Search for nuclear energy-density functional

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- **From effective interaction to energy density functional**
- **Extensions of Skyrme functional**
- **Surface-peaked effective mass**

Methods in nuclear structure

- **Basic methods and their applicability**

Ab initio	Light nuclei
Shell model	Medium nuclei
Mean-field methods	Heavy nuclei

Hartree-Fock method

- **Ritz variational principle**

$$H = T_{\mu\mu'} a^+_\mu a_{\mu'} + \frac{1}{4} V_{\mu\nu\mu'\nu'} a^+_\mu a^+_\nu a_{\nu'} a_{\mu'}$$

$$\delta \langle \psi | H | \psi \rangle = 0 \qquad | \psi \rangle = a^+_N \ldots a^+_1 | 0 \rangle$$

- **Density matrix and energy**

$$\rho_{\mu'\mu} = \langle \psi | a^+_\mu a_{\mu'} | \psi \rangle \qquad E = T_{\mu\mu'} \rho_{\mu'\mu} + \frac{1}{4} V_{\mu\nu\mu'\nu'} \rho_{\nu'\nu} \rho_{\mu'\mu}$$

- **Mean field**

$$h_{\mu\mu'} = T_{\mu\mu'} + V_{\mu\nu\mu'\nu'} \rho_{\nu'\nu} = \frac{\partial E}{\partial \rho_{\mu'\mu}}$$

- **Hartree-Fock equations and solution**

$$[\rho, h] = 0 \qquad h \rightarrow \rho \rightarrow h \rightarrow \rho \rightarrow \ldots$$

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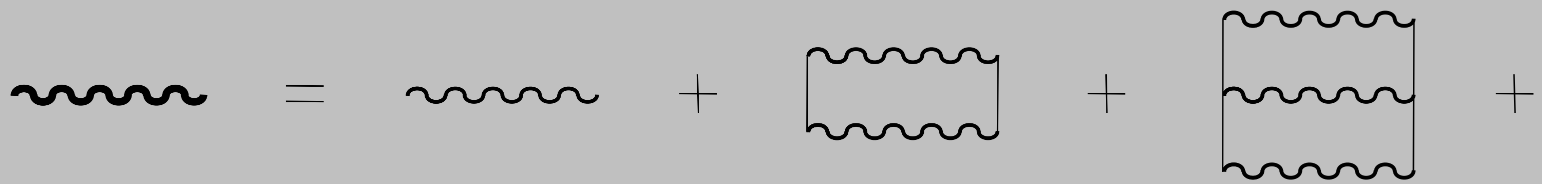
Effective interaction

- **Ladder diagrams**
- **Bethe-Goldstone equation**



- **Brueckner-Hartree-Fock method**
- **Phenomenological Gogny and Skyrme interactions**

$$V(\boldsymbol{r}-\boldsymbol{r}') \sim \mathrm{e}^{-(\boldsymbol{r}-\boldsymbol{r}')^2/a^2} \qquad V(\boldsymbol{r}-\boldsymbol{r}') \sim \delta(\boldsymbol{r}-\boldsymbol{r}')$$

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Skyrme force

- **Lord Tony Hilton Royle Skyrme (1922-1987)**
  Philosophical Magazine **1** (1956) 1043

$$
\begin{aligned}
V(\boldsymbol{r},\boldsymbol{r}') &= t_0(1+x_0 P_\sigma)\delta(\boldsymbol{r}-\boldsymbol{r}') \\
&+ \frac{1}{2}t_1(1+x_1 P_\sigma)\left[\boldsymbol{k}^2\delta(\boldsymbol{r}-\boldsymbol{r}')+\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k}^2\right] \\
&+ t_2(1+x_2 P_\sigma)\boldsymbol{k}\,\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k} \\
&+ \frac{1}{6}t_3(1+x_3 P_\sigma)\delta(\boldsymbol{r}-\boldsymbol{r}')\rho\left(\frac{1}{2}(\boldsymbol{r}+\boldsymbol{r}')\right) \\
&+ iW_0(\boldsymbol{\sigma}+\boldsymbol{\sigma}')\boldsymbol{k}\times\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k}
\end{aligned}
$$

- **Relative momentum (derivative) operator**

$$\boldsymbol{k}=\frac{1}{2i}(\nabla-\nabla')$$

Skyrme functional

- **Interaction energy**

$$E=\frac{1}{4}V_{\mu\nu\mu'\nu'}\rho_{\nu'\nu}\rho_{\mu'\mu}=\int d^3\boldsymbol{r}\,\Re(\boldsymbol{r})$$

- **Energy density**

$$\begin{aligned}\Re &= C^{\rho\rho}\rho^2+C^{\rho\Delta\rho}\rho\Delta\rho+C^{\tau\rho}\tau\rho+C^{JJ}\bar{J}^2+C^{\rho\nabla J}\rho\boldsymbol{\nabla}\boldsymbol{J}\\ &+ C^{ss}\boldsymbol{s}^2+C^{s\Delta s}\boldsymbol{s}\Delta\boldsymbol{s}+C^{sT}\boldsymbol{sT}+C^{jj}\boldsymbol{j}^2+C^{s\nabla j}\boldsymbol{s}(\boldsymbol{\nabla}\times\boldsymbol{j})\end{aligned}$$

Local densities

- **Local densities**

Particle	$\rho(\boldsymbol{r})=\left[\rho(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}$
Spin	$\boldsymbol{s}(\boldsymbol{r})=\left[\boldsymbol{s}(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}$
Kinetic	$\tau(\boldsymbol{r})=\left[\boldsymbol{\nabla}\boldsymbol{\nabla}'\rho(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}$
Vector kinetic	$\boldsymbol{T}(\boldsymbol{r})=\left[\boldsymbol{\nabla}\boldsymbol{\nabla}'\boldsymbol{s}(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}$
Momentum	$\boldsymbol{j}(\boldsymbol{r})=\frac{1}{2i}\left[(\boldsymbol{\nabla}-\boldsymbol{\nabla}')\rho(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}$
Spin-current	$J_{\mu\nu}(\boldsymbol{r})=\frac{1}{2i}\left[(\nabla_{\mu}-\nabla_{\nu}')s_{\nu}(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}$

Coupling constants

- **Linear functions of Skyrme force parameters**

$$64\begin{pmatrix} C_0^{\Delta\rho} \\ C_1^{\Delta\rho} \\ C_0^{\tau} \\ C_1^{\tau} \\ C_0^{\Delta s} \\ C_1^{\Delta s} \\ C_0^{T} \\ C_1^{T} \end{pmatrix} = \begin{pmatrix} -9 & 0 & 5 & 4 \\ 3 & 6 & 1 & 2 \\ 12 & 0 & 20 & 16 \\ -4 & -8 & 4 & 8 \\ 3 & -6 & 1 & 2 \\ 3 & 0 & 1 & 0 \\ -4 & 8 & 4 & 8 \\ -4 & 0 & 4 & 0 \end{pmatrix} \begin{pmatrix} t_1 \\ t_1 x_1 \\ t_2 \\ t_2 x_2 \end{pmatrix}.$$

- **Numbers of coupling constants**

Skyrme force	9
Skyrme functional	24

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Local density approximation

- Force range < density variation distance

- Expansion of full density matrix up to second order

- Energy density ...

$$\begin{aligned}\Re &= C^{\rho\rho}\rho^2 + C^{\rho\Delta\rho}\rho\Delta\rho + C^{\tau\rho}\tau\rho + C^{JJ}\bar{J}^2 + C^{\rho\nabla J}\rho\nabla \boldsymbol{J} \\ &+ C^{ss}\boldsymbol{s}^2 + C^{s\Delta s}\boldsymbol{s}\Delta\boldsymbol{s} + C^{sT}\boldsymbol{s}\boldsymbol{T} + C^{jj}\boldsymbol{j}^2 + C^{s\nabla j}\boldsymbol{s}(\nabla\times\boldsymbol{j})\end{aligned}$$

- Coupling constants are moments of interaction, e.g.

$$C^{\rho} \sim \int d^3\boldsymbol{r}\,\boldsymbol{r}^2 V(\boldsymbol{r})$$

- Spurious dependence on interaction !

Density functional theory

- General functional and its minimum

$$E = E(\rho) \qquad \delta E = 0$$

- Single-particle hamiltonian

$$h_{\mu\mu'} = \frac{\partial E}{\partial \rho_{\mu'\mu}}$$

- Kohn-Sham equations and their solution

$$[\rho, h] = 0 \qquad h \rightarrow \rho \rightarrow h \rightarrow \rho \rightarrow \ldots$$

Why functional and how

- **Hohenberg-Kohn theorem**

Exact functional exists

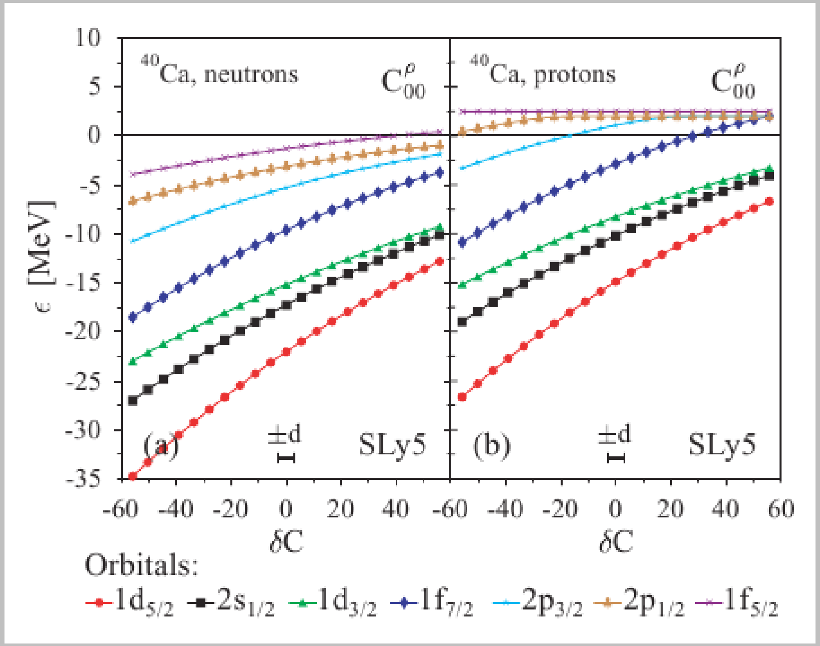
- **Includes effects beyond mean field**
- **More in spirit of effective field theory**
- **Unknown how to construct such functional**
- **Start from Skyrme and**
  - Treat C coupling constants as independent
  - Add new terms
  - Modify in any way

Skyrme functional

- Good description of bulk properties
  like masses and radii
- Unsatisfactory description of single-particle properties
- Search for spectroscopic-quality functionals

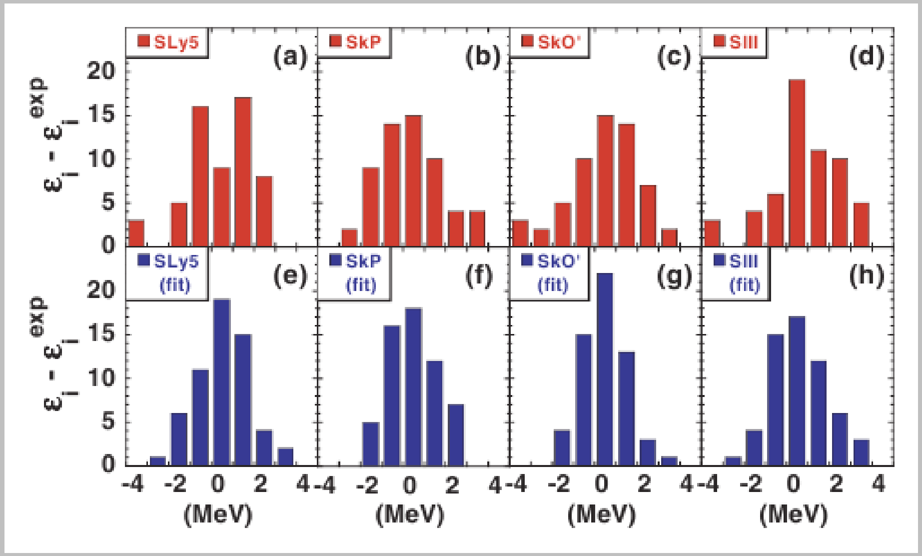
Can Skyrme functional describe single-particle data?

- **Kortelainen, Dobaczewski, Mizuyama, Toivanen** Phys. Rev. C **77** (2008) 064307
- **Linear dependence of single-particle energies on coupling constants**



Can Skyrme functionals describe single-particle data?

- **Linear fit problem solvable via Singular Value Decomposition of the Regression Matrix**
- **Deviations in single-particle energies:**



- **Skyrme functionals not sufficient – extensions needed**

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Next-to-next-to-next-to Leading Order (N^3LO)

- **Carlsson, Dobaczewski, Kortelainen**
  Phys. Rev. C **78** (2008) 044326
- **Functional quadratic in density derivatives up to sixth order**

LO	ρ^2	Delta force
NLO	$\rho \nabla^2 \rho$	Skyrme
N^3LO	$\rho \nabla^6 \rho$	

- **Nucleon-nucleon scattering well described by nucleon-pion Lagrangian up to N^3LO**

Next-to-next-to-next-to Leading Order (N^3LO)

- **Numbers of coupling constants**

Skyrme	24
N^3LO	376
+ galilean + gauge symmetry	42
+ spherical + time-reversal symmetry	22

- **Several tens of thousands of observables described (including single-particle data)**

Definition of effective mass

- **Standard single-particle Hamiltonian**

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(r)$$

- **Space and time nonlocality incorporated into the kinetic term**

$$\hat{H} = -\nabla \frac{\hbar^2}{2m^*(r)}\nabla + U(r)$$

- **Effective mass:** $m^*(r)/m$

- **Mass parameter:** $M(r) = \frac{\hbar^2}{2m^*(r)}$

Effective mass in infinite nuclear matter and in finite nuclei

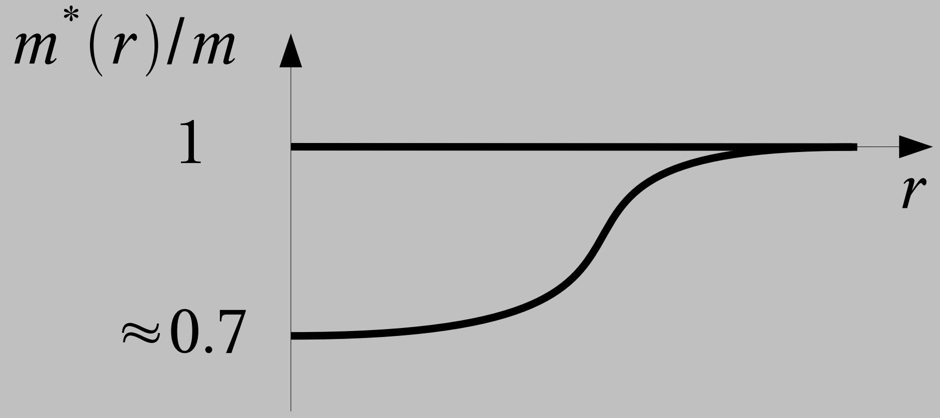
- **Infinite nuclear matter requires**

$$m^*(r)/m \approx 0.6 \div 0.9$$

- **S.p. level density in finite nuclei requires**

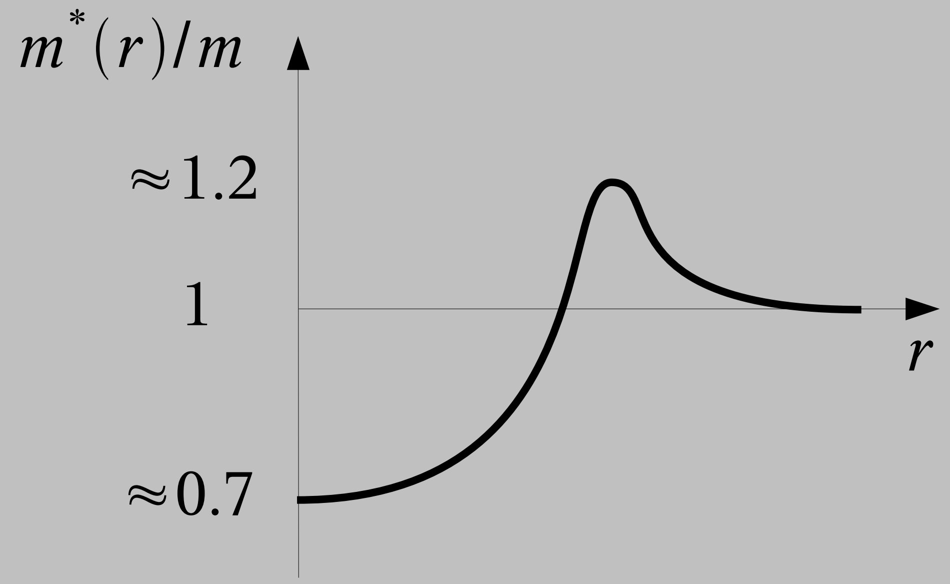
$$m^*(r)/m \approx 1$$

- **Typical radial dependence**



Surface-peaked effective mass and particle-vibration coupling

- Surface-peaked effective mass



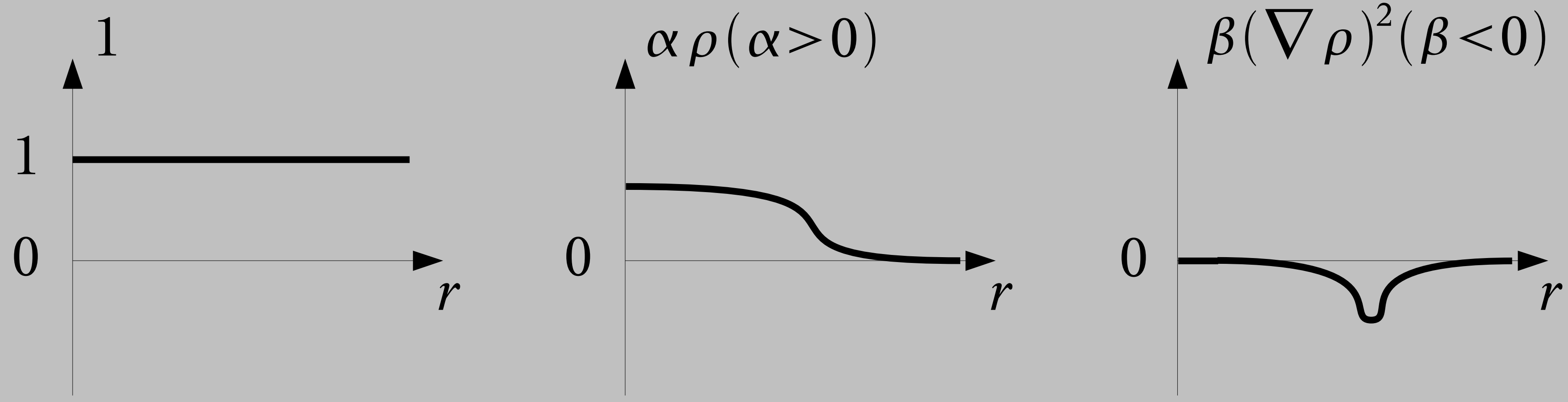
- Low inside, unit on average

- Peak may account for coupling to surface vibrations

Surface-peaked effective mass in Woods-Saxon potential

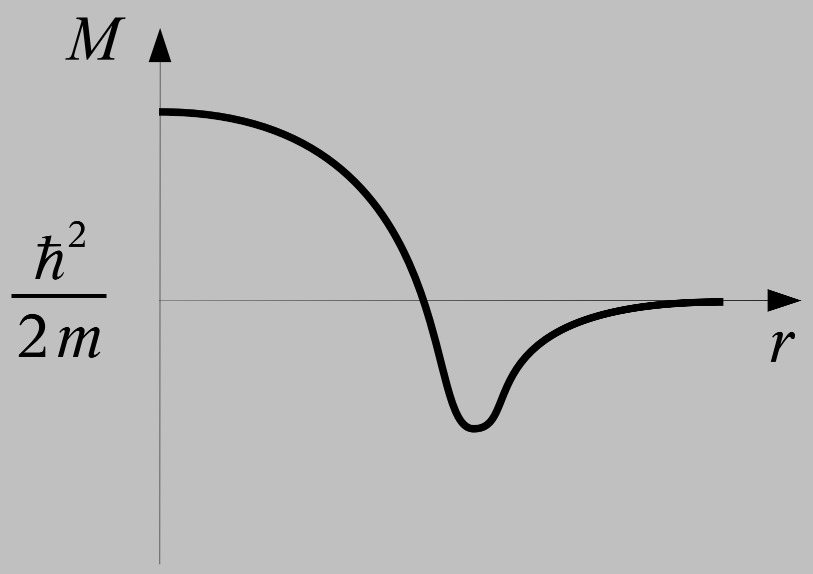
- **Kurpeta**
  MSc Thesis
- **Mass parameter**

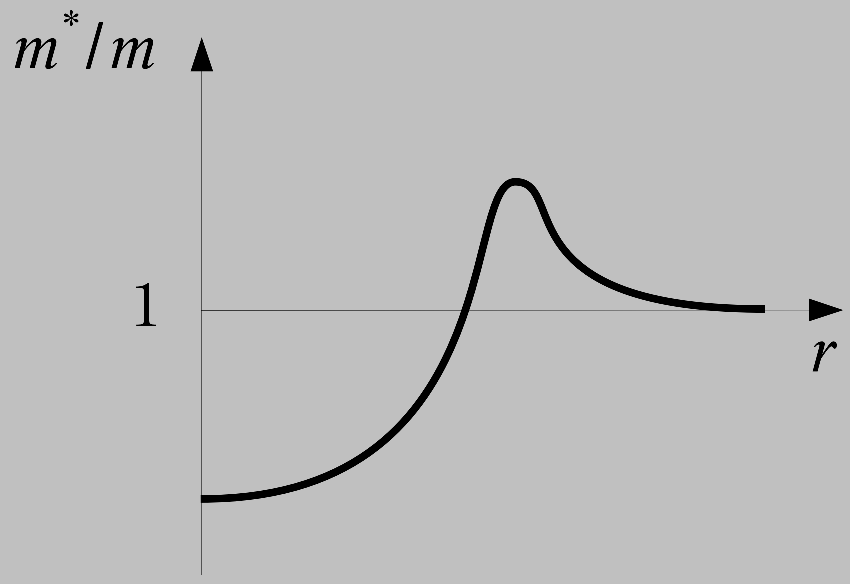
$$M(r)=\frac{\hbar^2}{2m}\left(1+\alpha\rho(r)+\beta(\nabla\rho)^2\right) \qquad \rho(r)\sim V_{\mathrm{WS}}(r)$$



Surface-peaked effective mass in Woods-Saxon potential

- **Mass parameter and effective mass**





Surface-peaked effective mass in Woods-Saxon potential

- **Ma, Wambach**
  Nucl. Phys. A **402** (1983) 275
- **Inspired by Green function approach**

$$\frac{m^*(r)}{m} = \left(1 - \alpha\, g(r)\right)\left(1 + \beta \frac{\mathrm{d}g}{dr}\right) \qquad g(r) \sim V_{\mathrm{WS}}(r)$$

k-mass
space nonlocality
mass lower inside

E-mass
time nonlocality
peak at surface

Effective mass in the Skyrme functional

- **Mass parameter in functional approach**

$$M=\frac{\delta\Re}{\delta\tau}$$

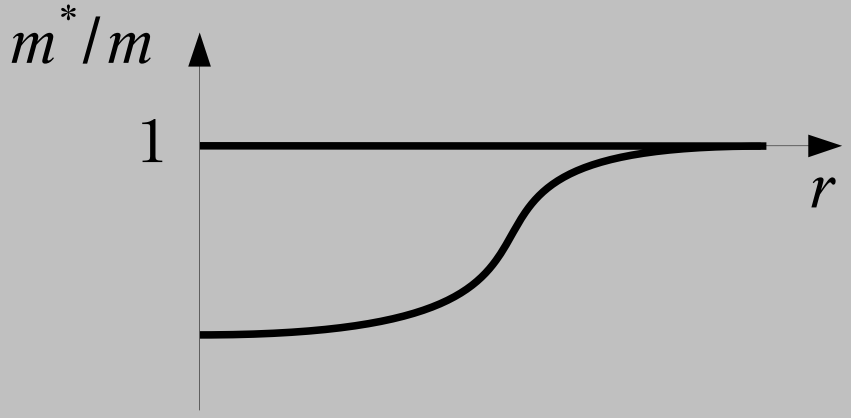
- **Part of the Skyrme functional containing τ**

$$\Re=\frac{\hbar^2}{2m}\tau+C^{\tau\rho}\tau\rho+\dots$$

- **Effective mass in the Skyrme functional**

$$M=\frac{\hbar^2}{2m}+C^{\tau\rho}\rho$$

$$C^{\tau\rho}>0$$



Surface-peaked effective mass in the Skyrme force

- **Farine, Pearson, Tondeur**
  Nucl. Phys. A 696 (2001) 396
- **New term in Skyrme force, analogous to t_1, x_1**

$$V(\boldsymbol{r},\boldsymbol{r}')=\frac{1}{2}t_4(1+x_4P_\sigma)\left(\boldsymbol{k}^2\rho(\boldsymbol{r})^\beta\delta(\boldsymbol{r}-\boldsymbol{r}')+\delta(\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r})^\beta\boldsymbol{k}^2\right)+\ldots$$

- **Functional**

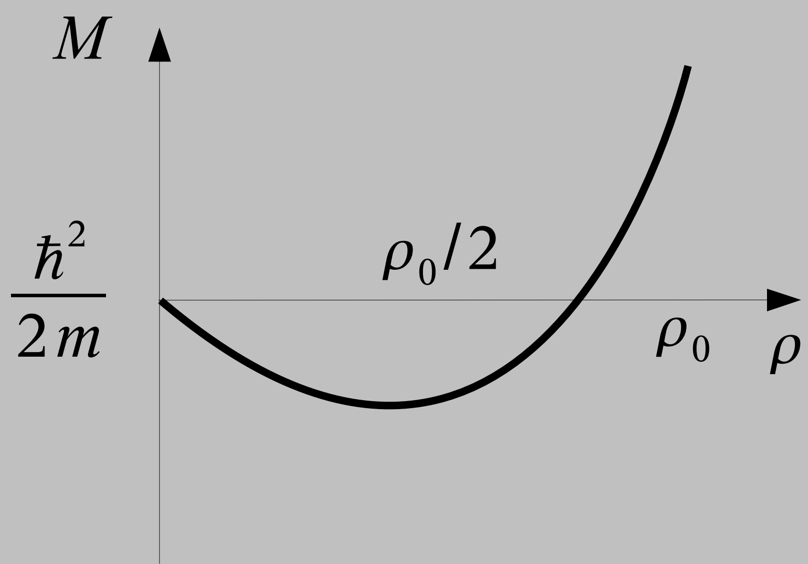
$$\Re=\frac{\hbar^2}{2m}\tau+C^{\tau\rho}\tau\rho+\boldsymbol{C}^{\boldsymbol{\tau}\boldsymbol{\rho}^{\boldsymbol{\beta}+\mathbf{1}}}\boldsymbol{\tau}\boldsymbol{\rho}^{\boldsymbol{\beta}+\mathbf{1}}+\ldots$$

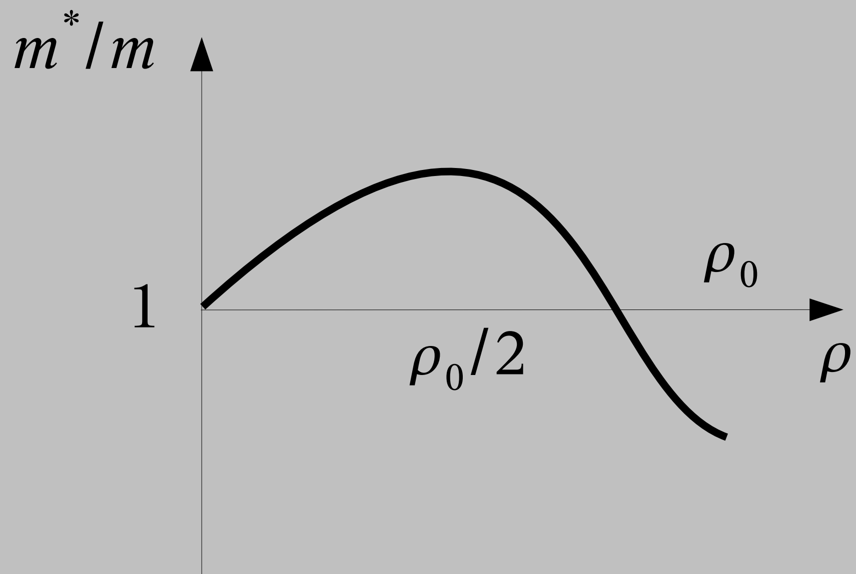
$$M=\frac{\hbar^2}{2m}+C^{\tau\rho}\rho+\boldsymbol{C}^{\boldsymbol{\tau}\boldsymbol{\rho}^{\boldsymbol{\beta}+\mathbf{1}}}\boldsymbol{\rho}^{\boldsymbol{\beta}+\mathbf{1}}$$

Surface-peaked effective mass in the Skyrme force

- **Mass parameter and effective mass**

$$M = \frac{\hbar^2}{2m} + C^{\tau\rho}\rho + \boldsymbol{C^{\tau\rho^{\beta+1}}}\boldsymbol{\rho^{\beta+1}} \qquad \beta = 0.4 \quad C^{\tau\rho} < 0 \quad C^{\tau\rho^{\beta+1}} > 0$$





Surface-peaked effective mass in the energy density functional

- **Quadratic term a la Kurpeta**

$$\Re=\frac{\hbar^2}{2m}\tau+C^{\tau\rho}\tau\rho+\boldsymbol{C}^{\boldsymbol{\tau}(\nabla\boldsymbol{\rho})^2}\boldsymbol{\tau}(\nabla\boldsymbol{\rho})^2+\dots$$

$$M=\frac{\hbar^2}{2m}+C^{\tau\rho}\rho+\boldsymbol{C}^{\boldsymbol{\tau}(\nabla\boldsymbol{\rho})^2}(\nabla\boldsymbol{\rho})^2$$

- **Linear term a la Ma & Wambach**
  only for spherical symmetry

$$\Re=\frac{\hbar^2}{2m}\tau+C^{\tau\rho}\tau\rho+\boldsymbol{C}^{\boldsymbol{\tau}\frac{\partial\boldsymbol{\rho}}{\partial\boldsymbol{r}}}\boldsymbol{\tau}\frac{\partial\boldsymbol{\rho}}{\partial\boldsymbol{r}}+\dots$$

$$M=\frac{\hbar^2}{2m}+C^{\tau\rho}\rho+\boldsymbol{C}^{\boldsymbol{\tau}\frac{\partial\boldsymbol{\rho}}{\partial\boldsymbol{r}}}\frac{\partial\boldsymbol{\rho}}{\partial\boldsymbol{r}}$$

Details of the calculations

- **Even-Even N=Z nuclei: ^{40}Ca, ^{56}Ni, ^{100}Sn**
  No time-odd nor isovector terms
- **SkXc force**
  Effective mass ≈ 1, emphasis on s.p. levels
- **Code Spherius by PO**
  Spherical and time-reversal symmetry, coordinate space
- **Calculations by MZ, coordination by WS**

Varying radial profile of effective mass

- **Constraint on mean effective mass**

$$\int \frac{m^*(\boldsymbol{r})}{m}\frac{\rho(\boldsymbol{r})}{A}\,\mathrm{d}^3\boldsymbol{r}=1$$

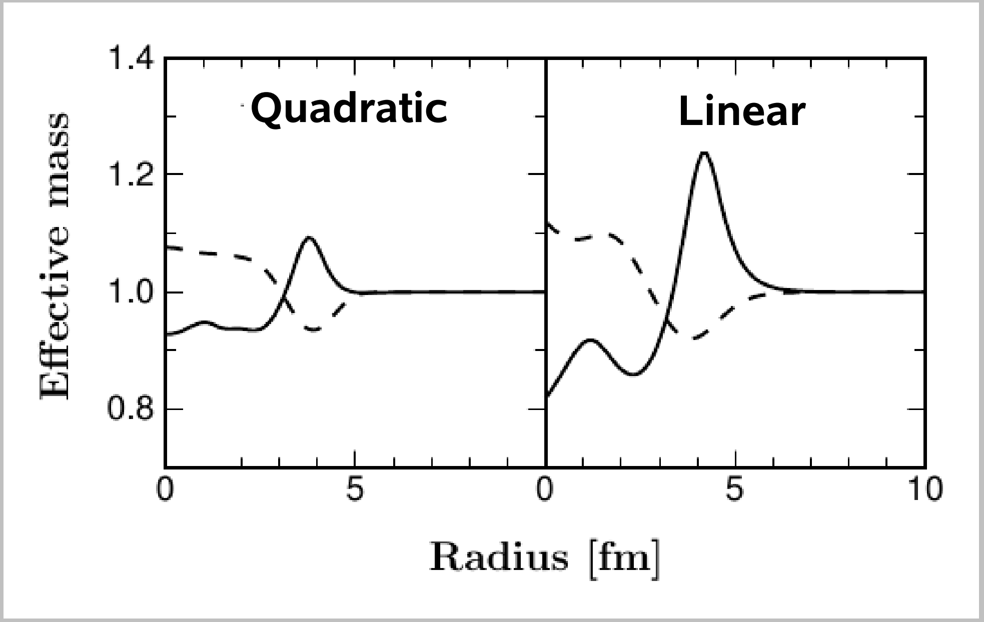
- **Treatment of coupling constants**

$C^{\tau(\nabla\rho)^2}$ or $C^{\tau\frac{\partial\rho}{\partial r}}$	Varied freely
$C^{\tau\rho}$	Adjusted to ensure unit effective mass on average
Remaining ones	Unchanged

Radial dependence of effective mass

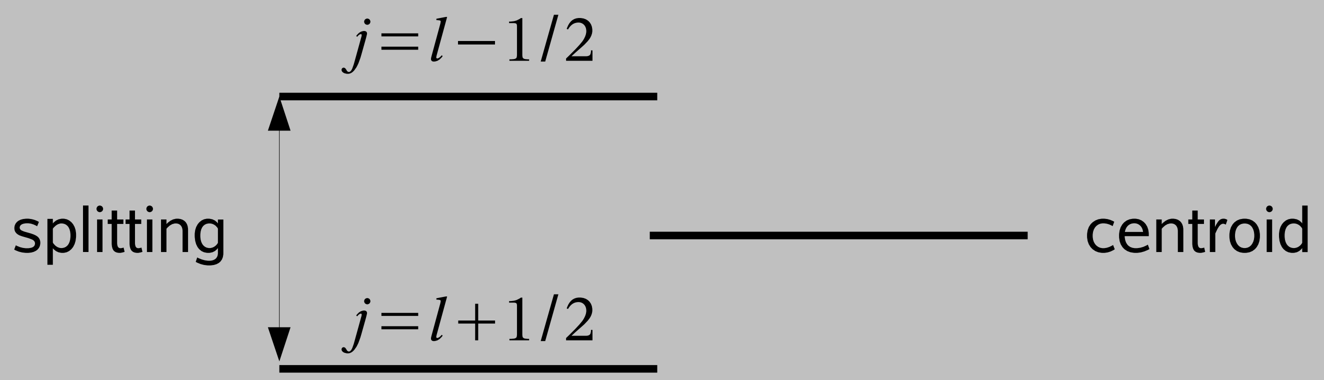
- **Zalewski, Olbratowski, Satuła**
  To be published

- **Largest peaks in ^{40}Ca**



Spin-orbit coupling

- **Spin-orbit splitting and centroid**

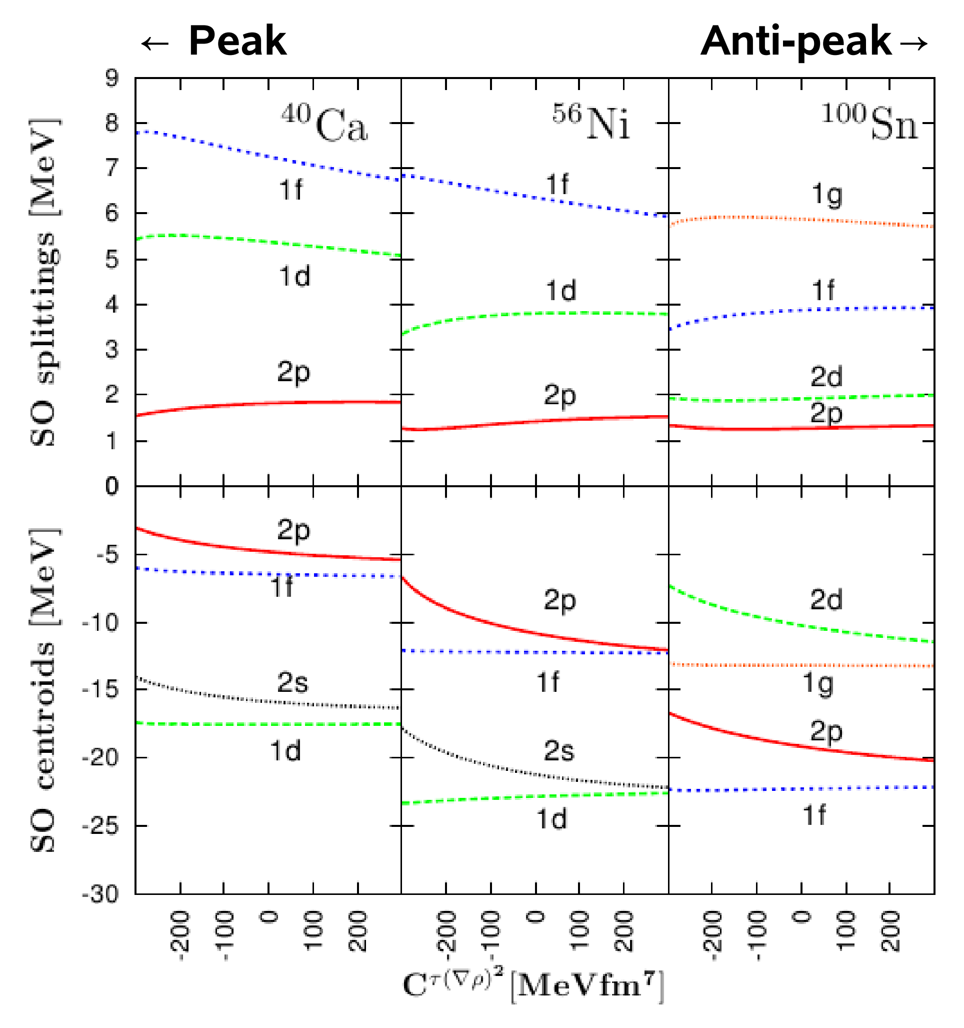


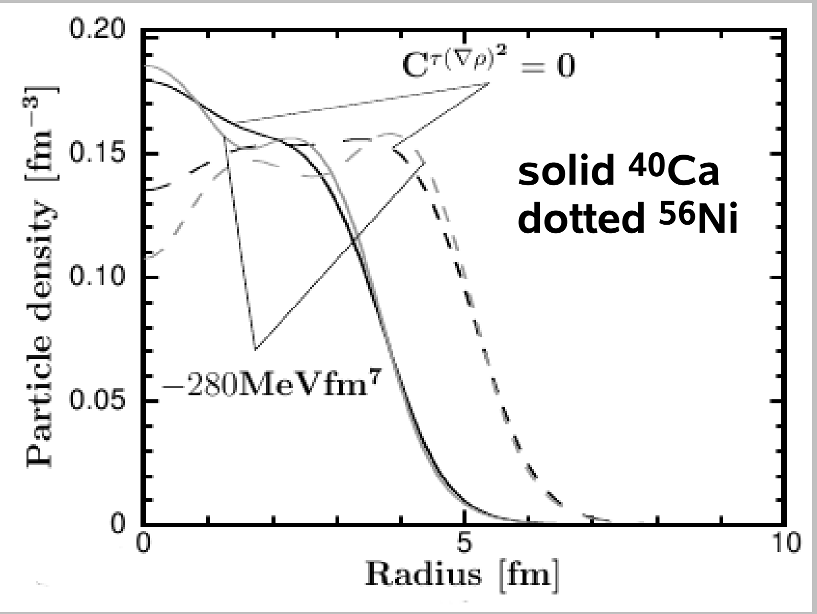
- **Spin-orbit field**

$$\bar{B} = \frac{\delta \Re}{\delta \bar{J}} \qquad \Re = C^J \bar{J}^2 + C^{\nabla J} \rho \boldsymbol{\nabla} \boldsymbol{J} + \ldots$$

$$\bar{B} = 2 C^J \bar{J} - C^{\nabla J} \bar{\nabla} \rho \qquad B_r = 2 C^J J_r - C^{\nabla J} \nabla_r \rho$$

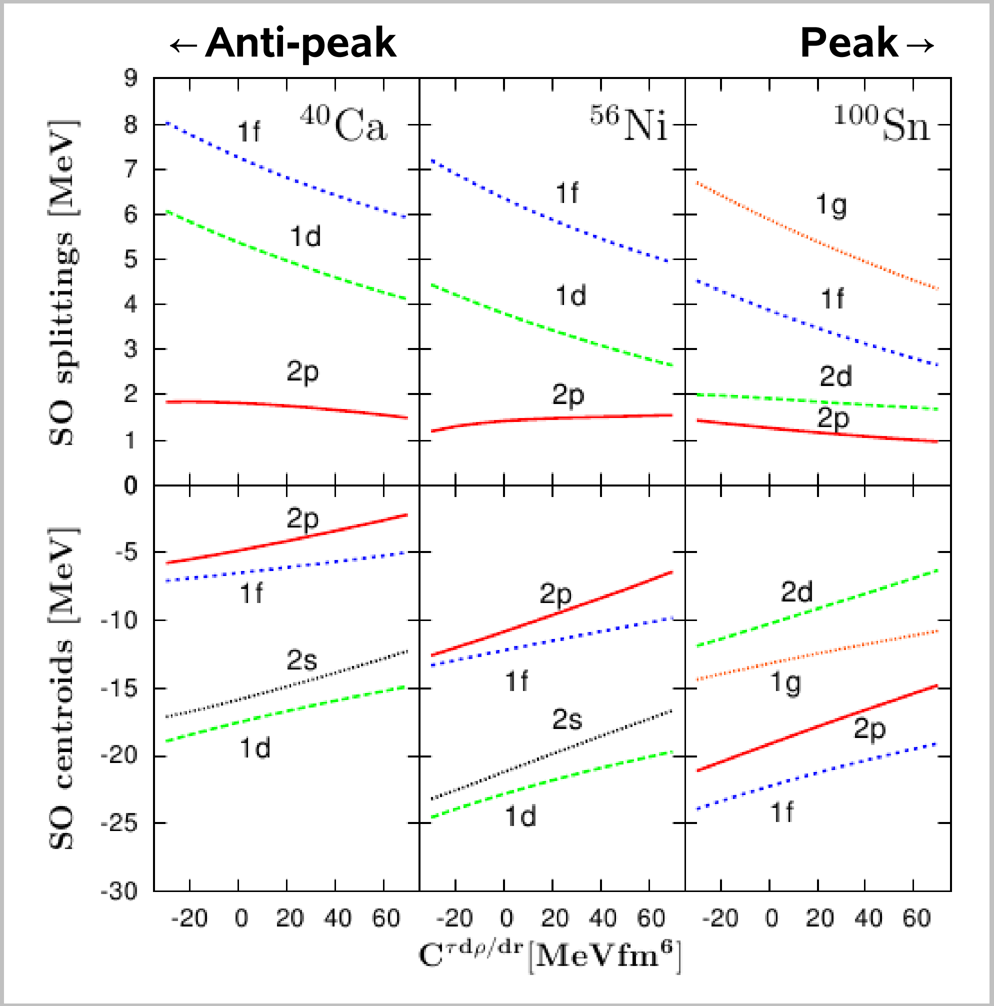
Single-particle levels with quadratic term

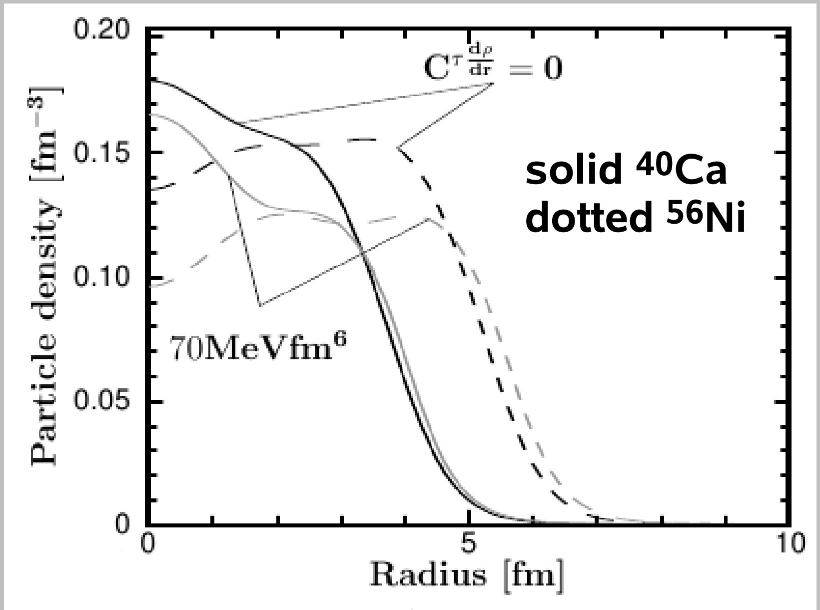




- Weak influence on s.p. levels
- No modifications at surface, more fluctuations inside - touches low-l states
- Incorrect trend in 1f splitting

Single-particle levels with linear term





- Decrease in high-l splittings, increase in all centroids
- Surface moved outwards, lower density inside
- Correct trend in 1f splitting

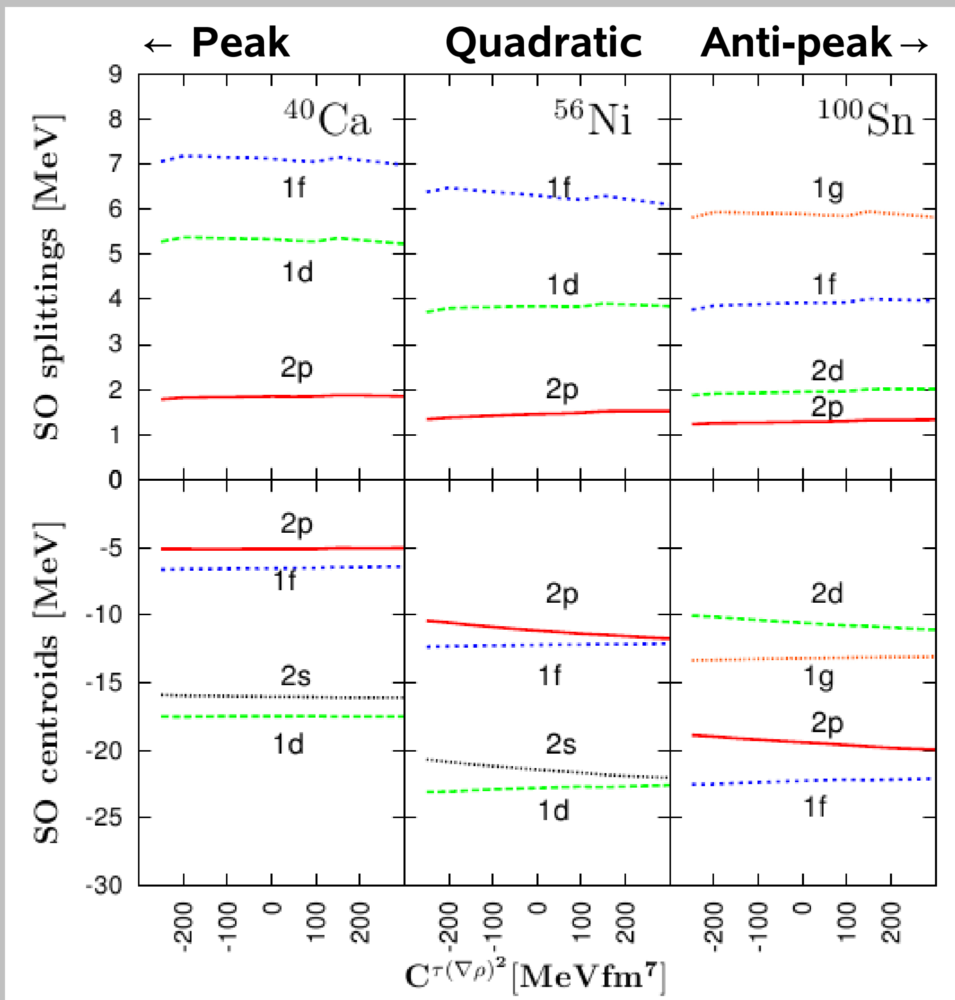
Fit to masses and radii

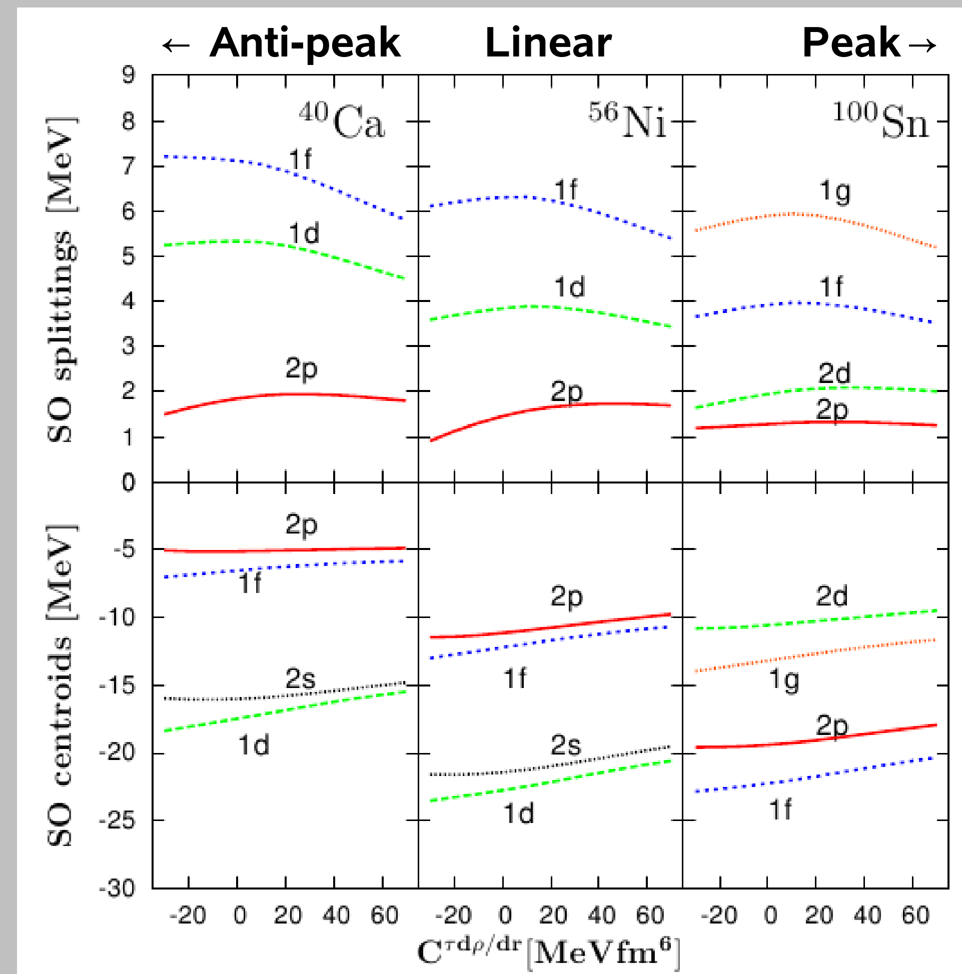
- New constants deteriorate description of masses and radii – refit needed
- Treatment of coupling constants

$C^{\tau(\nabla\rho)^2}$ or $C^{\tau\frac{\partial\rho}{\partial r}}$	Varied freely
$C^{\tau\rho}$	Adjusted to ensure unit effective mass on average
$C^{\rho\rho}$ and $C^{\rho\Delta\rho}$	Fitted to masses and radii of ^{40}Ca, ^{56}Ni, ^{100}Sn
C^{JJ} and $C^{\rho\nabla J}$	Unchanged

- Small changes in fitted constants and original SkXc masses and radii nearly reproduced over whole range of new constants

Single-particle levels after fit





- Correct trend in splittings retained for linear term

Conclusions

- Possible to obtain surface-peaked effective mass in functional approach, but height of peak limited
- Possible to retain quality of masses and radii
- Linear term gives correct trend in spin-orbit splittings
- Surface-peaked effective mass will probably interplay nicely with tensor term