Spin Densities and Currents in the Routhian Approximation

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- Spin densities and spin-currents
- Semiclassical functionals in the generalised routhian approach
- **ETF** spin-up and spin-down densities
- Application to rotating nuclei
- Continuity equation for quantum and **ETF** densities

Spin densities and spin currents

Study of an N particle system subject to an external vector field $\vec{\beta}$

Solve the variational problem for the N-body Routhian

$$\hat{\mathcal{R}} = \hat{\mathcal{H}} + \sum_{i=1}^{N} \frac{1}{2} \left[\vec{\beta}(\hat{\vec{r}}_i) \cdot \hat{\vec{p}}_i + \hat{\vec{p}}_i \cdot \vec{\beta}(\hat{\vec{r}}_i) \right] - \sum_{i=1}^{N} \vec{\Omega}(\hat{\vec{r}}_i) \cdot \hat{\vec{s}}_i$$

where

$\hat{\mathcal{H}}$ many-body Hamiltonien of the N-particle system,

$\hat{\vec{p}}_i$ momentum operator of particle i,

$\vec{\Omega}$ collective potential (generated by $\vec{\beta}$) which couples to the spin

- <u>System of N electrons subject to a uniform magnetic field $\vec{B}$</u>

$$\vec{\beta}(\vec{r}) = -\frac{|e|}{2m}\left(\vec{r}\times\vec{B}\right) \qquad \text{and} \qquad \vec{\Omega}(\vec{r}) = -\text{rot}\,\vec{\beta} = -\frac{|e|}{m}\vec{B}$$

$$\Downarrow$$

$$\hat{\mathcal{R}} = \hat{\mathcal{H}} + \frac{|e|}{2m}\vec{B}\cdot\left(\hat{\vec{L}} + 2\hat{\vec{S}}\right)$$

- <u>rotating N particle system</u>

$$\vec{\beta}(\vec{r}) = \vec{r}\times\vec{\omega} \qquad \text{and} \qquad \vec{\Omega}(\vec{r}) = -\frac{1}{2}\,\text{rot}\,\vec{\beta} = \vec{\omega}$$

$$\Downarrow$$

$$\hat{\mathcal{R}} = \hat{\mathcal{H}} - \vec{\omega}\cdot\hat{\vec{L}} - \vec{\omega}\cdot\hat{\vec{S}} = \hat{\mathcal{H}} - \vec{\omega}\cdot\hat{\vec{J}}$$

Complete treatment of the variational problem can be formulated through the <u>one-body reduced density matrix operator</u>

$$\hat{\rho} = \frac{1}{2}\left(\hat{\rho}_0 + \hat{\vec{\rho}} \cdot \hat{\vec{\sigma}}\right)$$

with the coordinate representations

$$\rho_0(\vec{r},\vec{r}\,') = \sum_{\sigma} \rho(\vec{r},\sigma;\vec{r}\,',\sigma) = \sum_{k}\sum_{\sigma} n_k\, \varphi_k(\vec{r},\sigma)\, \varphi_k^*(\vec{r}\,',\sigma)$$

and

$$\vec{\rho}(\vec{r},\vec{r}\,') = \sum_{\sigma,\sigma'} \rho(\vec{r},\sigma;\vec{r}\,',\sigma')\langle \sigma'|\vec{\sigma}|\sigma \rangle = \sum_{k}\sum_{\sigma,\sigma'} n_k\, \varphi_k(\vec{r},\sigma)\, \varphi_k^*(\vec{r}\,',\sigma')\, \langle \sigma'|\vec{\sigma}|\sigma \rangle$$

At $T = 0$ one has

$$n_k = \Theta(\varepsilon_F - \varepsilon_k)$$

one can similarly define the <u>current density matrix</u>

$$\vec{j}(\vec{r},\sigma;\vec{r}\,',\sigma') = \frac{1}{2i}\left(\vec{\nabla}_r - \vec{\nabla}_{r'}\right)\rho(\vec{r},\sigma;\vec{r}\,',\sigma')$$

and which can be written

$$\vec{j}(\vec{r},\sigma;\vec{r}\,',\sigma') = \frac{1}{2}\,\vec{j}_0(\vec{r},\vec{r}\,')\,\delta_{\sigma,\sigma'} + \frac{1}{2}\sum_{\nu=1}^{3}\vec{J}_\nu(\vec{r},\vec{r}\,')\,\langle\sigma|\sigma_\nu|\sigma'\rangle$$

where

$$\vec{j}_0(\vec{r},\vec{r}\,') = \frac{1}{2i}\left(\vec{\nabla}_r - \vec{\nabla}_{r'}\right)\rho_0(\vec{r},\vec{r}\,')$$

and

$$\vec{J}_\nu(\vec{r},\vec{r}\,') = \frac{1}{2i}\left(\vec{\nabla}_r - \vec{\nabla}_{r'}\right)\rho_\nu(\vec{r},\vec{r}\,') \quad , \qquad \nu = 1,2,3$$

The 9 components of the vectors $(\vec{J}_1, \vec{J}_2, \vec{J}_3)$ may be understood as the components of a 3×3 spin current tensor [1]

$$J_{\mu\,\nu}(\vec{r},\vec{r}\,') = \frac{1}{2i}\left(\vec{\nabla}_r - \vec{\nabla}_{r'}\right)_\mu \rho_\nu(\vec{r},\vec{r}\,')$$

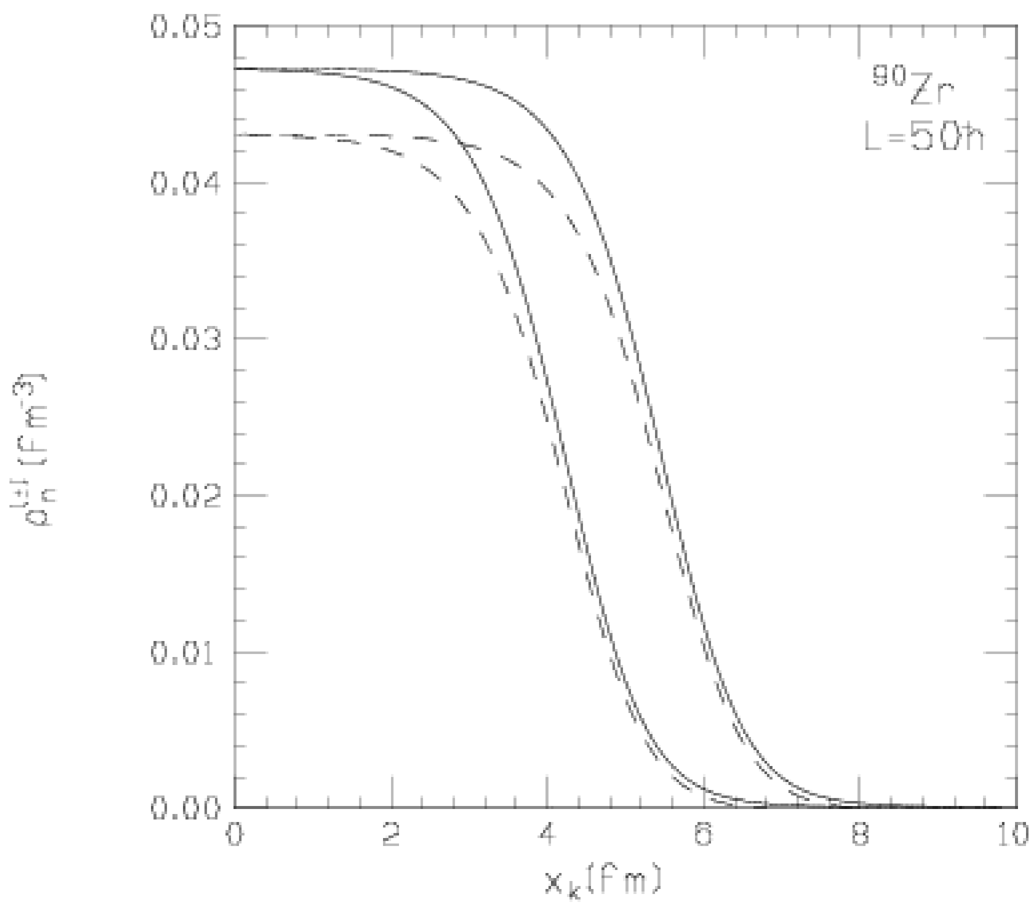
Don't confuse with the so-called spin-orbit density $\vec{J}$, which is the antisymmetric part of the tensor $J_{\mu\,\nu}$

$$J_\lambda = \sum_{\mu\nu}\varepsilon_{\lambda\mu\nu}J_{\mu\nu}$$

[1] Y.M. Engel, D.M. Brink, K. Göke, S.J. Krieger, D. Vautherin, Nucl. Phys. A249 (1975) 215

one may them study the local behaviour of spin-up $\rho_\uparrow(\vec{r})$ and spin-down $\rho_\downarrow(\vec{r})$ densities, defined through

$$\begin{aligned} \rho_0(\vec{r}) &= \rho_\uparrow(\vec{r}) + \rho_\downarrow(\vec{r}) \\ \rho_3(\vec{r}) &= \rho_\uparrow(\vec{r}) - \rho_\downarrow(\vec{r}) \end{aligned} \quad \Longrightarrow \quad \begin{aligned} \rho_\uparrow(\vec{r}) &= \frac{1}{2}\left[\rho_0(\vec{r}) + \rho_3(\vec{r})\right] \\ \rho_\downarrow(\vec{r}) &= \frac{1}{2}\left[\rho_0(\vec{r}) - \rho_3(\vec{r})\right] \end{aligned}$$



and similarly

$$\vec{j}_\uparrow(\vec{r}) = \frac{1}{2}\left[\vec{j}_0(\vec{r}) + \vec{J}_3(\vec{r})\right]$$

$$\vec{j}_\downarrow(\vec{r}) = \frac{1}{2}\left[\vec{j}_0(\vec{r}) - \vec{J}_3(\vec{r})\right]$$

Semiclassical functionals in the generalised routhian approach

Study the local behaviour of above densities by evaluating the expectation value of the routhian $\hat{\mathcal{R}}$ in the independent-particle approximation.

Using Skyrme type effective forces $\langle \hat{\mathcal{R}} \rangle$ can be written as

$$\langle \hat{\mathcal{R}} \rangle = \int \left\{ \mathcal{E} \left[\rho_q, \vec{\rho}_q, \vec{j}_q, \vec{J}_q, \tau_q \right] - \hbar \, \vec{\beta} \cdot \vec{j} - \frac{\hbar}{2} \vec{\Omega} \cdot \vec{\rho} \right\} d^3 r$$

Minimizing this expectation value with respect to all single-particle wave functions one obtains the following set of equations

$$\left\{ -\frac{\hbar^2}{2m} \vec{\nabla} \cdot f_q \vec{\nabla} + V_q + \frac{\hbar}{2i} (\vec{\alpha_q} \cdot \vec{\nabla} + \vec{\nabla} \cdot \vec{\alpha_q}) \right.$$
$$\left. + \frac{1}{2i} (\vec{W}_q \times \vec{\nabla} - \vec{\nabla} \times \vec{W}_q) \cdot \vec{\sigma} + \hbar \vec{S}_q \cdot \vec{\sigma} \right\} | \varphi_j^{(q)} \rangle = \varepsilon_j^{(q)} | \varphi_j^{(q)} \rangle$$

Semiclassical ETF functionals :

Perform selfconsistent semiclassical calculation for given constraint $\rho_n \; ; \; \rho_p$

Solve system of equations for $\vec{\rho}_n$ and $\vec{\rho}_p$

Solve system of equations for $\vec{j}_n$ and $\vec{j}_p$

$$\Downarrow$$

Form factors : effective mass f_q, spin-orbit potential $\vec{W}_q$,

cranking field $\vec{\alpha}_q$, spin field $\vec{S}_q$ [2,3]

are determined

$$\Longrightarrow \qquad J_{\mu\nu} = -\frac{m}{\hbar^2 f}\,\rho_0 \sum_{\lambda=1}^{3} \varepsilon_{\mu\nu\lambda} W_\lambda - \frac{m}{\hbar^2 f}\,\alpha_\mu\,\rho_\nu$$

[2] K. Bencheikh, P. Quentin, J. Bartel, Nucl. Phys. A571 (1994) 518

[3] J. Bartel, K. Bencheikh, P. Quentin, Nucl. Phys. A in print

ETF spin-up and spin-down densities

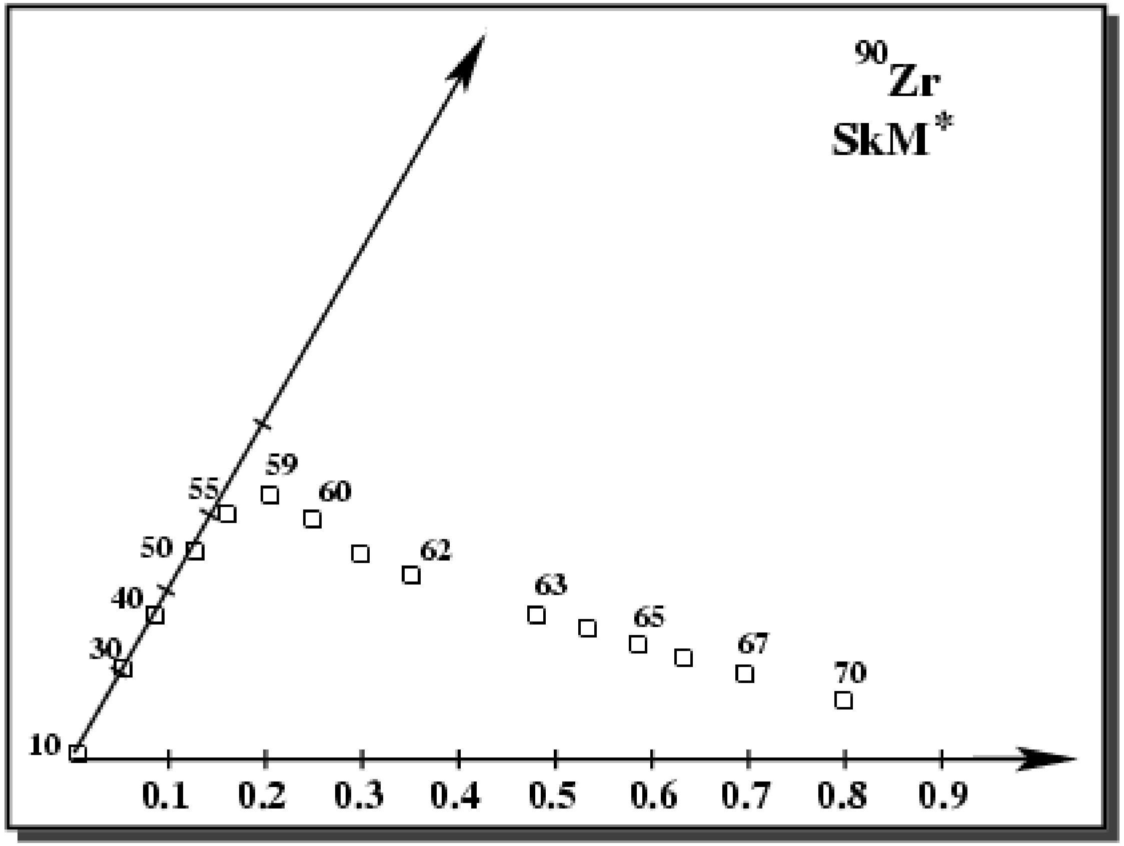
$$\rho_\uparrow(\vec{r}) = \frac{1}{2}\left[\rho_0(\vec{r}) + \rho_3(\vec{r})\right]$$
$$\rho_\downarrow(\vec{r}) = \frac{1}{2}\left[\rho_0(\vec{r}) - \rho_3(\vec{r})\right]$$

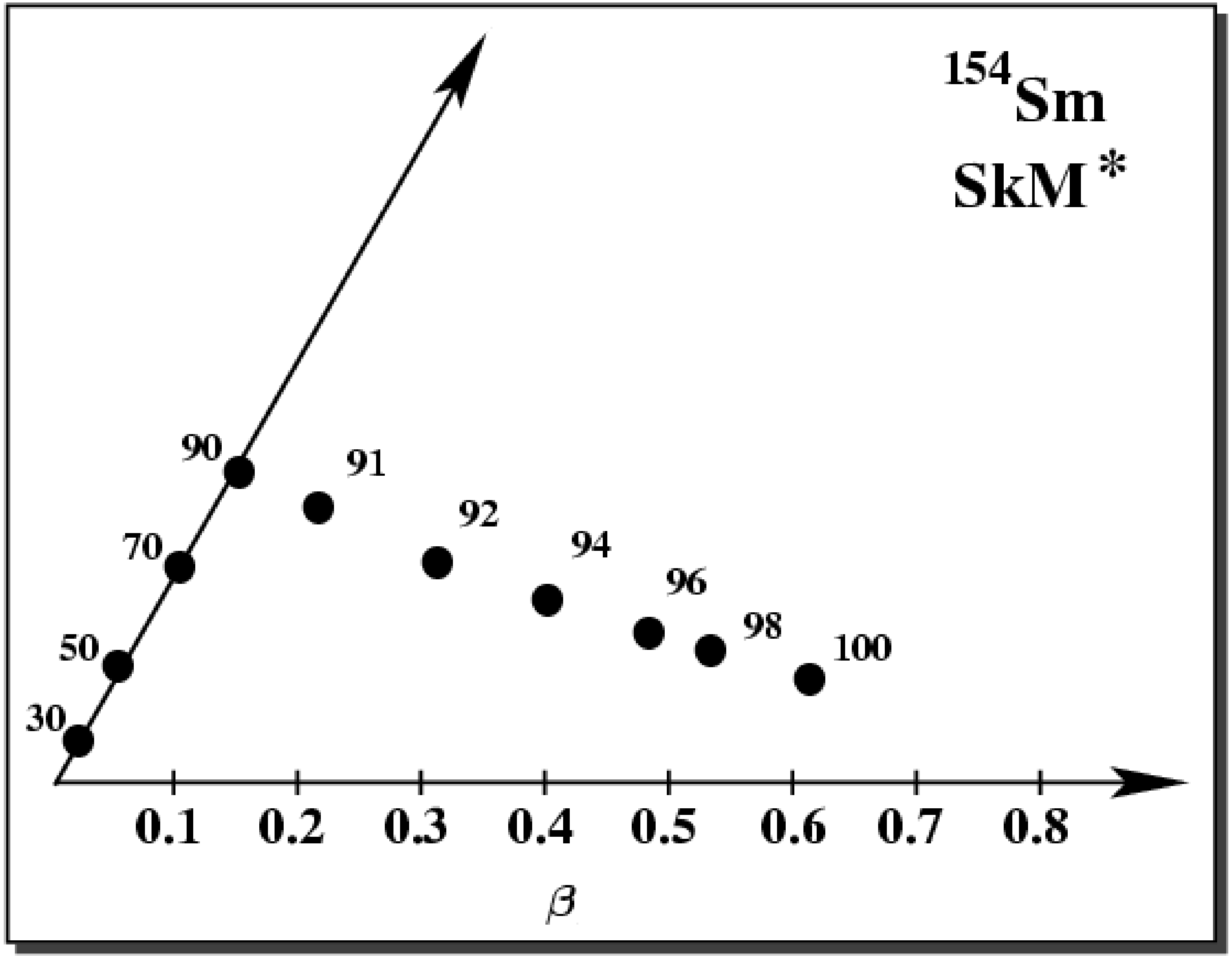
and one finds

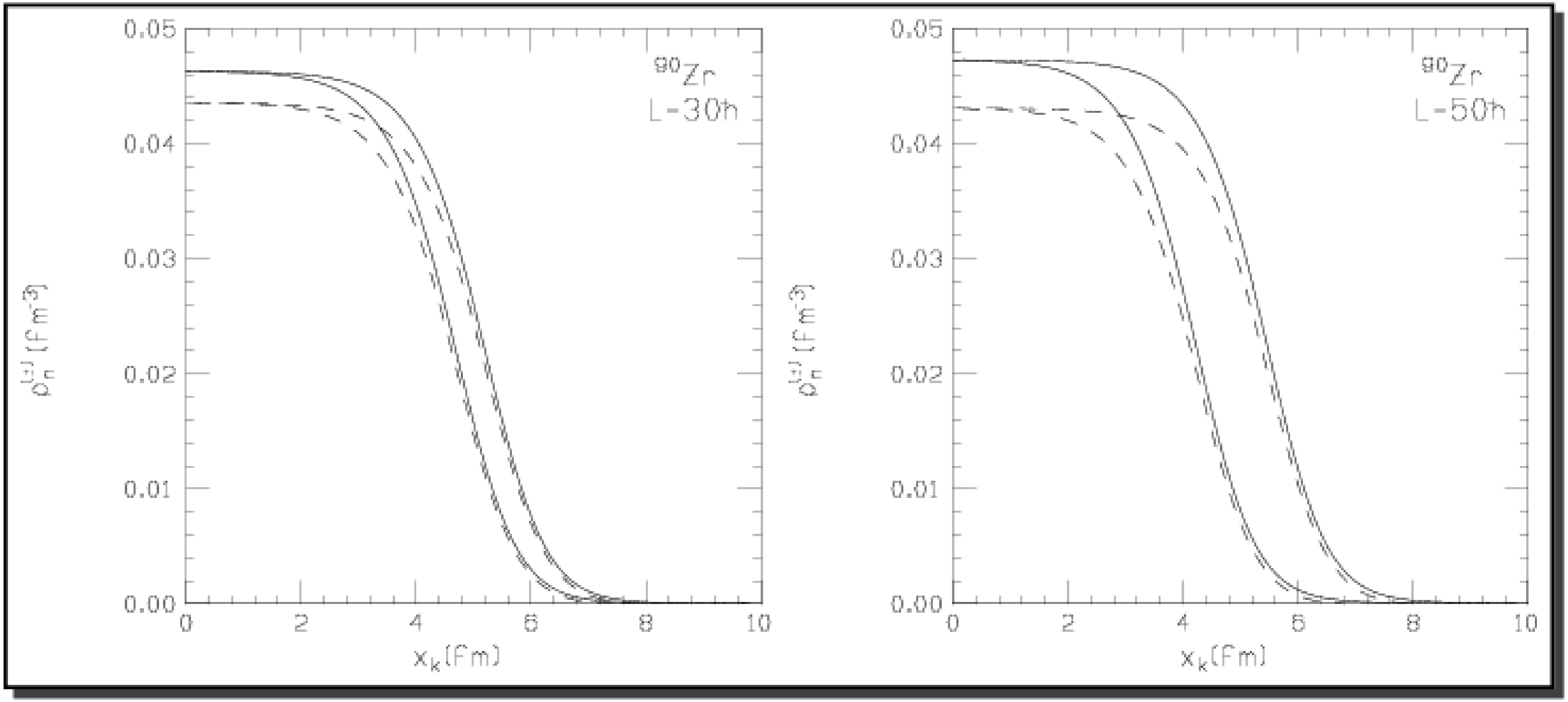
$$\vec{j}_\uparrow = \frac{1}{2}\left[\vec{j}_0 + \frac{m}{\hbar^2 f}\,\rho_0\left(\boldsymbol{W}_2\,\vec{e}_1 - \boldsymbol{W}_1\,\vec{e}_2\right) - \frac{m}{\hbar^2}\,\rho_3\,\vec{\beta}\right]$$
$$\vec{j}_\downarrow = \frac{1}{2}\left[\vec{j}_0 - \frac{m}{\hbar^2 f}\,\rho_0\left(\boldsymbol{W}_2\,\vec{e}_1 - \boldsymbol{W}_1\,\vec{e}_2\right) + \frac{m}{\hbar^2}\,\rho_3\,\vec{\beta}\right]$$

Application to rotating nuclei

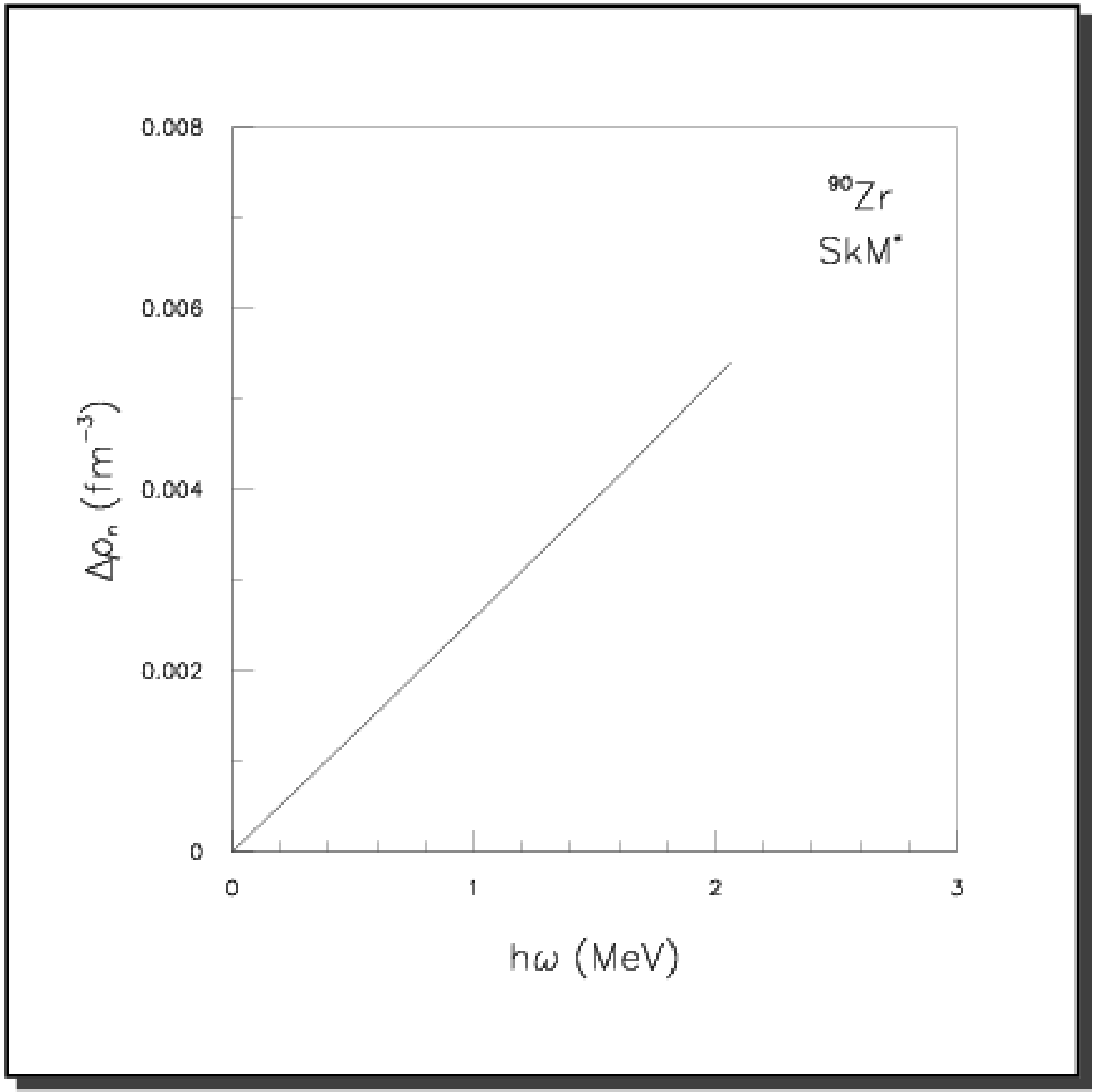
Perform selfconsistent semiclassical calculations for given $\langle \hat{\vec{J}} \rangle$

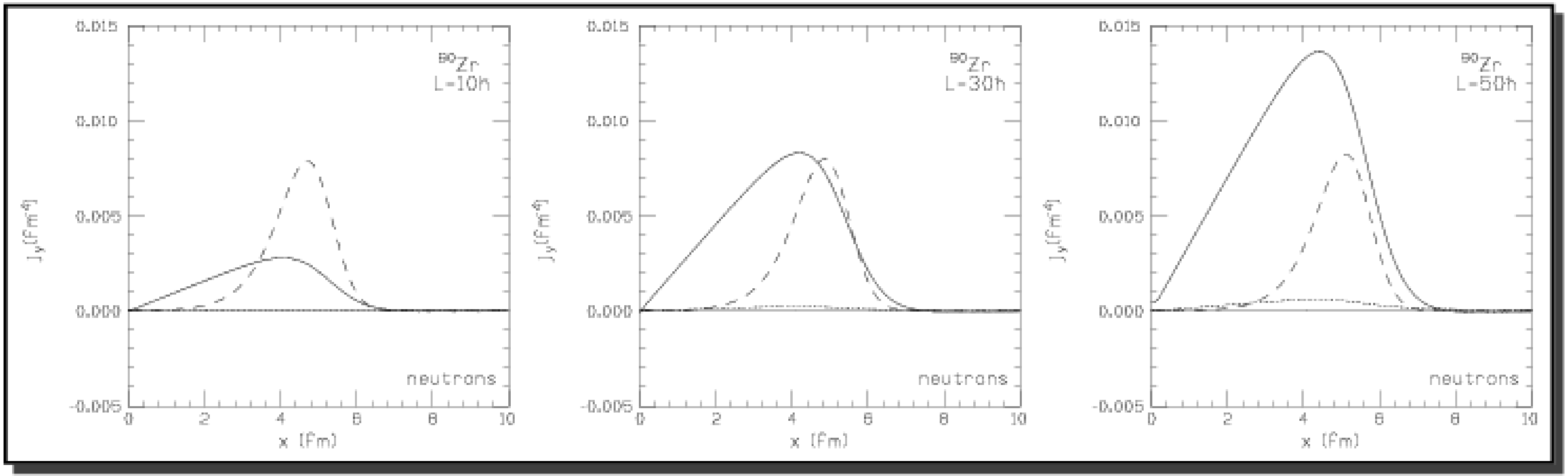



154Sm
SkM*
90
91
92
94
96
98
100
70
50
30
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
β



90Zr
L-30h
90Zr
L-50h
x_k(fm)
x_k(fm)
0.00
0.01
0.02
0.03
0.04
0.05
0
2
4
6
8
10


0.008
0.006
0.004
0.002
0
Δρn (fm-3)
90Zr
SkM*
0
1
2
3
hω (MeV)

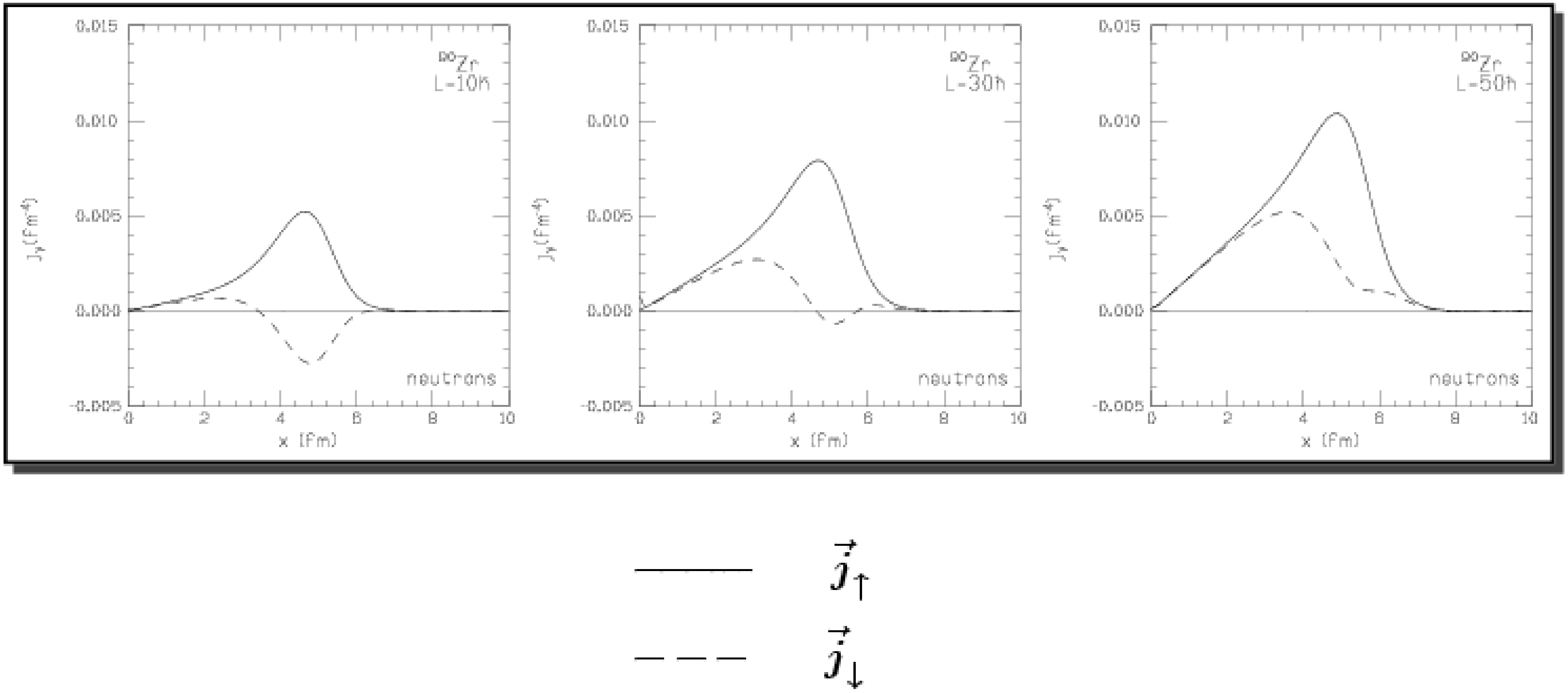


Contributions to spin-up and spin-down currents:

——— (1) total current density

– – – (2) spin-orbit contribution

· · · · · · (3) vector-field coupling



90Zr
L-10ħ
L-30ħ
L-50ħ
neutrons
j_y (fm^-4)
x (fm)
0.015
0.010
0.005
0.000
-0.005
0
2
4
6
8
10
$\vec{j}_\uparrow$
$\vec{j}_\downarrow$

Continuity equation for quantum and ETF densities

Start from s.-p. Hartree-Fock equation

$$\Big\{ -\frac{\hbar^2}{2m}\vec{\nabla}\cdot f_q\vec{\nabla} + V_q + \frac{\hbar}{2i}(\vec{\alpha}_q\cdot\vec{\nabla} + \vec{\nabla}\cdot\vec{\alpha}_q) + \frac{1}{2i}(\vec{W}_q\times\vec{\nabla} - \vec{\nabla}\times\vec{W}_q)\cdot\vec{\sigma} + \hbar\vec{S}_q\cdot\vec{\sigma}\Big\} \mid \varphi_j^{(q)}> = \varepsilon_j^{(q)} \mid \varphi_j^{(q)}>$$

one can then easily prove ther following continuity equation

$$\vec{\nabla}\left[f\,\vec{j} + \frac{m\rho}{\hbar^2}\hbar\vec{\alpha} + \frac{m}{\hbar^2}\left(\vec{\rho}\times\vec{W}\right)\right] = 0$$

It is now interesting to notice that this equation is also satisfied by the semiclassical ETF densities and fields

$\Longrightarrow$ severe test for our semiclassial ETF densities

Conclusions

What can this be usefull for ?

- effect of rotation much more pronounced on $\vec{j}_\uparrow \, \vec{j}_\downarrow$ than on $\rho_\uparrow \, \rho_\downarrow$
- any magnetic property in rotating nuclei
- dynamical effects of pairing correlations in rotating nuclei well described within a **HF** Routhian approach upon imposing well defined intrinsic vortical currents [4]

[4] P. Quentin, H. Lafchiev, D. Samsoen, I.N. Mikhailov, Phys. Rev. C69 (2004) 054315