T. Lesinski et al., Phys. Rev. C **74**, 044315 (2006)
  - C. García-Recio et al., Ann. Phys. **214**, 293 (1992)