Spin-orbit-tensor terms in the Skyrme energy density functional

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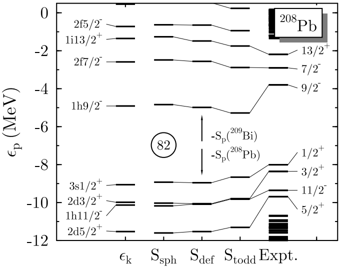
DISCLAIMER

- Shell structure is usually discussed in terms of the spectrum of eigenvalues of the single-particle Hamiltonian ϵ_μ in even-even nuclei

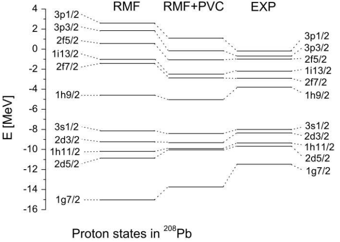
$$\hat{h}\,\psi_\mu = \epsilon_\mu\,\psi_\mu$$

- The ϵ_μ provide at best a zeroth-order approximation to empirical single-particle energies, that are obtained as separation energies (i.e. differences of total binding energies)
- The two many-body states that are compared with S_n are significantly different
- Rearrangement effects of the mean field, the different structure of the mean-field state of an even-even and an odd-A nucleus (blocking, additional mean fields that originate from interactions involving currents and spin densities in the odd-A nucleus from broken time-reversal invariance, . . .) different amount correlations beyond the mean field in magic and non-magic nuclei add significant corrections

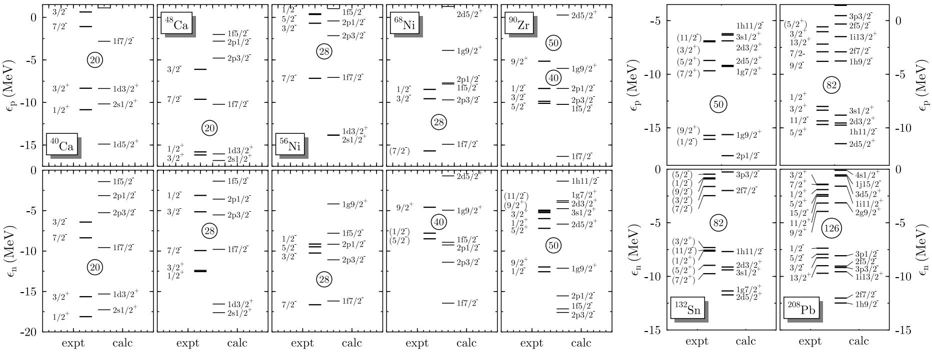
K. Rutz, M. B., P.-G. Reinhard, J. A. Maruhn and W. Greiner, Nucl. Phys. A634 (1998) 67



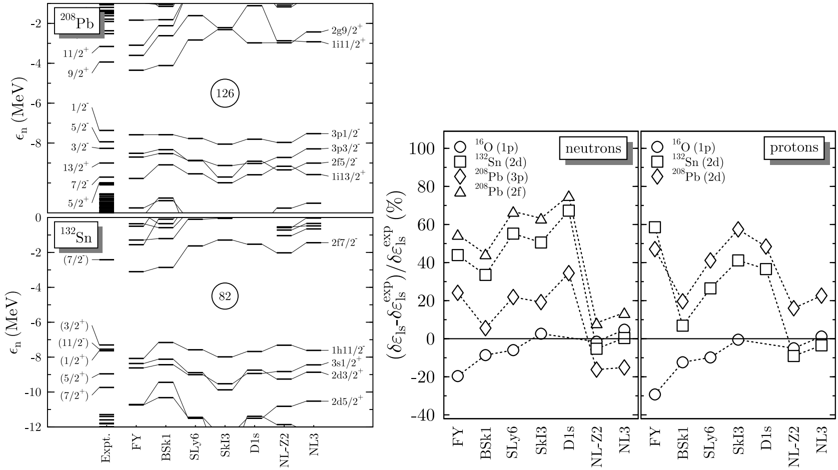
E. Litvinova, P. Ring, Phys. Rev. C 73 (2006) 044328



Open problems: single-particle spectra of doubly magic nuclei



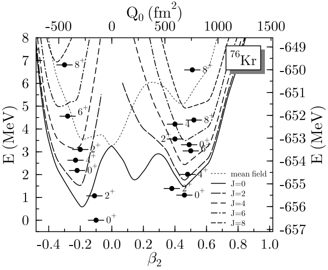
Open problems: single-particle spectra

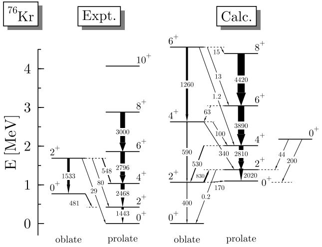


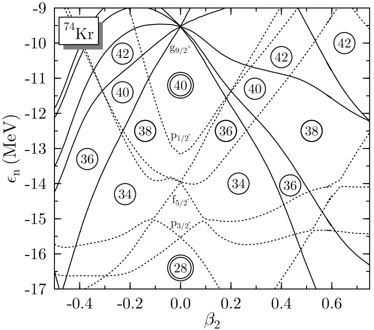
M. B., P.-H. Heenen, P.-G. Reinhard, Rev. Mod. Phys. 75 (2003) 121.

Open problems: collectivity

M. B., P. Bonche, P.-H. Heenen, Phys. Rev. C 74 (2006) 024312

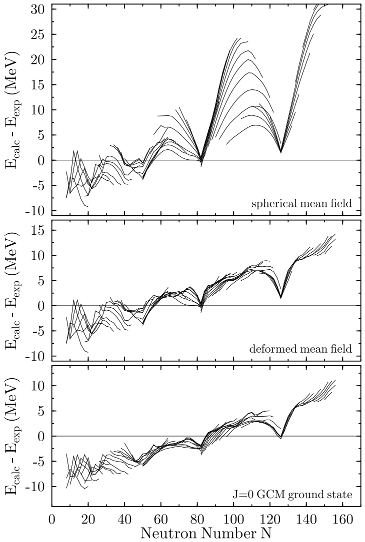


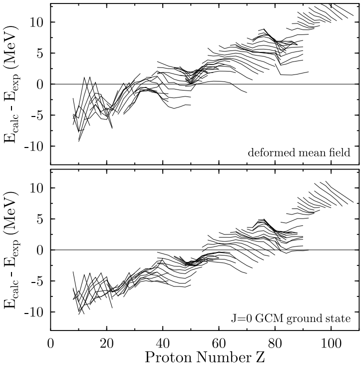




- relative position of collective states can be traced back to the underlying single-particle spectrum

Open problems: masses





M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73, 034322 (2006).

- deep ravines in the mass resisuals of heavy nuclei when plotted for isotopic chains against neutron number
- much smoother behaviour when plotted for isotonic chains against proton number

Where to start?

- It would be naive to expect a single explanation for all problems
- Still, one can hope that a limited number of modifications of the effective interaction and/or the fit protocol gives a major improvement
- If many little changes are necessary, we have an obvious uncurable problem.

What to look at?

- density dependences of coupling constants?
- three-body force (including momentum-dependent terms)?
- tensor force?
- higher-order derivative terms?
- Finite range? Finite non-locality?

The degrees of freedom associated with a zero-range tensor force are the obvious missing piece in – and of the same order as - the standard Skyrme interaction, and it is known to cause local modifications of shell structure, not global ones.

Skyrme's zero-range tensor force

$$
\begin{aligned}
v^{\text{tensor}} &= \tfrac{1}{2}\, t_e \, [3\,(\boldsymbol{\sigma}_1 \cdot \mathbf{k}')\,(\boldsymbol{\sigma}_1 \cdot \mathbf{k}') - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)\,\mathbf{k}'^2\,\delta \\
&\qquad + 3\,\delta\,(\boldsymbol{\sigma}_1 \cdot \mathbf{k})\,(\boldsymbol{\sigma}_1 \cdot \mathbf{k}) - \delta\,(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)\,\mathbf{k}^2] \\
&\quad + t_o\, [3\,(\boldsymbol{\sigma}_1 \cdot \mathbf{k}')\,\delta\,(\boldsymbol{\sigma}_1 \cdot \mathbf{k}) - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)\,\mathbf{k}' \cdot \,\delta\,\mathbf{k}]
\end{aligned}
$$

T. H. R. Skyrme, Philos. Mag. 1, 1043 (1956); Nucl. Phys. 9, 635 (1959).

General properties of any tensor force

- vanishes for relative S states
- only acts in spin-triplet states

Particular properties of Skyrme's zero-range tensor force

- even isospin-singlet t_e term mixes S and D waves
- odd isospin-triplet t_o term mixes P and F waves

The two-body tensor force gives the energy functional

$$
\begin{aligned}
\mathcal{E}^{\text{tensor}} = & \int d^3r \sum_{t=0,1} \Big\{ B_t^T \Big(\mathbf{s}_t \cdot \mathbf{T}_t - \sum_{\mu,\nu=x,y,z} J_{t,\mu\nu} J_{t,\mu\nu} \Big) \\
& + B_t^F \Big[\mathbf{s}_t \cdot \mathbf{F}_t - \tfrac{1}{2} \Big(\sum_{\mu=x,y,z} J_{t,\mu\mu} \Big)^2 - \tfrac{1}{2} \sum_{\mu,\nu=x,y,z} J_{t,\mu\nu} J_{t,\nu\mu} \Big] \\
& + B_t^{\Delta s} \mathbf{s}_t \cdot \Delta \mathbf{s}_t + B_t^{\nabla s} (\nabla \cdot \mathbf{s}_t)^2 \Big\}
\end{aligned}
$$

Definition of the local densities

$$
\begin{aligned}
B_0^T &= -\tfrac{1}{8}(t_e + 3t_o) & B_1^T &= \tfrac{1}{8}(t_e - t_o) \\
B_0^F &= \tfrac{3}{8}(t_e + 3t_o) & B_1^F &= -\tfrac{3}{8}(t_e - t_o) \\
B_0^{\Delta s} &= \tfrac{3}{32}(t_e - t_o) & B_1^{\Delta s} &= \tfrac{9}{32}(t_e - t_o) \\
B_0^{\nabla s} &= \tfrac{9}{32}(t_e - t_o) & B_1^{\nabla s} &= -\tfrac{3}{32}(3t_e + t_o)
\end{aligned}
$$

- Two new terms proportional to B_t^F and $B_t^{\nabla s}$

Don't confuse the tensor force with the J^2 terms from the central force

The central Skyrme force

$$\begin{aligned} v^{\text{central}} &= t_0\,(1 + x_0\hat{P}_\sigma)\,\delta + \tfrac{1}{6}\,t_3\,(1 + x_3\hat{P}_\sigma)\,\rho^\alpha\,\delta \\ &+ \tfrac{1}{2}\,t_1\,(1 + x_1\hat{P}_\sigma)\big(\hat{\mathbf{k}}'^2\,\delta + \delta\,\hat{\mathbf{k}}^2\big) \\ &+ t_2\,(1 + x_2\hat{P}_\sigma)\,\hat{\mathbf{k}}'\cdot\delta\,\hat{\mathbf{k}} \end{aligned}$$

and the spin-orbit force

$$v^{\text{LS}} = iW_0\,(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2)\cdot\hat{\mathbf{k}}'\times\delta\,\hat{\mathbf{k}}$$

combined give the energy functional

$$\begin{aligned} \mathcal{E} &= \int \mathrm{d}^3r \sum_{t=0,1} \Big[A_t^\rho \rho_t^2 + A_t^s \mathbf{s}_t^2 + A_t^{\Delta\rho}\rho_t\Delta\rho_t + A_t^{\Delta s}\mathbf{s}_t\cdot\Delta\mathbf{s}_t + A_t^\tau(\rho_t\tau_t - \mathbf{j}_t^2) \\ &+ A_t^T\Big(\mathbf{s}_t\cdot\mathbf{T}_t - \sum_{\mu,\nu=x,y,z} J_{t,\mu\nu}J_{t,\mu\nu}\Big) + A_t^{\nabla\cdot J}(\rho_t\nabla\cdot\mathbf{J}_t + \mathbf{s}_t\cdot\nabla\times\mathbf{j}_t)\Big]. \end{aligned}$$

where A_t^ρ and A_t^s are density-dependent.

Definition of the local densities

What J^2 term ???

It is often neglected in parameterizations of Skyrme's interaction and/or calculations because

- *the resulting mean field is difficult to derive and implement in deformed codes and very time-consuming to calculate*
- *the term sometimes gives bizarre solutions*, as "the presence of this term often favors an energetically lowest HF solution where unoccupied levels are below the Fermi surface", as pointed out in Sect. 2.4. of M. Beiner, H. Flocard, Nguyen Van Giai, and P. Quentin, Nucl. Phys. A238, 29 (1975).
- By contrast, in (Q)RPA codes these terms are often included even for parameterizations where they should not, as it is difficult to take them out when the Skyrme force is used directly as residual interaction.

Combined central + LS + tensor energy functional I

$$
\begin{aligned}
\mathcal{E}^{\text{Skyrme}} &= \mathcal{E}^{\text{central}} + \mathcal{E}^{\text{LS}} + \mathcal{E}^{\text{tensor}} \\
&= \int \mathrm{d}^3 r \sum_{t=0,1} \Big\{ C_t^{\rho} \rho_t^2 + C_t^{s} \mathbf{s}_t^2 + C_t^{\Delta\rho} \rho_t \Delta \rho_t \\
&\quad + C_t^{\nabla s} (\nabla \cdot \mathbf{s}_t)^2 + C_t^{\Delta s} \mathbf{s}_t \cdot \Delta \mathbf{s}_t + C_t^{\tau} (\rho_t \tau_t - \mathbf{j}_t^2) \\
&\quad + C_t^{T} \Big(\mathbf{s}_t \cdot \mathbf{T}_t - \sum_{\mu,\nu=x,y,z} J_{t,\mu\nu} J_{t,\mu\nu} \Big) \\
&\quad + C_t^{F} \Big[\mathbf{s}_t \cdot \mathbf{F}_t - \tfrac{1}{2} \Big(\sum_{\mu=x,y,z} J_{t,\mu\mu} \Big)^2 - \tfrac{1}{2} \sum_{\mu,\nu=x,y,z} J_{t,\mu\nu} J_{t,\nu\mu} \Big] \\
&\quad + C_t^{\nabla \cdot J} (\rho_t \nabla \cdot \mathbf{J}_t + \mathbf{s}_t \cdot \nabla \times \mathbf{j}_t) \Big\}.
\end{aligned}
$$

This functional contains all possible terms up to second order in the derivatives that can be constructed from local densities that are invariant under spatial and time inversion, rotations, and gauge transformations.

▸ Definition of the local densities ▸ Definition of the coupling constants

Single-particle Hamiltonian

$$
\begin{aligned}
\hat{h}_q \quad = \quad & U_q(\mathbf{r}) - \boldsymbol{\nabla} \cdot B_q(\mathbf{r}) \boldsymbol{\nabla} - \tfrac{i}{2}[\mathbb{W}_q(\mathbf{r}) \otimes \nabla\sigma + \nabla\sigma \otimes \mathbb{W}_q(\mathbf{r})] \\
& + \mathbf{S}_q(\mathbf{r}) \cdot \hat{\boldsymbol{\sigma}} - \boldsymbol{\nabla} \cdot [\hat{\boldsymbol{\sigma}} \cdot \mathbf{C}_q(\mathbf{r})] \boldsymbol{\nabla} - \boldsymbol{\nabla} \cdot \mathbf{D}_q(\mathbf{r})\, \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{\nabla} \\
& - \tfrac{i}{2}[\mathbf{A}_q(\mathbf{r}) \cdot \boldsymbol{\nabla} + \boldsymbol{\nabla} \cdot \mathbf{A}_q(\mathbf{r})]
\end{aligned}
$$

- The tensor force contributes to $\mathbb{W}$, **S**, **C**, and **D**.
- **D** is a new term that appears only with a tensor force
- The tensor force also gives a contribution with a new structure to $\nabla\sigma \otimes \mathbb{W}_q(\mathbf{r})$

$\Rightarrow$ too complicated to start with
$\Rightarrow$ go step by step: spherical, deformed with parity, deformed with broken parity, deformed with broken time-reversal invariance

- sphericity imposes time-reversal symmetry $\mathbf{s} = \mathbf{T} = \mathbf{F} = \mathbf{j} = 0$
- all vectors are proportional to to the radial unit vector $\mathbf{J} = J_r \mathbf{e}_r$.
- For symmetry reasons $J^{(0)} = J^{(2)} = 0$

Skyrme energy functional

$$\mathcal{E}^{\text{Sk}} = \int d^3r \sum_{t=0,1} \Big\{ C_t^\rho[\rho_0]\,\rho_t^2 + C_t^{\Delta\rho}\,\rho_t\Delta\rho_t + C_t^\tau\,\rho_t\tau_t + \tfrac{1}{2}\,C_t^J\,\mathbf{J}_t^2 + C_t^{\nabla\cdot J}\,\rho_t\nabla\cdot\mathbf{J}_t \Big\}$$

Tensor term

$$\mathcal{E}^T = \int d^3r \sum_{t=0,1} \tfrac{1}{2}\,C_t^J\,\mathbf{J}_t^2 = \int d^3r \sum_{t=0,1} \Big(-\tfrac{1}{2}\,C_t^T + \tfrac{1}{4}\,C_t^F\Big)\,\mathbf{J}_t^2.$$

with $C_t^J = A_t^J + B_t^J$

$$A_0^J = \tfrac{1}{8}\,t_1\left(\tfrac{1}{2} - x_1\right) - \tfrac{1}{8}\,t_2\left(\tfrac{1}{2} + x_2\right) \qquad A_1^J = \tfrac{1}{16}\,t_1 - \tfrac{1}{16}\,t_2$$

$$B_0^J = \tfrac{5}{16}\,(t_e + 3t_o) = \tfrac{5}{48}\,(T + 3U) \qquad B_1^J = \tfrac{5}{16}\,(t_o - t_e) = \tfrac{5}{48}\,(U - T)$$

Alternatively, the energy functional can be formulated with proton and neutron densities, for the tensor term one obtains

$$\mathcal{E}^T = \int d^3r \left\{ \tfrac{1}{2}\,\alpha\,(\mathbf{J}_n^2 + \mathbf{J}_p^2) + \beta\,\mathbf{J}_n \cdot \mathbf{J}_p \right\}$$

with

$$\begin{aligned} C_0^J &= \tfrac{1}{2}\,(\alpha+\beta) \\ C_1^J &= \tfrac{1}{2}\,(\alpha-\beta). \end{aligned} \tag{1}$$

Again $\alpha = \alpha_C + \alpha_T$

$$\alpha_C = \tfrac{1}{8}\,(t_1 - t_2) - \tfrac{1}{8}\,(t_1 x_1 + t_2 x_2) \qquad \beta_C = -\tfrac{1}{8}\,(t_1 x_1 + t_2 x_2)$$

$$\alpha_T = \tfrac{5}{4}\,t_o = \tfrac{5}{12}\,U \qquad \beta_T = \tfrac{5}{8}\,(t_e + t_o) = \tfrac{5}{24}\,(T + U)$$

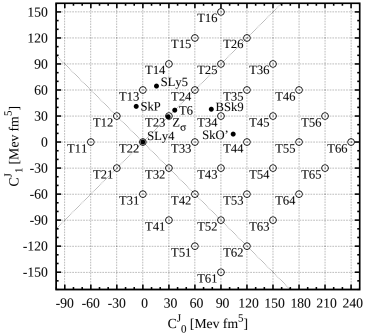
A brief history of tensor forces in self-consistent mean-field models

Skyrme

- a zero-range tensor force was contained in Skyrme, Philos. Mag. 1 (1956) 1043; Nucl. Phys. 9 (1959) 615
- $\mathbf{J}^2$ terms added to SIII without refit by Stancu, Brink, and Flocard, Phys. Lett. 68B (1977) 108
- Fit with unconstrained $\mathbf{J}^2$ terms by Tondeur, Phys. Lett. 123B (1983) 139
- generalized Skyrme force with tensor force by Liu, Luo, Ma, Shen, and Moszkowski, Nucl. Phys. A534 (1991) 1
- Brown, Duguet, Otsuka, Abe and Suzuki, Phys. Rev. C 74 (2006) 061303: fit of a Skyrme force with a tensor force constrained by *ab-initio* arguments
- Dobaczewski, nucl-th/0604043, $\mathbf{J}^2$ terms added without refit to SLy4
- Colo, Sagawa, Fracasso, and Bortignon Phys. Lett. **B** (2007) in press: tensor force added without refit to SLy5; GT giant resonance energy estimated using a sum-rule approach

Gogny

- calculation of matrix elements of a Gaussian finite range tensor force discussed in Gogny's seminal paper Nucl. Phys. A237 (1975) 399
- Onishi and Negele, Nucl. Phys. A301, 336 (1978) propose a finite- range force of Gogny type with a finite-range tensor force and zero-range three-body forces, including momentum-dependent terms.
- Otsuka, Matsuo, and Abe, Phys. Rev. Lett. 97 (2006) 162501, Gogny force with finite-range tensor force.



- Values of C_0^J and C_1^J for our set of parameterizations.
- Diagonal lines indicate $\alpha = C_0^J + C_1^J = 0$ (pure neutron-proton coupling) and $\beta = C_0^J - C_1^J = 0$ (pure like-particle coupling).
- Values for classical parameter sets are also indicated, with SLy4 representing all parameterizations for which $\mathbf{J}^2$ terms have been omitted in the fit.

Fit protocol and quality

- Fit protocol nearly identical with that of the Saclay-Lyon parameterizations SLyx
- E and r_{ch} of ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{132}Sn and ^{208}Pb; E of ^{100}Sn; the spin-orbit splitting of the neutron $3p$ state in ^{208}Pb; the empirical E/A and ρ at the saturationpoint; E/A of neutron matter as predicted by Wiringa *et al.*
- constrained: $K_\infty = 230$ MeV, $a_\tau = 32$ MeV. Thomas-Reiche-Kuhn sum-rule enhancement factor $\kappa_v = 0.25$
- Using a single density-dependent term, m_0^*/m cannot be chosen independently from K_∞ for a given exponent of $\rho_0^\alpha(\mathbf{r})$. We follow the prescription used for the SLy parameterizations and use $\alpha = 1/6$, which leads to $m_0^*/m \approx 0.7$
- no constraint $x_2 = -1$ (stability of neutron matter against ferromagnetism)

Fit protocol and quality

- Fit protocol nearly identical with that of the Saclay-Lyon parameterizations SLy*x*
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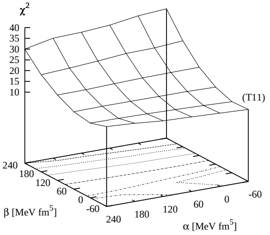
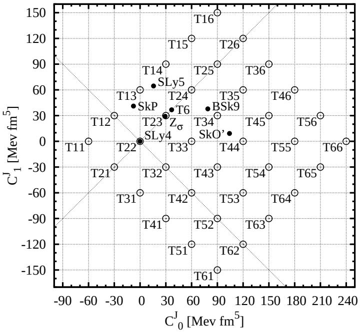


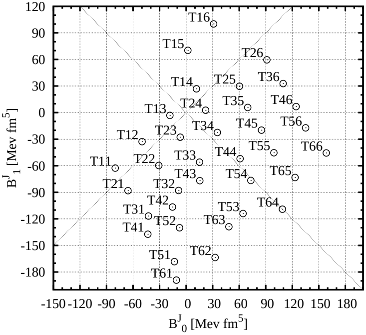
- cost function χ^2 as defined in the fit
- Contour at $\chi^2 = 11$, 12, 15, 20, 25, and 30
- minimum: T21 ($\chi^2 = 10.05$), maximum: T61 ($\chi^2 = 37.11$)

Tensor term contribution to the J^2 term coupling constant at sphericity

total coupling constant $C_t^J = A_t^J + B_t^J$

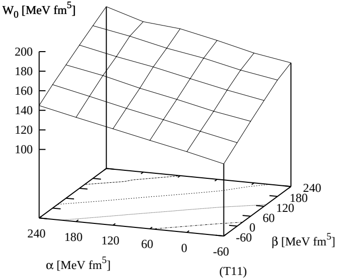


tensor contribution B_t^J



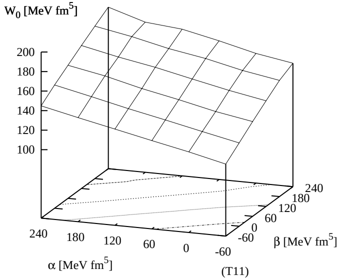
- The contribution from the central force is mainly of like-particle type and very similar for all our parameterizations
- The little scatter of the central force contribution is not surprising, the coupling constants A_t^J are depend on those that determine the effective mass and surface tension A_t^τ and $A_t^{\Delta\rho}$

Do the other coupling constants significantly change?



- Example: spin-orbit coupling constant W_0
- The contour lines differ by 20 MeV fm^5.
- T11: 103.7 MeV fm^5
  T66: 195.3 MeV fm^5

Do the other coupling constants significantly change?

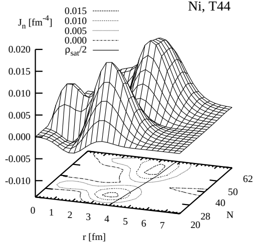


- Example: spin-orbit coupling constant W_0
- The contour lines differ by 20 MeV fm^5.
- T11: 103.7 MeV fm^5
  T66: 195.3 MeV fm^5

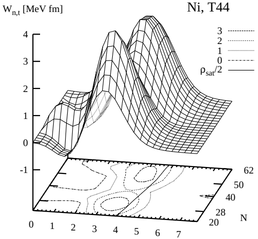
- yes, they do!
- Strong rearrangement of other coupling constants
- It is advised not to add a tensor force to an existing parameterizations without refitting the entire parameter set
- The origin of the correlation between W_0 and the C^J will be explained in a few slides

Contribution of the J^2 terms to the spin-orbit potential in Ni isotopes I

neutron spin-orbit density

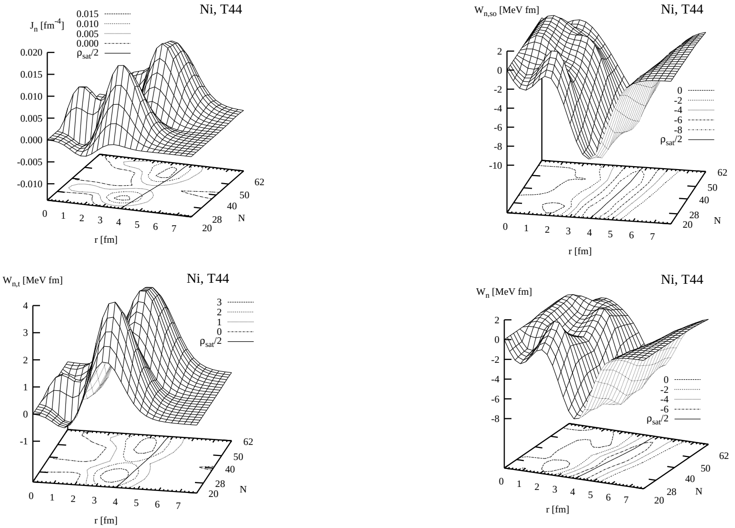


tensor term contribution to the neutron spin-orbit potential



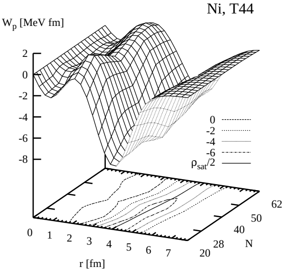
- spin-orbit density oscillates between near zero values for the spin-saturated $N = 20$ and $N = 40$ isotopes and large values when the $1f_{7/2}$ and $1g_{9/2}$ are filled
- for "spin-saturated" nuclei $\mathbf{J}$ is not exactly zero
- oscillations at small radii from the filling of orbits with one node ($2p$ and $2d$))
- The tensor term contributions (central and tensor forces) to the spin-orbit potential is strictly proportional to $\mathbf{J}_n$ and $\mathbf{J}_p$

Contribution of the J^2 terms to the spin-orbit potential in Ni isotopes II

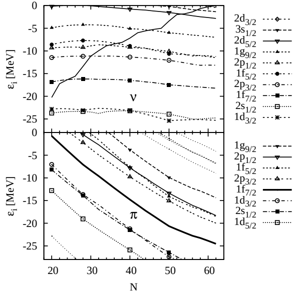


Contribution of the J^2 terms to the spin-orbit potential in Ni isotopes III

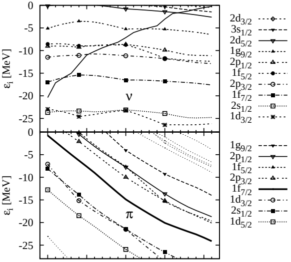
proton spin-orbit potential



single-particle spectra with T22 (no $\mathbf{J}^2$ term)

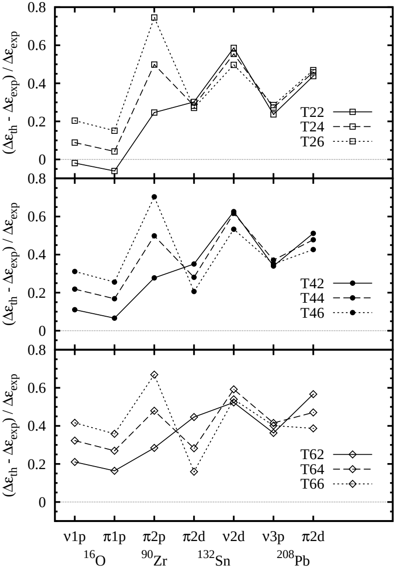


single-particle spectra with T44 (proton-neutron + like-particle $\mathbf{J}^2$ terms)

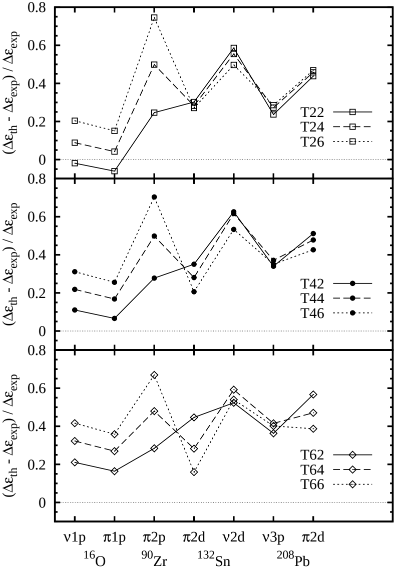


- proton spin-orbit potential more robust
- influence on single-particle energies stays subtle (for Ni isotopes with this parameterization T44)

Spin-orbit splittings I. within a major shell



Spin-orbit splittings I. within a major shell



- Relative error of spin-orbit splittings within a major shell in doubly-magic nuclei for $\ell \leq 2$ levels.
- staying within the same major shell, the empirical splittings are relatively robust against correlations
- all but the 1p states in ^{16}O have one or more nodes.
- Spin-orbit splittings are too large
- a known problem that is even amplified in the presence of tensor terms

Where does the correlation between W_0 and C_0^J come from?

Define the combined spin-orbit and tensor term contribution to the binding energy

$$E_0^{spin}(N,Z) = C_0^{\nabla J}\,\mathcal{C}_0^{\nabla J}(N,Z) + C_0^J\,\mathcal{C}_0^J(N,Z)$$

with

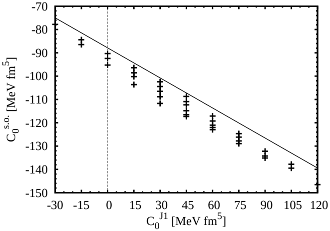
$$\begin{aligned}\mathcal{C}_0^{\nabla J}(N,Z) &= \int \mathrm{d}^3r\; \rho_0 \nabla \cdot \mathbf{J}_0 \\ \mathcal{C}_0^{J}(N,Z) &= \int \mathrm{d}^3r\; \mathbf{J}_0^2.\end{aligned}$$

The integrals are fairly independent on the parameterization
Look at difference between ^{56}Ni and ^{40}Ca

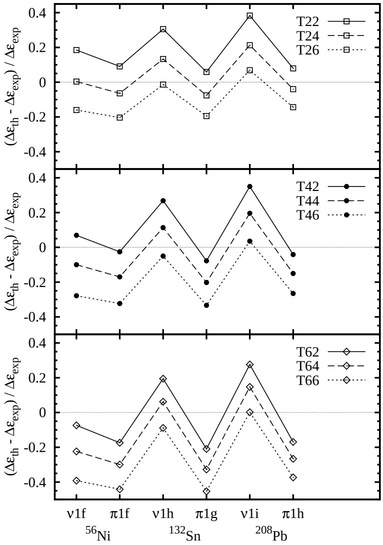
$$\Delta E^{spin} = E_0^{spin}\left(^{56}\mathrm{Ni}\right) - E_0^{spin}\left(^{40}\mathrm{Ca}\right)$$

and set-up the estimate for $C_0^{\nabla J}$ as a function of C_0^{J1}

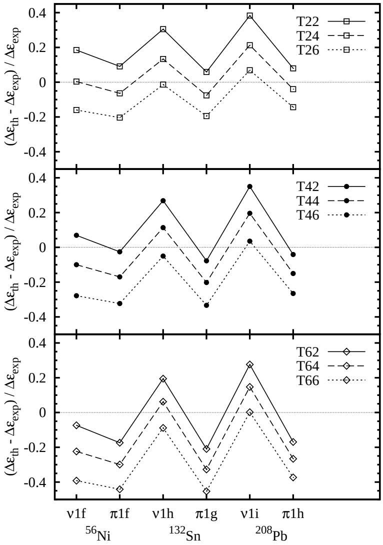
$$C_0^{\nabla J} = \frac{\Delta E^{spin} - C_0^{J1}\langle \mathcal{C}_0^J\left(^{56}\mathrm{Ni}\right) - \mathcal{C}_0^J\left(^{40}\mathrm{Ca}\right)\rangle}{\langle \mathcal{C}_0^{\nabla J}\left(^{56}\mathrm{Ni}\right) - \mathcal{C}_0^{\nabla J}\left(^{40}\mathrm{Ca}\right)\rangle}.$$



- Correlation between the of spin-orbit coupling constant $C_0^{\nabla J}$ and the isoscalar spherical effective spin-current coupling constant C_0^{J1}. Dots: values for the actual parameterizations TIJ, solid line: trend estimated


T22
T24
T26
T42
T44
T46
T62
T64
T66
$(\Delta\varepsilon_{th} - \Delta\varepsilon_{exp}) / \Delta\varepsilon_{exp}$
0.4
0.2
0
-0.2
-0.4
ν1f
π1f
ν1h
π1g
ν1i
π1h
^{56}Ni
^{132}Sn
^{208}Pb

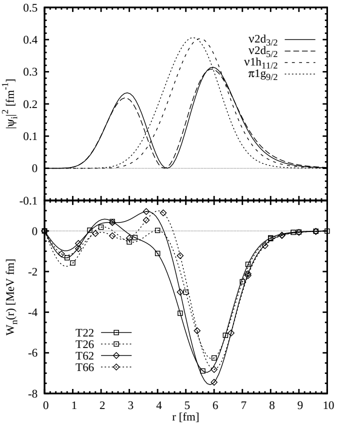
Spin-orbit splittings II. intruder states



- spin-orbit splittings of intruder levels across the Fermi energy
- This quantity is *not* robust against correlations, which will pull down levels above and push up levels below the Fermi energy and significantly decrease the calculated values
- empirical value establishes a lower limit for what should be found with the eigenvalues of the spherical mean- field Hamiltonian $\hat{h}$
- calculated values are often even *smaller*
- large tensor terms amplify this deficiency
- We have to re-evaluate above's finding: spin-orbit splittings are not too large in general. There is a missing trend with angular momentum and/or the number of nodes
- proton-neutron staggering ⇒ missing isospin trend?

Where does the trend with node number come from?

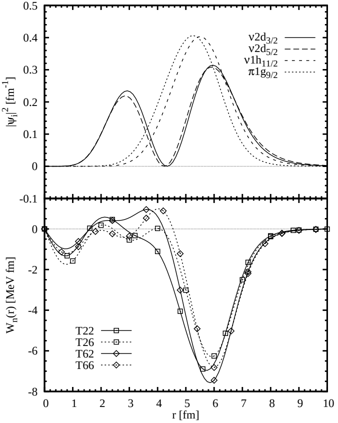
see also B. A. Brown, T. Duguet, T. Otsuka, D. Abe, T. Suzuki, Phys. Rev. C74 (2006) 061303



Neutron spin-orbit potential (bottom) and the radial wave function of selected orbitals (top) in ^{132}Sn.

Where does the trend with node number come from?

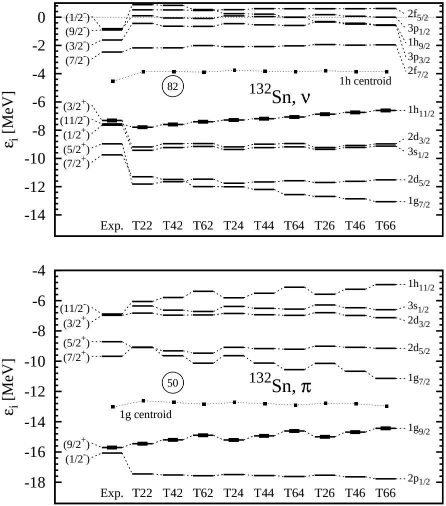
see also B. A. Brown, T. Duguet, T. Otsuka, D. Abe, T. Suzuki, Phys. Rev. C74 (2006) 061303



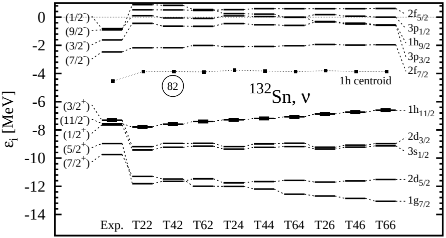
Neutron spin-orbit potential (bottom) and the radial wave function of selected orbitals (top) in ^{132}Sn.

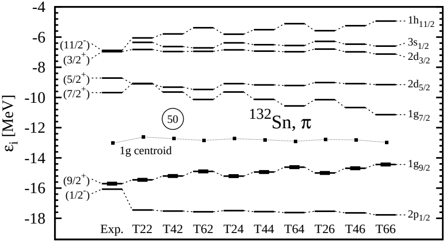
- might be geometrical effect from overlap with spin-orbit potential
- larger sensitivity of the nodeless levels to the $\mathbf{J}^2$ terms as the major contribution to $\mathbf{J}$ is most often from nodeless states; hence the nodeless states have large overlap with the tensor term contribution (we use zero-range interactions, after all) while levels with nodes have their nodes where
- Note that the refit of the other coupling constants increases the spin-orbit force such that the depth of the spin-orbit potential stays the same; mainly its width changes for our parameterizations
- No, we do not want to change the sign of the tensor contribution. This leads to instabilities that will be discussed below.

Single-particle spectra of ^{132}Sn



Single-particle spectra of ^{132}Sn



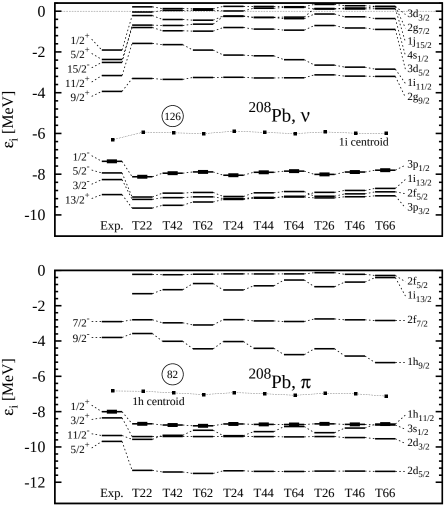


- notorious for wrong relative order of the last occupied neutron levels $1h_{11/2}$, $2d_{3/2}$ and $3s_{1/2}$.
- underestimated spin-orbit splitting of the intruder for large tensor terms amplifies the problems
- centroid

$$\varepsilon_{qn\ell}^{\text{cent}} = \frac{\ell+1}{2\ell+1}\,\varepsilon_{qn\ell,j=\ell+1/2} + \frac{\ell}{2\ell+1}\,\varepsilon_{qn\ell,j=\ell-1/2}.$$

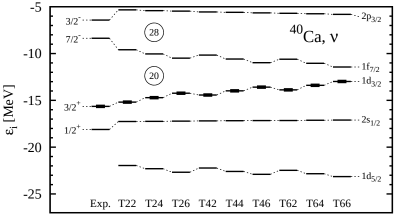
of the intruder seems to be too high for the neutrons (attention, might not be robust)

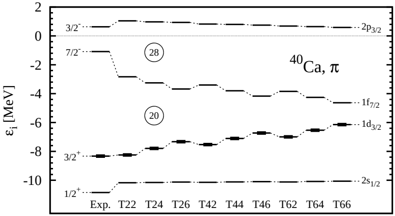
Single-particle spectra of ^{208}Pb



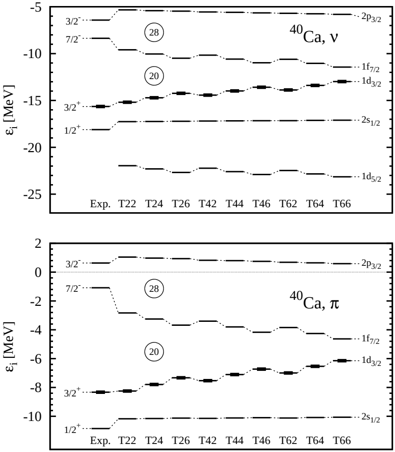
- similar problems as for ^{132}Sn, only sligthly more subtle

Single-particle spectra of ^{40}Ca



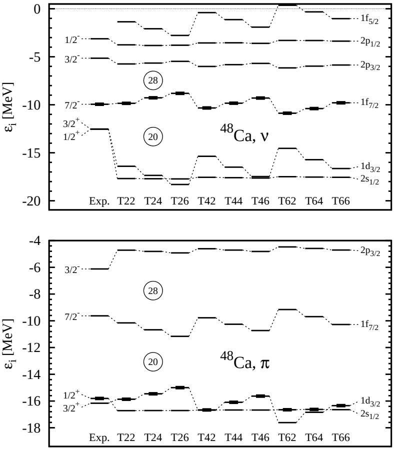


Single-particle spectra of ^{40}Ca

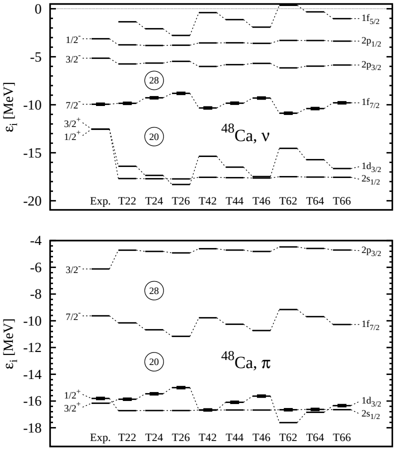


- spin-saturated nucleus ($N = Z = 20$)
- the evolution of levels seen is the *background* from the readjustment of all coupling constants
- genuine spin-orbit interaction too large
- gap at 20 too small, even disappears for large J^2 coupling constants
- for large J^2 coupling constants the also large spin-orbit term pulls the $1f_{7/2}$ intruder (the J^2 terms always near zero)
- For not spin-saturated doubly-magic nuclei the intruders are pushed up: the J^2 contribution overcompsensates the larger spin-orbit coupling W_0
- with our fit protocol, W_0 is correlated to C_0^J, such that (T24, T42) and (T26, T44, T62) give similar single-particle spectra for ^{40}Ca

Single-particle spectra of ^{48}Ca

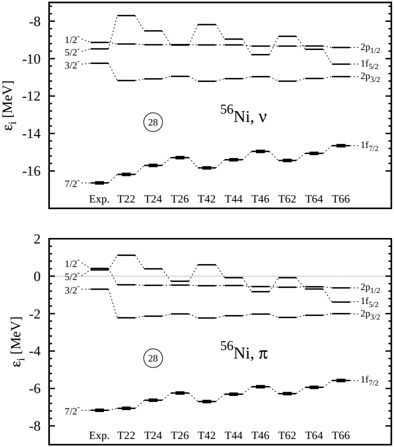


Single-particle spectra of ^{48}Ca

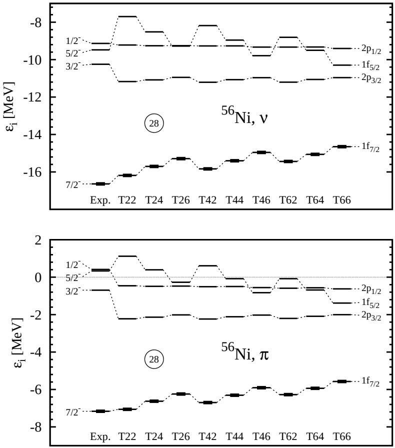


- protons spin saturated ($Z = 20$)
- large neutron $\mathbf{J}_n$ ($1f_{7/2}$ filled, $1f_{5/2}$ empty)
- depending on the combination of proton-neutron and like-particle coupling constants, $\mathbf{J}_n^2$ contributes to the spin-orbit potential of the neutrons or the protons or both
- pure proton-neutron $\mathbf{J}^2$ term (T42, T62): same problems for protons from readjustment of W_0 as for ^{40}Ca, at the same time neutron $N = 20$ gap too much opened, $N = 28$ gap too small
- pure like-particle $\mathbf{J}^2$ term (T24, T26): opposite effect: $Z = 20$ gap opened (overcompensation of increased W_0), neutron gaps more realistic
- comibations of both give anything in between

Single-particle spectra of ^{56}Ni

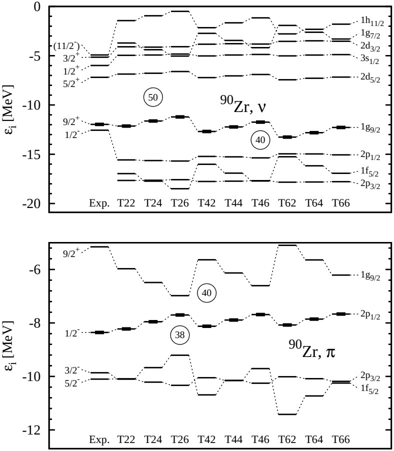


Single-particle spectra of ^{56}Ni

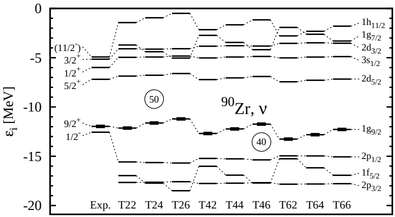


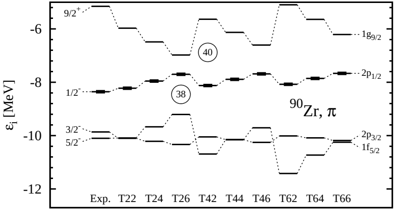
- large proton and neutron $\mathbf{J}$ ($1f_{7/2}$ filled, $1f_{5/2}$ empty for both)
- $N = Z$: spectra of ^{56}Ni depend only on C_0^J.
- This statement is less trivial than it seems: for the contribution of the $\mathbf{J}^2$ it is obvious, but the the background shift from the rearrangement of the other coupling constants is mainly correlated to C_0^J as well.
- gap at 28 too small for all parameterizations
- smaller shifts of the single-particle than for ^{40}Ca $\Rightarrow$ $\mathbf{J}^2$ contributions compensate background shift from increasing W_0

Single-particle spectra of ^{90}Zr



Single-particle spectra of ^{90}Zr





- protons: $N = 40$ spin saturated
- neutrons: very large $\mathbf{J}_n$ (highly degenerate $1g_{9/2}$ filled, $1g_{7/2}$ empty)
- depending on the combination of proton-neutron and like-particle coupling constants, $\mathbf{J}_n^2$ contributes to the spin-orbit potential of the neutrons or the protons or both
- pure proton-neutron $\mathbf{J}^2$ term (T42, T62):

Instability – phase transition - coexistence phenomena

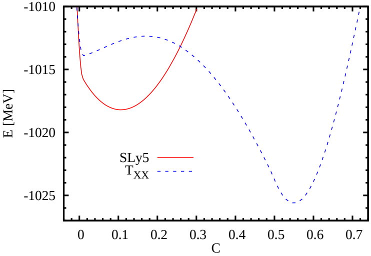
(0) $\mathbf{J}_q$ is not a bulk property, but a shell effect. It varies rapidly between near-zero and substantial values. (1) Multiplying a large $\mathbf{J}_q$ with a large coupling constant leads (2) to a large contribution to the spin-orbit potential

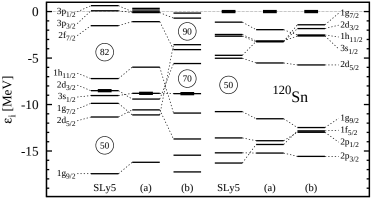
$$W_n(r) = -\frac{W_0}{2}\,(2\nabla\rho_n + \nabla\rho_p) + \alpha\, J_n + \beta\, J_p$$

which (3) might switch levels originating from different j shells, which further increases $\mathbf{J}$. Feed this back to (1) and you have an instability towards unrealistic spectra

- fits in many regions of the parameter space not covered by our parameter sets have this instability
- there is even "spin-orbit current coexistence"
- constraint on

$$C = \int d^3r\, \mathbf{J}_n \cdot \nabla\rho_n$$





- TXX: parameter set with large negative α and β

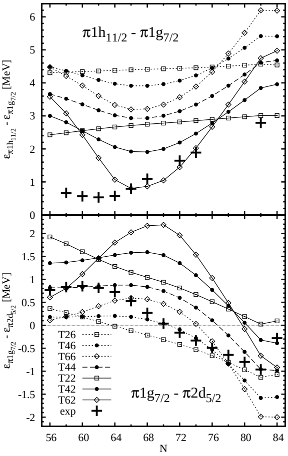
What we have learnt so far

Within the Skyrme energy functional and the fit protocol we use

- the spin-orbit coupling constant W_0 is correlated to C_0^T trough the masses of ^{40}Ca and ^{56}Ni in the fit
- the spin-orbit and J^2 terms are misused in the fit to get the masses of ^{40}Ca and ^{56}Ni right, simulating missing physics (which is not the Wigner term)
- without $\mathbf{J}^2$ terms, the spin-orbit splittings within a major shell (states with 1 or more nodes) are too large, those of the intruders across the gap are too small.
- positive proton-neutron and like-particle coupling constants of the $\mathbf{J}^2$ terms make this usually worse
- negative coupling constants of the $\mathbf{J}^2$ terms (might) lead to instabilities towards unphysical single-particle spectra
- in lowest order, the deficiency of the splittings does probably not originate from the $\mathbf{J}^2$ terms, but the spin-orbit force (which always dominates the splittings)
- centroids of the neutron intruder states in heavy doubly-magic nuclei might be placed too high

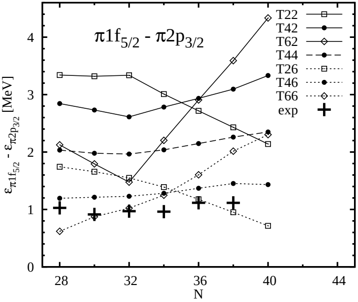
. . . and we have not looked into tensor term specific observables yet.

Evolution of spin-orbit splittings: proton levels in Sn ($Z = 50$)



- $2d_{5/2}$ and $\pi\ 1g_{7/2}$: change of ground state spin of odd-A Sb isotopes between $N = 70$ and 72
- $1g_{7/2}$ and $1h_{11/2}$: PRL by Schieffer *et al.*
- these are open-shell nuclei, unclear effect of correlations on the "single-particle energies".
- How to compare calculation with empirical data in view of the deficiencies of the single-particle spectra in doubly-magic nuclei outlined above?
- absolute energy difference is arbitrary (can be normalized out, see papers by Otsuka *et al.*)
- look at the bend of the curves
- but: if the bend is determined by the proton-neutron $\mathbf{J}_p \cdot \mathbf{J}_n$ terms, then it sets in up to 4 mass units too large, as the $\nu\ 1h_{11/2}$ is occupied too late (see spectrum of ^{132}Sn above)
- positive $\mathbf{J}_p \cdot \mathbf{J}_n$ coupling constant needed in both cases

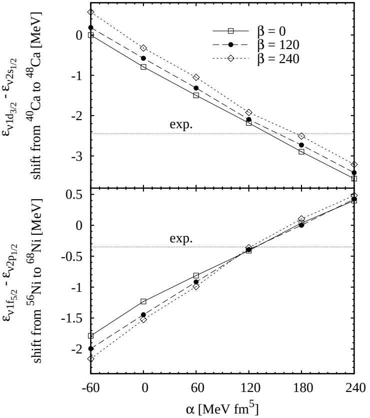
Evolution of spin-orbit splittings: proton levels in Ni ($Z = 28$)



- distance between $1f_{5/2}$ and $2p_{3/2}$ levels
- compensation of two effect: without $\mathbf{J}^2$ terms at sphericity (see T22), the spin-orbit splittings are reduced by the increasing diffuseness of the neutron surface
- positive $\mathbf{J}_p \cdot \mathbf{J}_n$ coupling constant needed to compensate this effect to obtain the flat curve

Evolution of spin-orbit splittings: neutron levels in Ca and Ni

- How to narrow down the like-particle coupling strength?
- $\Rightarrow$ look at neutron states in doubly-magic nuclei in an isotopic chain



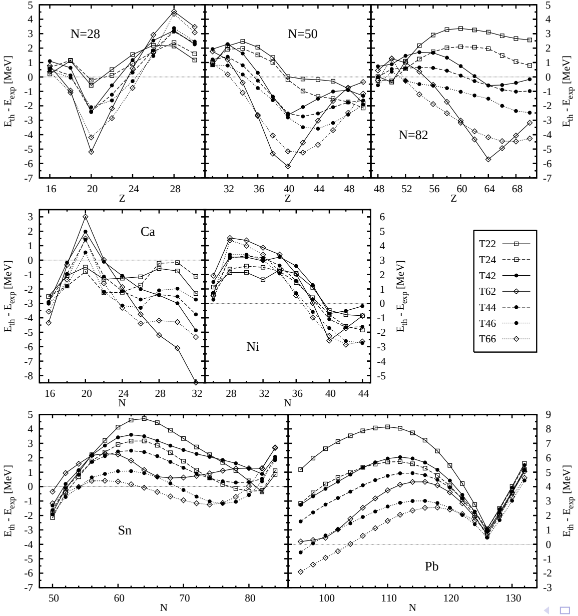
$$\delta^{\mathrm{Ca}} = \left(\varepsilon^{48\mathrm{Ca}}_{1d_{3/2}} - \varepsilon^{48\mathrm{Ca}}_{2s_{1/2}}\right) - \left(\varepsilon^{40\mathrm{Ca}}_{1d_{3/2}} - \varepsilon^{40\mathrm{Ca}}_{2s_{1/2}}\right).$$

- double difference takes out deficiencies from central and spin-orbit force
- separated by more than 2 MeV in ^{40}Ca, nearly degenerate in ^{48}Ca

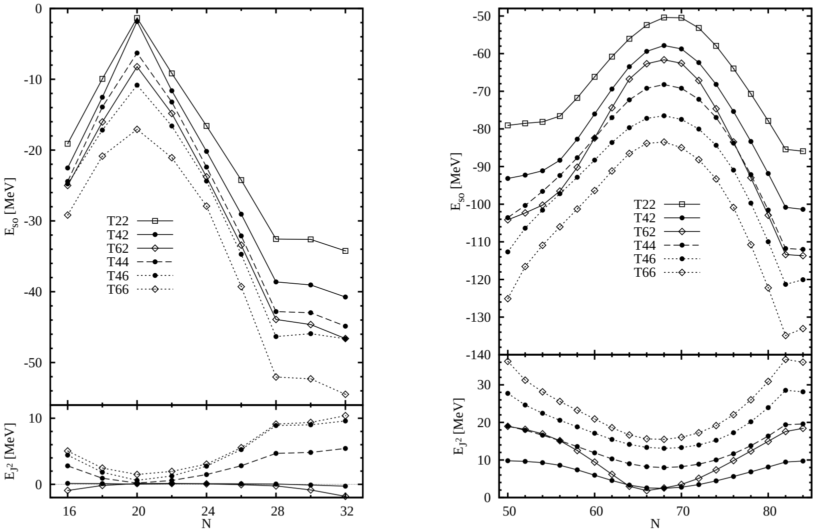
$$\delta^{\mathrm{Ni}} = \left(\varepsilon^{68\mathrm{Ni}}_{1f_{5/2}} - \varepsilon^{68\mathrm{Ni}}_{2p_{1/2}}\right) - \left(\varepsilon^{56\mathrm{Ni}}_{1f_{5/2}} - \varepsilon^{56\mathrm{Ni}}_{2p_{1/2}}\right)$$

- $1f_{5/2}$ level comes further down than the $2p_{1/2}$ level when going from ^{56}Ni to ^{68}Ni
- both differences aare reproduced $\alpha \approx 120$ MeV fm^5

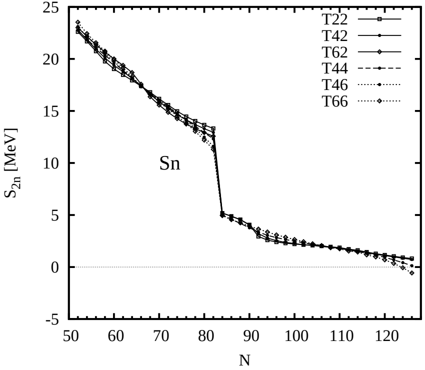
Mass residuals



contribution of the spin-orbit and tensor terms to the total binding energy

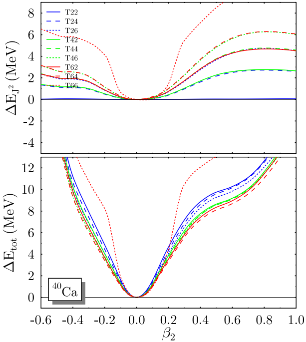


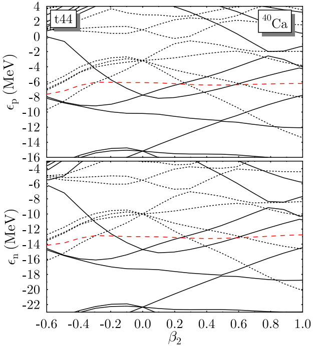
S_{2n} in the Sn isotopic chain



- differences for neutron-rich systems not larger than around the valley of stability

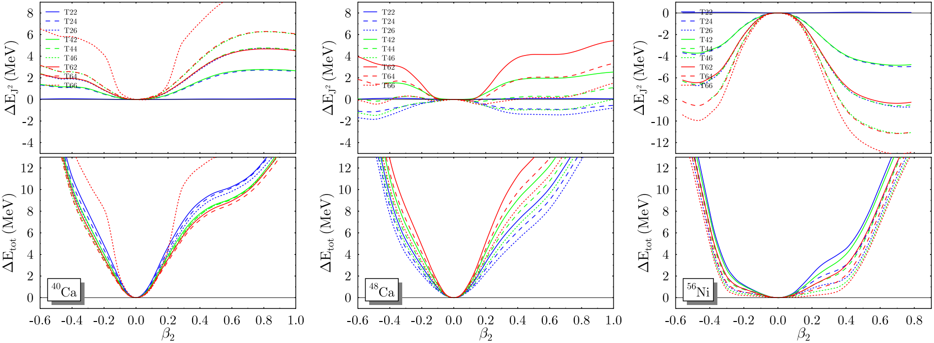
Deformation energy from a quadrupole constraint I





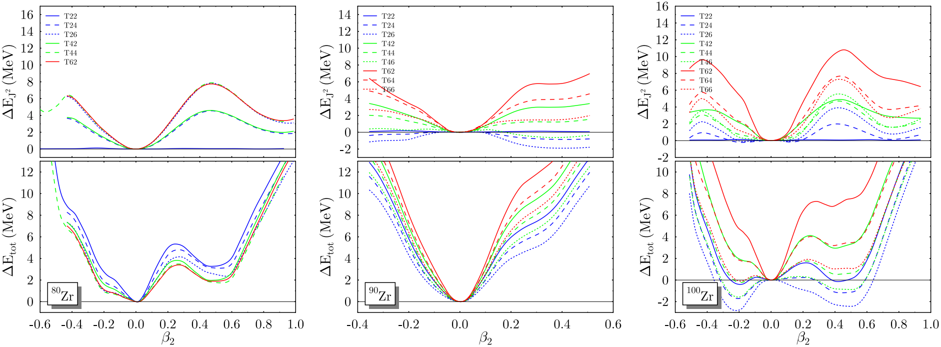
- deformation modifies the amount of spin saturation that determined the contribution of the $\mathbf{J}^2$ terms discussed for spherical configurations above

Deformation energy from a quadrupole constraint I



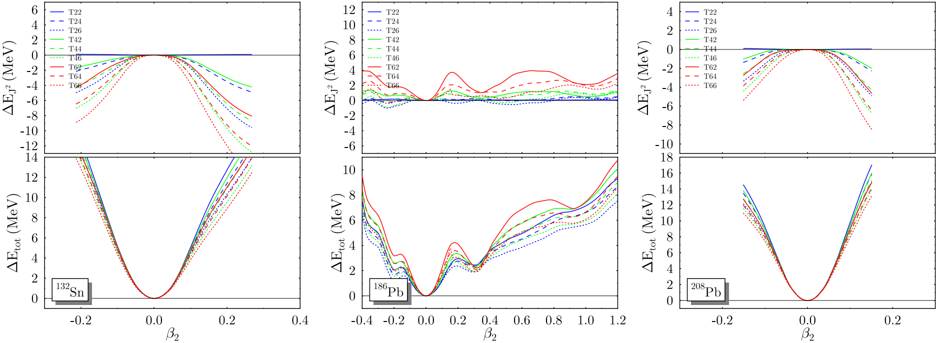
- nuclei become stiffer of softer depending on their spin-saturation

Deformation energy from a quadrupole constraint II



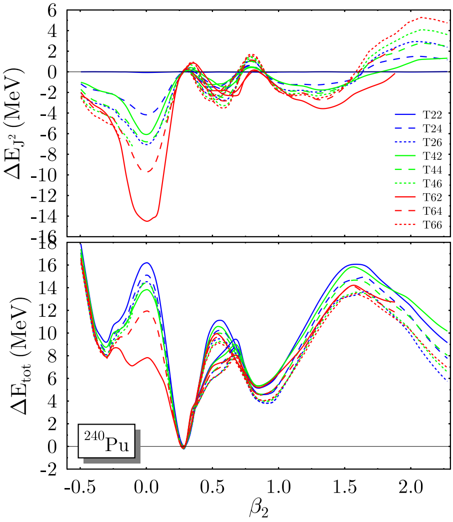
- nuclei become stiffer of softer depending on their spin-saturation

Deformation energy from a quadrupole constraint II



- nuclei become stiffer of softer depending on their spin-saturation

Fission barriers - axial - triaxial - reflection asymmetric



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Paul Bonche	SPhT, CEA Saclay, France
Thomas Duguet	NSCL/Michigan State University, USA
Jacques Meyer,	IPN Lyon, France

Intermezzo: local densities and currents I

$$
\begin{aligned}
\rho_q(\mathbf{r}) &= \sum_k v_k^2 \, \Psi_k^\dagger(\mathbf{r})\Psi_k(\mathbf{r}) \\
\tau_q(\mathbf{r}) &= \sum_k v_k^2 \, [\boldsymbol{\nabla}\Psi_k(\mathbf{r})]^\dagger \cdot \boldsymbol{\nabla}\Psi_k(\mathbf{r}) \\
\mathbf{j}_q(\mathbf{r}) &= -\tfrac{i}{2}\sum_k v_k^2 \, \{\Psi_k^\dagger(\mathbf{r})\,[\boldsymbol{\nabla}\Psi_k(\mathbf{r})] - [\boldsymbol{\nabla}\Psi_k(\mathbf{r})]^\dagger\,\Psi_k(\mathbf{r})\} \\
\mathbf{s}_q(\mathbf{r}) &= \sum_k v_k^2 \, \Psi_k^\dagger(\mathbf{r})\,\hat{\boldsymbol{\sigma}}\,\Psi_k(\mathbf{r}) \\
T_{q\mu}(\mathbf{r}) &= \sum_k v_k^2 \, [\nabla\Psi_k(\mathbf{r})]^\dagger\;\hat{\boldsymbol{\sigma}}_\mu \cdot [\nabla\Psi_k(\mathbf{r})] \\
J_{q,\mu\nu}(\mathbf{r}) &= -\tfrac{i}{2}\sum_k v_k^2 \, \{\Psi_k^\dagger(\mathbf{r})\,\sigma_\nu\,[\nabla_\mu\Psi_k(\mathbf{r})] - [\nabla_\mu\Psi_k(\mathbf{r})]^\dagger\,\sigma_\nu\,\Psi_k(\mathbf{r})\} \\
F_{q,\mu}(\mathbf{r}) &= \tfrac{1}{2}\sum_k v_k^2 \, \{[\boldsymbol{\nabla}\cdot\hat{\boldsymbol{\sigma}}\Psi_k(\mathbf{r})]^\dagger\,[\nabla_\mu\Psi_k(\mathbf{r})] + [\nabla_\mu\Psi_k(\mathbf{r})]^\dagger\,[\boldsymbol{\nabla}\cdot\hat{\boldsymbol{\sigma}}\Psi_k(\mathbf{r})]\}
\end{aligned}
$$

The tensor-kinetic pseudovector density $\mathbf{F}(\mathbf{r})$ was intruduced in H. Flocard's thesis in 1975, but afterwards forgotten.

back to the functional from the central force   back to the functional from the tensor force

Intermezzo: recoupling of the spin-orbit tensor

The cartesian spin-orbit tensor can be decomposed into a pseudoscalar, pseudovector and traceless pseudotensor

$$J_{\mu\nu}(\mathbf{r}) = \tfrac{1}{3}\delta_{\mu\nu}\, J^{(0)}(\mathbf{r}) + \tfrac{1}{2} \sum_{\kappa=x,y,z} \epsilon_{\mu\nu\kappa}\, J^{(1)}_{\kappa}(\mathbf{r}) + J^{(2)}_{\mu\nu}(\mathbf{r})$$

The pseudovector part is the spin-orbit current known from the genuine spin-orbit force

$$\mathbf{J}(\mathbf{r}) = \sum_{\mu=x,y,z} J^{(1)}_{\mu}(\mathbf{r})\, \mathbf{e}_{\mu} = -\tfrac{i}{2} \sum_{k} v_k^2 \left\{ \Psi^{\dagger}_k(\mathbf{r}) \left[\boldsymbol{\nabla} \times \hat{\boldsymbol{\sigma}} \Psi_k(\mathbf{r}) \right] - \left[\boldsymbol{\nabla} \times \hat{\boldsymbol{\sigma}} \Psi_k(\mathbf{r}) \right]^{\dagger} \Psi_k(\mathbf{r}) \right\}$$

Dobaczewski *et al.* reformulate the density functional as

$$\begin{aligned}
\mathcal{E}^{\text{tensor}} \quad = \quad & \int d^3 r \sum_{t=0,1} \Bigg\{ B_t^T \Big[\mathbf{s}_t \cdot \mathbf{T}_t - \tfrac{1}{3} (J_t^{(0)})^2 - \tfrac{1}{2} (\mathbf{J}_t^{(1)})^2 - \sum_{\mu,\nu=x,y,z} J^{(2)}_{t,\mu\nu} J^{(2)}_{t,\mu\nu} \Big] \\
& + B_t^F \Big[\mathbf{s}_t \cdot \mathbf{F}_t - \tfrac{2}{3} (J_t^{(0)})^2 + \tfrac{1}{4} (\mathbf{J}_t^{(1)})^2 - \tfrac{1}{2} \sum_{\mu,\nu=x,y,z} J^{(2)}_{t,\mu\nu} J^{(2)}_{t,\mu\nu} \Big] \\
& + B_t^{\Delta s} \mathbf{s}_t \cdot \Delta \mathbf{s}_t + B_t^{\nabla s} (\nabla \cdot \mathbf{s}_t)^2 \Bigg\}
\end{aligned}$$

back to the functional from the central force

back to the functional from the tensor force

Auxiliary material: Combined central + LS + tensor energy functional

central + LS:

$$C_0^\rho = \tfrac{3}{8} t_0 + \tfrac{3}{48} t_3\, \rho_0^\alpha(\mathbf{r}) \qquad C_1^\rho = -\tfrac{1}{4} t_0 \left(\tfrac{1}{2} + x_0\right) - \tfrac{1}{24} t_3 \left(\tfrac{1}{2} + x_3\right) \rho_0^\alpha(\mathbf{r})$$

$$C_0^s = -\tfrac{1}{4} t_0 \left(\tfrac{1}{2} - x_0\right) - \tfrac{1}{24} t_3 \left(\tfrac{1}{2} - x_3\right) \rho_0^\alpha(\mathbf{r}) \qquad C_1^s = -\tfrac{1}{8} t_0 - \tfrac{1}{48} t_3\, \rho_0^\alpha(\mathbf{r})$$

$$C_0^\tau = \tfrac{3}{16}\, t_1 + \tfrac{1}{4} t_2 \, \left(\tfrac{5}{4} + x_2\right) \qquad C_1^\tau = -\tfrac{1}{8} \left[t_1 \left(\tfrac{1}{2} + x_1\right) - t_2 \left(\tfrac{1}{2} + x_2\right)\right]$$

$$C_0^{\Delta\rho} = -\tfrac{9}{64} t_1 + \tfrac{1}{16} t_2 \left(\tfrac{5}{4} + x_2\right) \qquad C_1^{\Delta\rho} = \tfrac{1}{32} \left[3 t_1 \left(\tfrac{1}{2} + x_1\right) + t_2 \left(\tfrac{1}{2} + x_2\right)\right]$$

$$C_0^{\nabla J} = -\tfrac{3}{4} W_0 \qquad C_1^{\nabla J} = -\tfrac{1}{4} W_0$$

tensor

$$C_0^F = \tfrac{3}{8}(t_e + 3 t_o) \qquad C_1^F = -\tfrac{3}{8}(t_e - t_o)$$

$$C_0^{\nabla s} = \tfrac{9}{32}(t_e - t_o) \qquad C_1^{\nabla s} = -\tfrac{3}{32}(3 t_e + t_o)$$

central + tensor

$$C_0^T = -\tfrac{1}{8}\left[t_1 \left(\tfrac{1}{2} - x_1\right) - t_2 \left(\tfrac{1}{2} + x_2\right)\right] - \tfrac{1}{8}(t_e + 3 t_o)$$

$$C_1^T = -\tfrac{1}{16}(t_1 - t_2) + \tfrac{1}{8}(t_e - t_o)$$

$$C_0^{\Delta s} = \tfrac{1}{32}\left[3 t_1 \left(\tfrac{1}{2} - x_1\right) + t_2 \left(\tfrac{1}{2} + x_2\right)\right] + \tfrac{3}{32}(t_e - t_o)\, 1$$

$$C_1^{\Delta s} = \tfrac{1}{64}(3 t_1 + t_2) - \tfrac{1}{32}(3 t_e + t_o)$$

back to the combined energy functional