CISS07 8/30/2007

Comprehensive treatment of correlations at different energy scales in nuclei using Green's functions

Lecture 1: 8/28/07	Propagator description of single-particle motion and the link with experimental data
Lecture 2: 8/29/07	From Hartree-Fock to spectroscopic factors < 1: inclusion of long-range correlations
Lecture 3: 8/29/07	Role of short-range and tensor correlations associated with realistic interactions
Lecture 4: 8/30/07	Dispersive optical model and predictions for nuclei towards the dripline
Adv. Lecture 1: 8/30/07	Saturation problem of nuclear matter & pairing in nuclear and neutron matter
Adv. Lecture 2: 8/31/07	Quasi-particle density functional theory

Wim Dickhoff
Washington University in St. Louis

Outline

- Dispersion relation for self-energy
- Self-energy and nucleon optical potential
- Description of elastic nucleon scattering
- Empirical information on optical potentials
- Subtracted dispersion relation
- Discussion of time and space nonlocality
- Dispersive optical model fits for ^{40}Ca and ^{48}Ca
- Extrapolation to the dripline
- Data-driven extrapolations & missing data
- Inclusion of nonlocal potentials

Theory & Framework

Theory
hard...

- Calculations: Include SRC and LRC as good as possible
- Compare with experiment; add more physics

Framework
"easy"

- Determine propagator from data!?!!
- Illustrated with (e,e′p) reaction below the Fermi energy
- Today also elastic scattering data

Answers:
What do nucleons do in the nucleus
and how does their behavior change
as a function of asymmetry

Correlations for nuclei with N very different from Z?
$\Rightarrow$ Radioactive beam facilities

Nuclei are TWO-component Fermi liquids

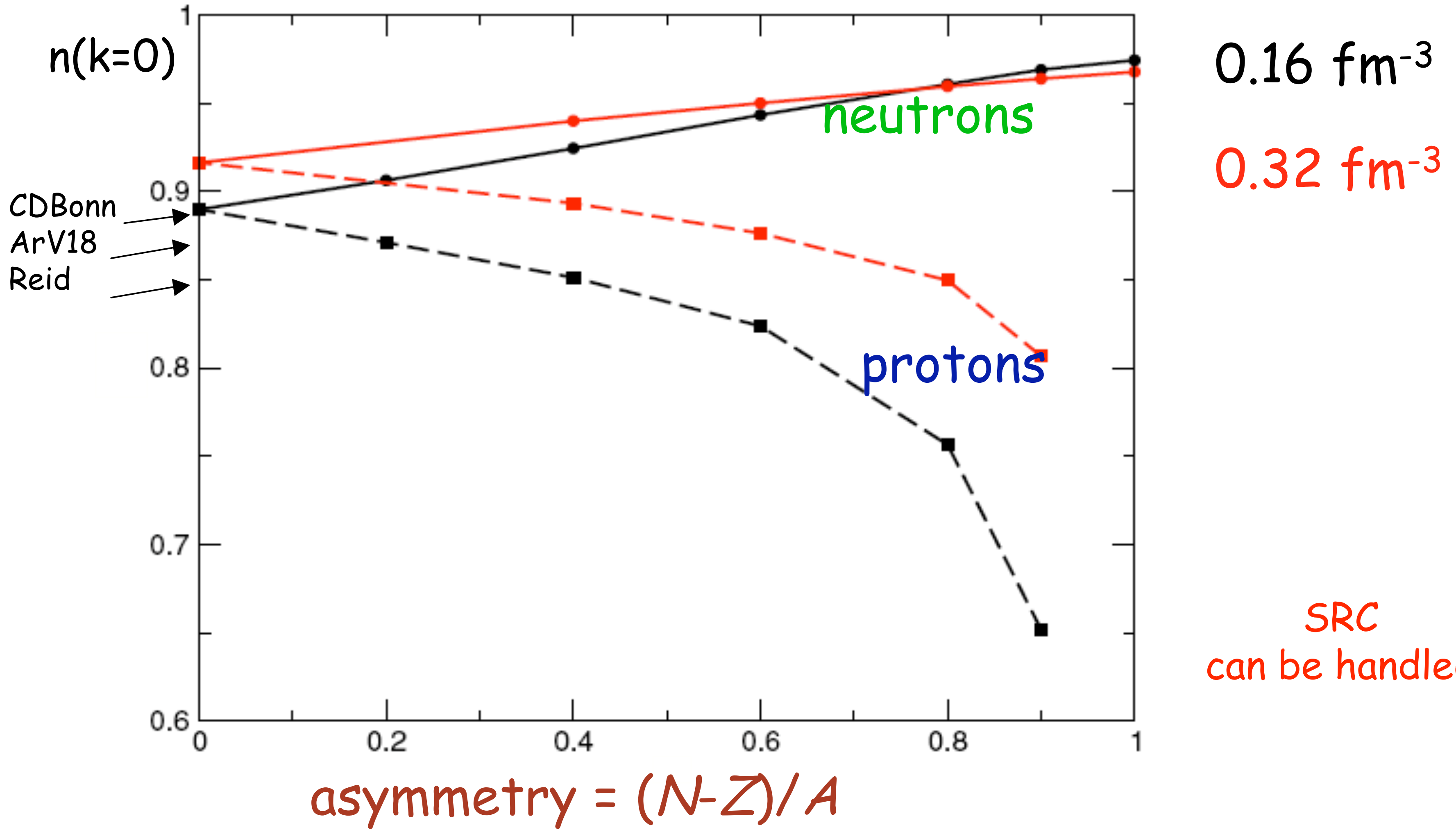
- SRC about the same between pp, np, and nn
- Tensor force disappears for n when N >> Z but …
- Empirically p more bound with increasing asymmetry (N-Z)/A

- Any surprises?
- Ideally: quantitative predictions based on solid foundation

Some pointers: one from theory and one from experiment

SCGF for isospin-polarized nuclear matter including SRC ⇒ momentum distribution

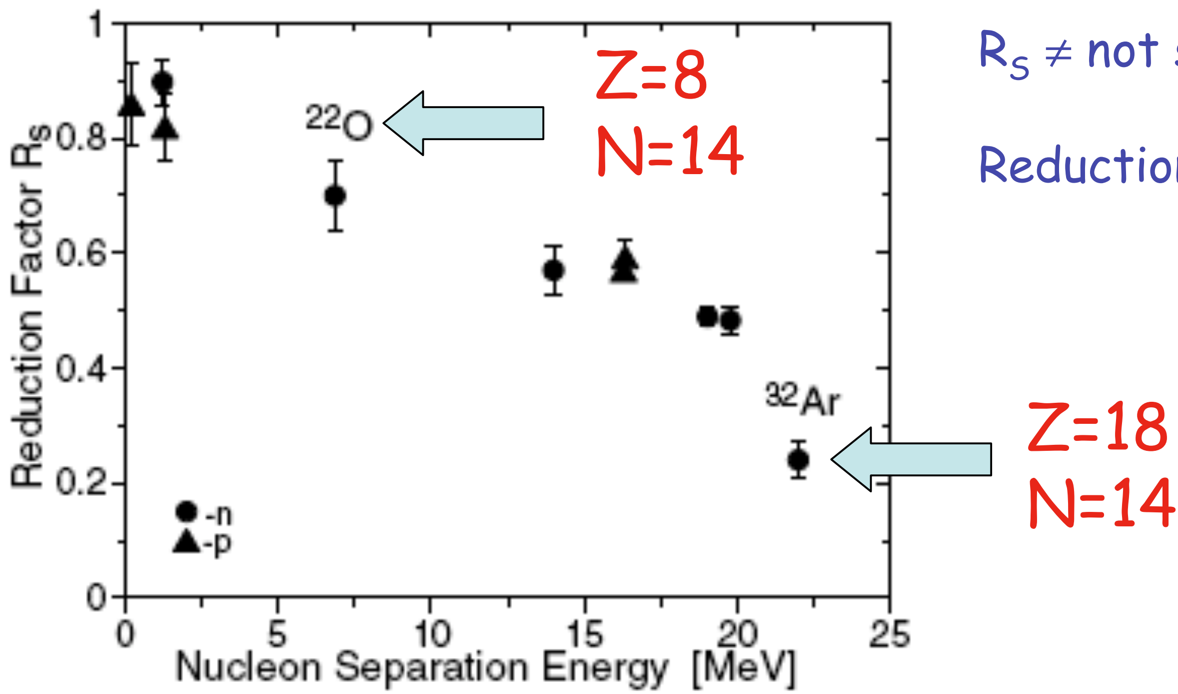
Frick *et al.* PRC71,014313(2005)



SRC
can be handled

A. Gade et al., Phys. Rev. Lett. 93, 042501 (2004)

Program at MSU initiated by Gregers Hansen
P. G. Hansen and J. A. Tostevin, Annu. Rev. Nucl. Part. Sci. **53**, 219 (2003)

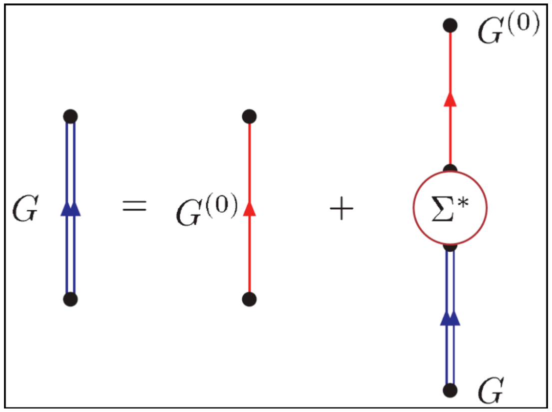


$R_S \neq$ not spectroscopic factor

Reduction w.r.t. shell model

neutrons more correlated with increasing proton number
and accompanying increasing separation energy.

Dyson Equation and "experiment"



Equivalent to …

Schrödinger-like equation with: $E_n^- = E_0^N - E_n^{N-1}$

Self-energy: non-local, energy-dependent potential
With energy dependence: spectroscopic factors < 1
$\Rightarrow$ as observed in (e,e'p)

$$-\frac{\hbar^2\nabla^2}{2m}\left\langle \Psi_n^{N-1}\middle| a_{\vec{r}m} \middle| \Psi_0^N \right\rangle + \sum_{m'} \int d\vec{r}\,' \Sigma'^*(\vec{r}m, \vec{r}\,'m'; E_n^-) \left\langle \Psi_n^{N-1}\middle| a_{\vec{r}\,'m'} \middle| \Psi_0^N \right\rangle = E_n^- \left\langle \Psi_n^{N-1}\middle| a_{\vec{r}m} \middle| \Psi_0^N \right\rangle$$

$$S = \left| \left\langle \Psi_n^{N-1}\middle| a_{\alpha_{qh}} \middle| \Psi_0^N \right\rangle \right|^2 = \frac{1}{1 - \left.\frac{\partial \Sigma'^*(\alpha_{qh}, \alpha_{qh}; E)}{\partial E}\right|_{E_n^-}}$$

α_{qh} solution of DE at E_n^-

DE yields

$$\left\langle \Psi_n^{N-1}\middle| a_{\vec{r}m} \middle| \Psi_0^N \right\rangle = \psi_n^{N-1}(\vec{r}m)$$ *Bound states in N-1*

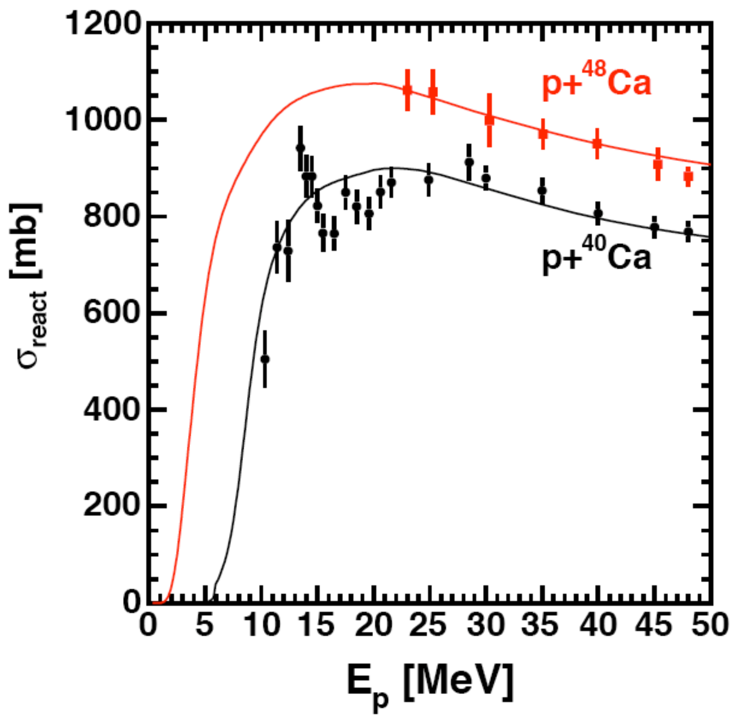
$$\left\langle \Psi_0^N\middle| a_{\vec{r}m} \middle| \Psi_k^{N+1} \right\rangle = \psi_k^{N+1}(\vec{r}m)$$ *Bound states in N+1*

$$\left\langle \Psi_E^{c,N-1}\middle| a_{\vec{r}m} \middle| \Psi_0^N \right\rangle = \chi_c^{N-1}(\vec{r}m; E)$$ *Scattering states in N-1*

$$\left\langle \Psi_0^N\middle| a_{\vec{r}m} \middle| \Psi_E^{c,N+1} \right\rangle = \chi_c^{N+1}(\vec{r}m; E)$$ *Elastic scattering in N+1*

Elastic scattering wave function for (*p*,*p*) or (*n*,*n*)

Does the nucleon self-energy also have an imaginary part above the Fermi energy?



Loss of flux in the elastic channel

Answer: YES!

FRAMEWORK FOR EXTRAPOLATIONS BASED ON EXPERIMENTAL DATA

"Mahaux analysis" ⇒ Dispersive Optical Model (DOM)

C. Mahaux and R. Sartor, Adv. Nucl. Phys. **20**, 1 (1991)

There is empirical information about the nucleon self-energy!!

⇒ Optical potential to analyze elastic nucleon scattering data

⇒ Extend analysis from A+1 to include structure information in A-1 ⇒ (e,e'p) data

⇒ Employ dispersion relation between real and imaginary part of self-energy

Recent extension

Combined analysis of protons in ^{40}Ca and ^{48}Ca

Charity, Sobotka, & WD nucl-ex/0605026, Phys. Rev. Lett. **97**, 162503 (2006)

Charity, Mueller, Sobotka, & WD, Phys. Rev. C (2007) submitted

Large energy window (> 200 MeV)

Goal: Extract asymmetry dependence ⇒ $\delta = (N - Z)/A$

⇒ **Predict** proton properties at large asymmetry ⇒ ^{60}Ca

⇒ **Predict** neutron properties … the dripline

based on data!

General dispersion relation

$$\mathrm{Re}\,\Sigma(\gamma,\delta;E)=\Sigma^{"HF"}(\gamma,\delta)-\frac{1}{\pi}P\int_{E_T^+}^{\infty}dE'\frac{\mathrm{Im}\,\Sigma(\gamma,\delta;E')}{E-E'}+\frac{1}{\pi}P\int_{-\infty}^{E_T^-}dE'\frac{\mathrm{Im}\,\Sigma(\gamma,\delta;E')}{E-E'}$$

At E_0 for example the Fermi energy

$$\mathrm{Re}\,\Sigma(\gamma,\delta;E_0)=\Sigma^{"HF"}(\gamma,\delta)-\frac{1}{\pi}P\int_{E_T^+}^{\infty}dE'\frac{\mathrm{Im}\,\Sigma(\gamma,\delta;E')}{E_0-E'}+\frac{1}{\pi}P\int_{-\infty}^{E_T^-}dE'\frac{\mathrm{Im}\,\Sigma(\gamma,\delta;E')}{E_0-E'}$$

Subtract

"HF" from Mahaux

$$\mathrm{Re}\,\Sigma(\gamma,\delta;E)=\mathrm{Re}\,\Sigma(\gamma,\delta;E_0)$$

$$-\frac{1}{\pi}(E_0-E)P\int_{E_T^+}^{\infty}dE'\frac{\mathrm{Im}\,\Sigma(\gamma,\delta;E')}{(E-E')(E_0-E')}+\frac{1}{\pi}(E_0-E)P\int_{-\infty}^{E_T^-}dE'\frac{\mathrm{Im}\,\Sigma(\gamma,\delta;E')}{(E-E')(E_0-E')}$$

Note here: $\mathrm{Im}\Sigma < 0$ for "2p1h" energies but >0 for "2h1p" energies

Diagonal approximation

Further simplification: assume no mixing between major shells

$$\Sigma^{(2)}(\alpha;E)=\frac{1}{2}\left\{\sum_{p_1p_2h_3}\frac{\left|\langle\alpha h_3|V|p_1p_2\rangle\right|^2}{E-\left(\varepsilon_{p_1}+\varepsilon_{p_2}-\varepsilon_{h_3}\right)+i\eta}+\sum_{h_1h_2p_3}\frac{\left|\langle\alpha p_3|V|h_1h_2\rangle\right|^2}{E-\left(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_3}\right)-i\eta}\right\}$$

Corresponding Dyson equation

$$G(\alpha;E)=G^{HF}(\alpha;E)+G(\alpha;E)\Sigma^{(2)}(\alpha;E)G^{HF}(\alpha;E)=\frac{1}{E-\varepsilon_\alpha-\Sigma^{(2)}(\alpha;E)}$$

Assume discrete poles in Σ, then discrete solution (poles of G) for

$$E_{n\alpha}=\varepsilon_\alpha+\Sigma^{(2)}(\alpha;E_{n\alpha})$$

With residue (spectroscopic factor) $$R_{n\alpha}=\frac{1}{1-\left.\frac{\partial\Sigma^{(2)}(\alpha;E)}{\partial E}\right|_{E_{n\alpha}}}$$

Employed equations

$$\Sigma(\boldsymbol{r}\mathrm{m},\boldsymbol{r}'\mathrm{m}';E) \Rightarrow \mathcal{U}(r,E) = -\mathcal{V}(r,E) + V_{so}(r) + V_C(r)$$
$$- iW_v(E)\, f(r,r_v,a_v) + 4ia_s W_s(E)\, f'(r,r_s,a_s)$$

$$f(r,r_i,a_i) = \left(1 + e^{\frac{r - r_i A^{1/3}}{a_i}}\right)^{-1}$$

Woods-Saxon form factor

$$\mathcal{V}(r,E) = V_{HF}(E)\, f(r,r_{HF},a_{HF}) + \Delta\mathcal{V}(r,E)$$

"*HF*" includes main effect of nonlocality $\Rightarrow$ *k*-mass

$$\Delta\mathcal{V}(r,E) = \Delta V_v(E)\, f(r,r_v,a_v) - 4a_s\, \Delta V_s(E)\, f'(r,r_s,a_s)$$

"Time" nonlocality $\Rightarrow$ *E*-mass

$$\Delta V_i(E) = \frac{P}{\pi}\int_{-\infty}^{\infty} W_i(E')\left(\frac{1}{E'-E} - \frac{1}{E'-E_F}\right) dE'$$

Subtracted dispersion relation
equivalent to earlier slide

Features of simultaneous fit to ^{40}Ca and ^{48}Ca data

- Surface contribution assumed symmetric around E_F
  - Represents coupling to low-lying collective states (GR)
- Volume term asymmetric w.r.t. E_F taken from nuclear matter
- Geometric parameters r_i and a_i fit but the same for both nuclei
- Decay (in energy) of surface term identical also
- Possible to keep volume term the same (consistent with exp) and independent of asymmetry
- *HF* and surface parameters different and can be extrapolated to larger asymmetry
- Surface potential stronger and narrower around E_F for ^{48}Ca

Locality and other approximations

Mahaux $$V_{HF}(\vec{r}m,\vec{r}'m') = \mathrm{Re}\,\Sigma(\vec{r}m,\vec{r}'m';E_F) \Rightarrow V_{HF}(r;E) = U_{HF}(E)f(X_{HF})$$

with

$$f(X_{HF}) = \left[1+\exp(X_{HF})\right]^{-1}$$

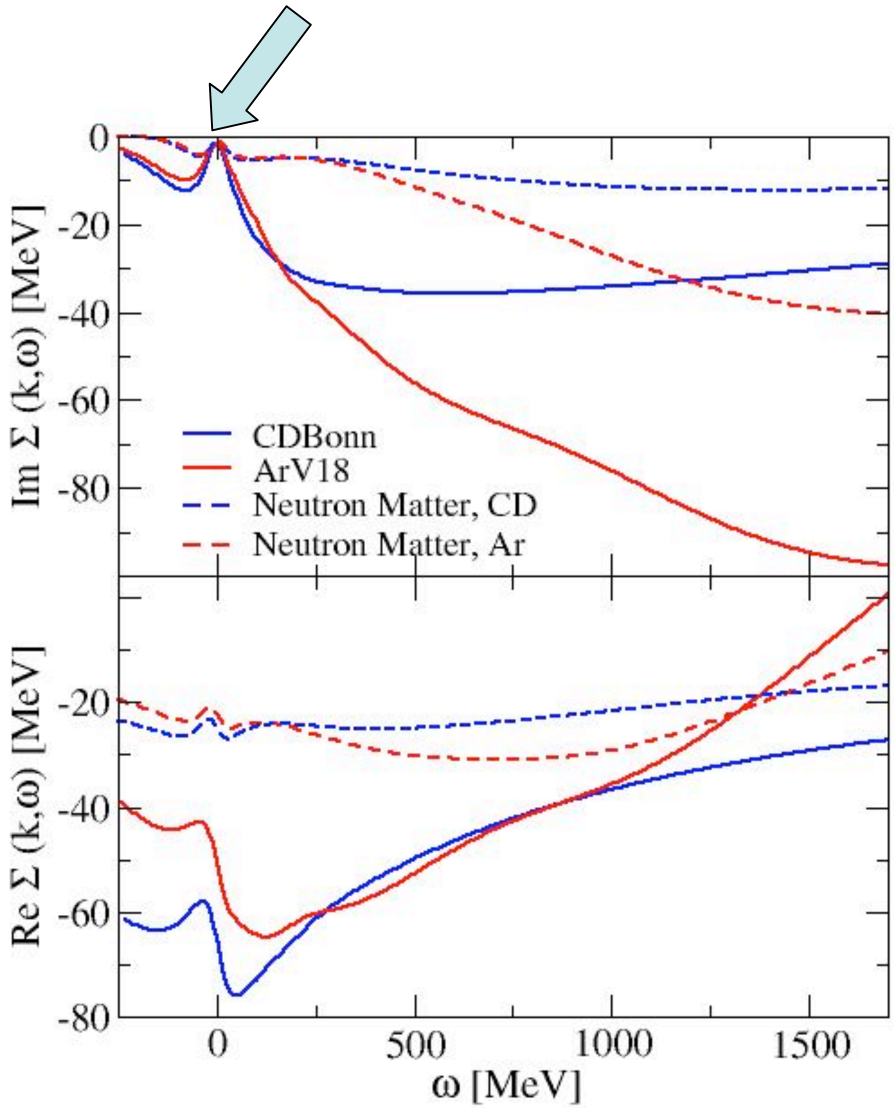
$$X_{HF} = \frac{r-R_{HF}}{a_{HF}}$$

$$R_{HF} = r_{HF}A^{1/3}$$

$$U_{HF}(E) = U_{HF}(E_F) + \left[1-\frac{m^*_{HF}}{m}\right](E-E_F)$$

Dispersive part: - assumed large E contribution and m^*_{HF} correlated
$\Rightarrow$ can use nuclear matter model
and introduces asymmetry in Im part
- nonlocality of Im Σ smooth
$\Rightarrow$ replace by local form identified with the imaginary part of the optical-model potential with volume and surface contributions

Infinite matter self-energy



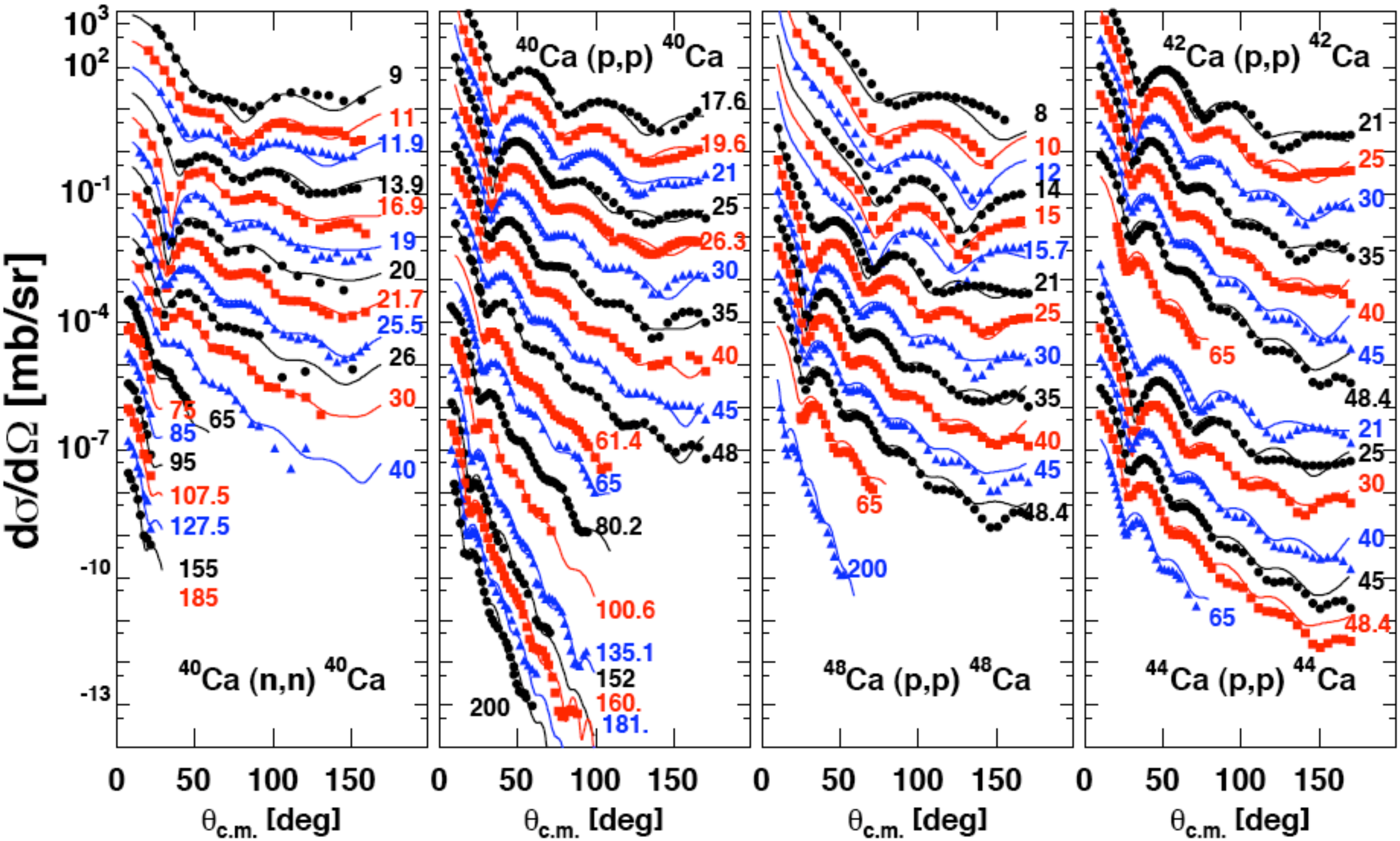
Real and imaginary part of the (retarded) self-energy

- k_F = 1.35 fm^{-1}
- T = 5 MeV
- k = 1.14 fm^{-1}

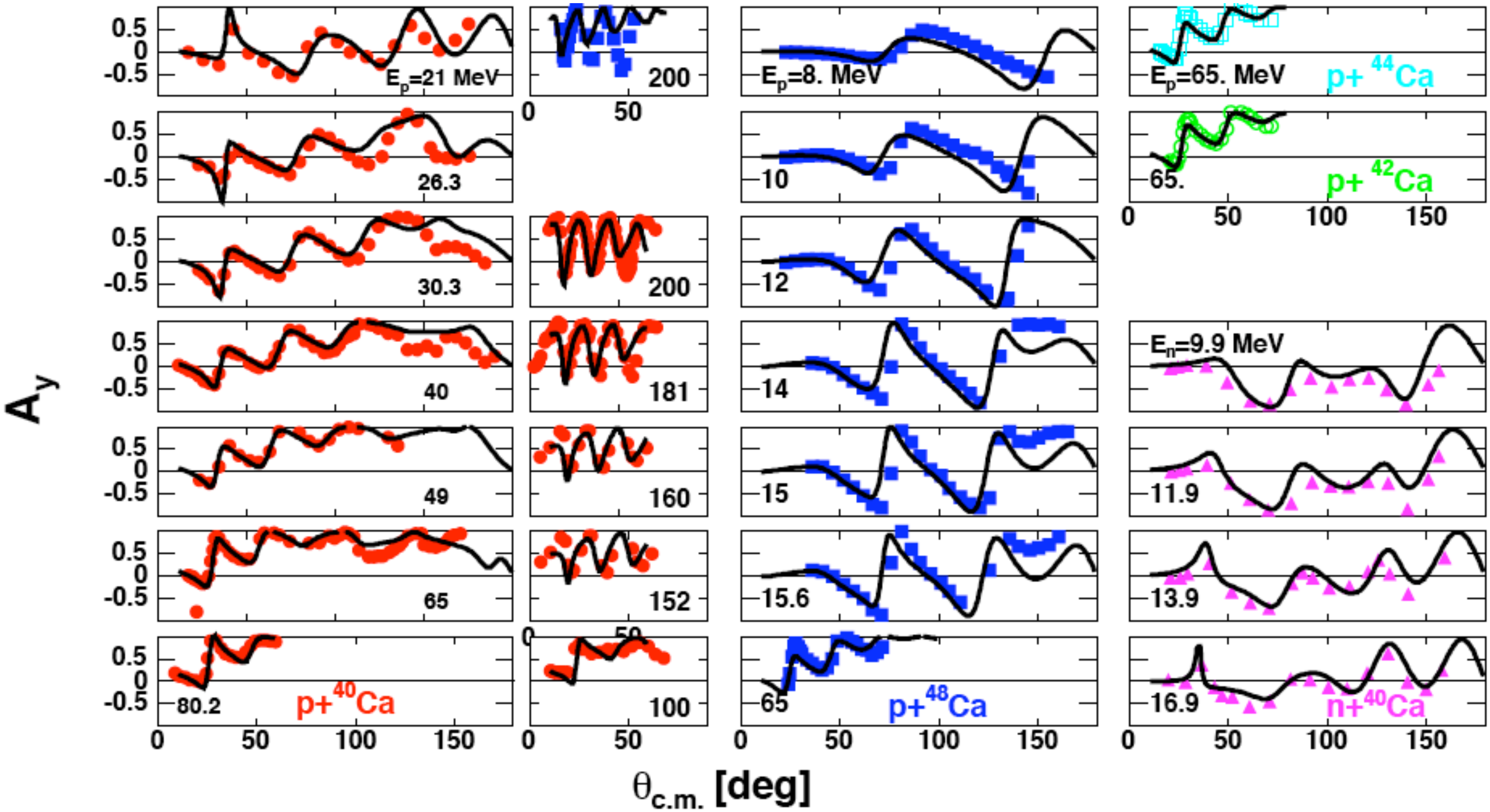
Note differences due to *NN* interaction

Asymmetry w.r.t. the Fermi energy related to phase space for *p* and *h*

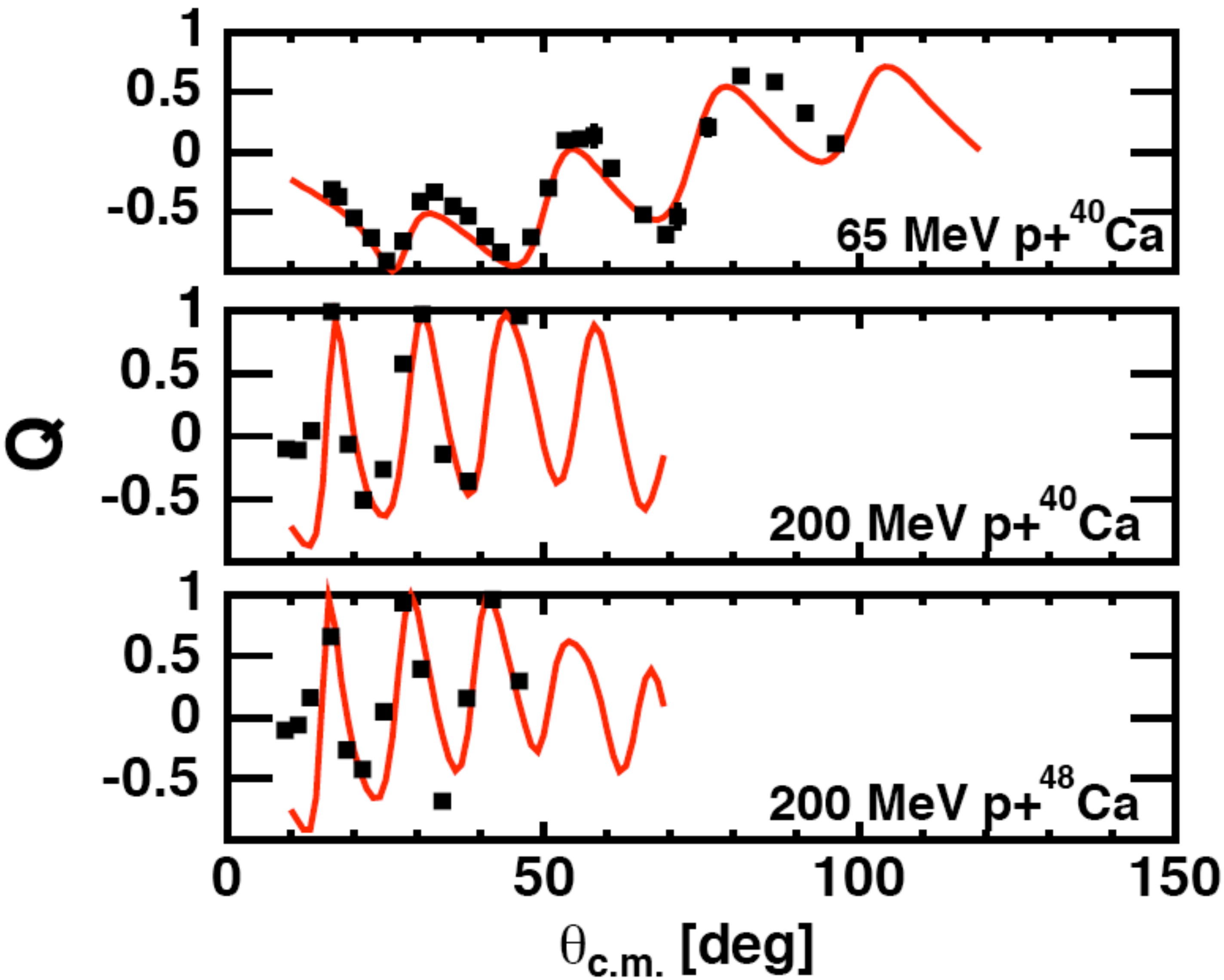
Fit and predictions of n & p elastic scattering cross sections



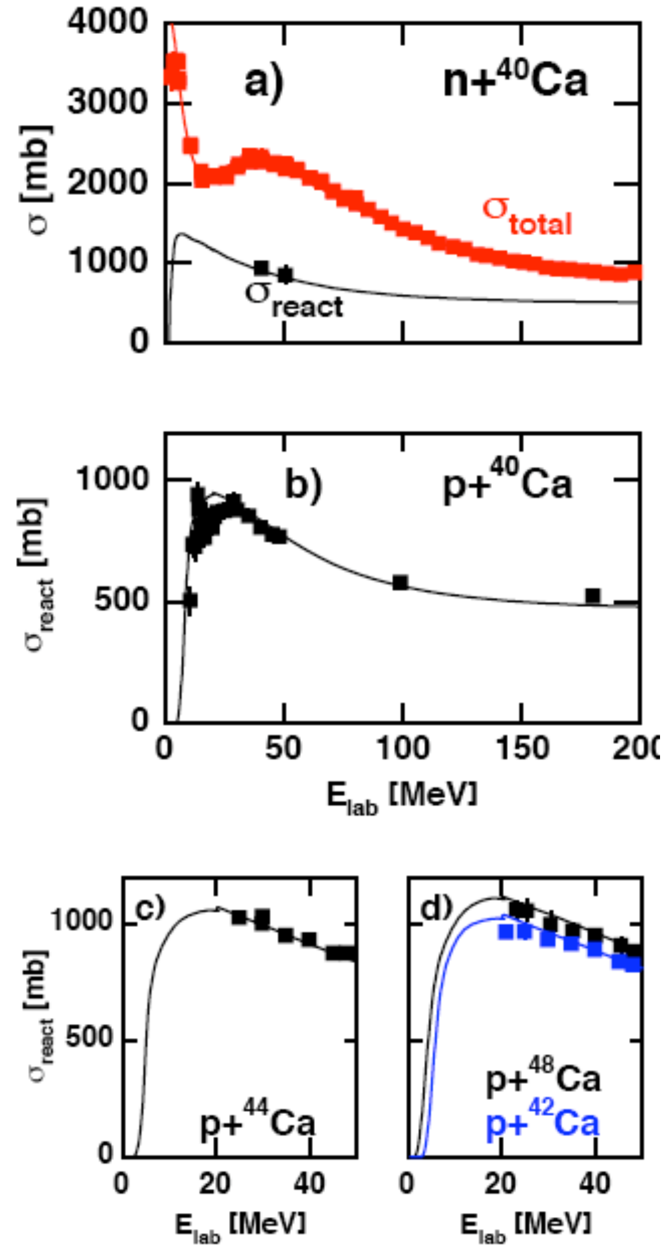
Present fit and predictions of polarization data



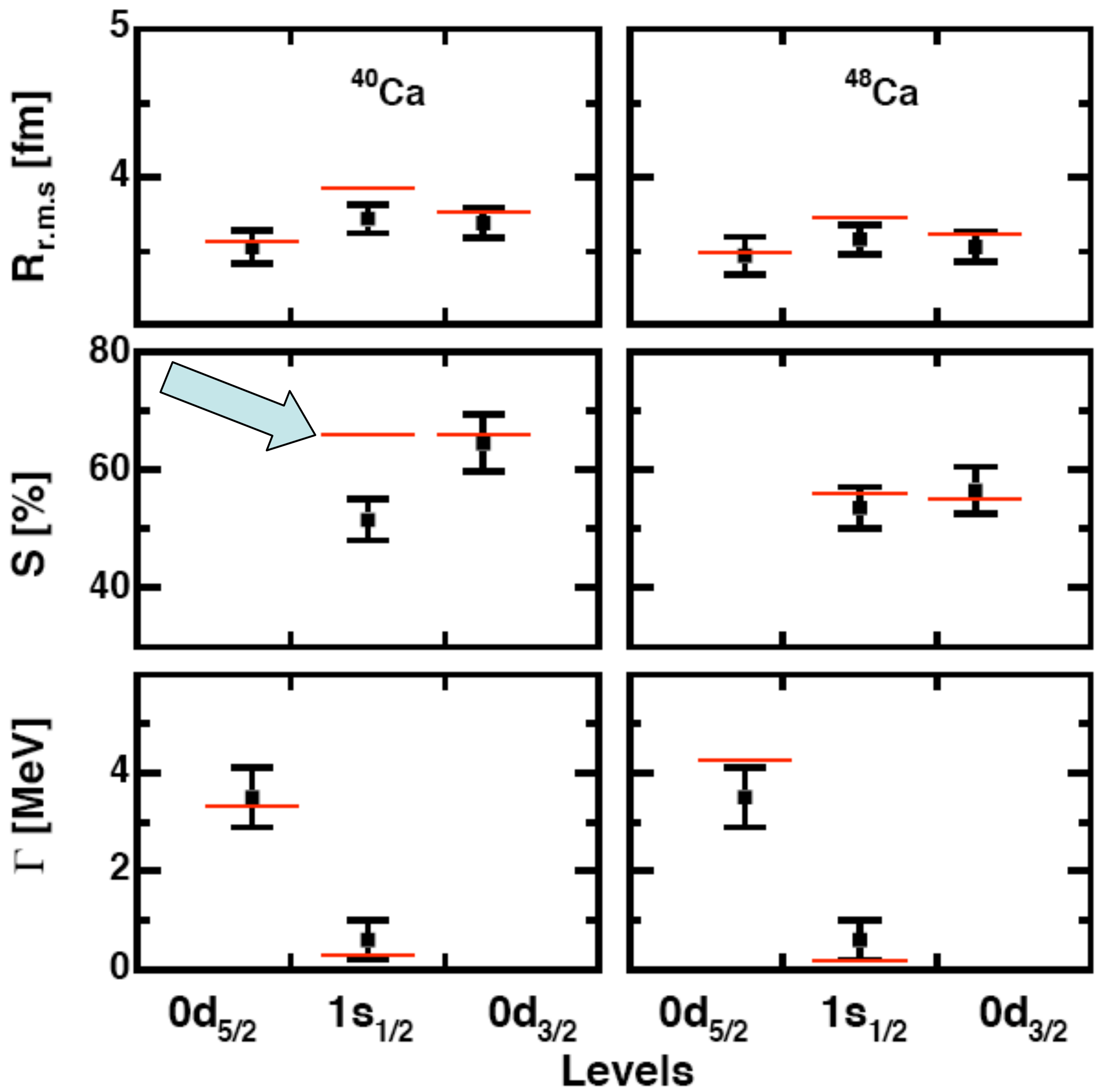
Spin rotation parameter (not fitted)



Fit and predictions
Of reaction cross sections



Present fit to (e,e′p) data



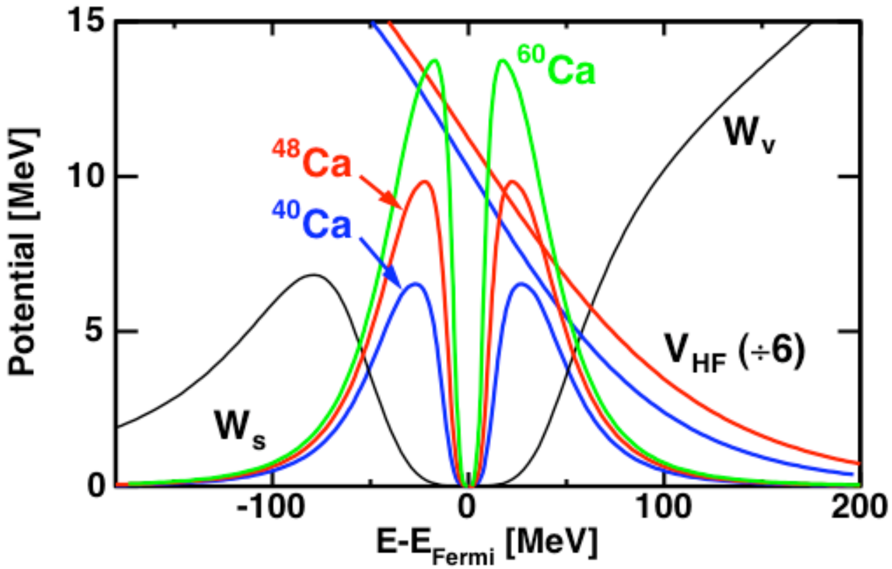
radii of bound state wave functions

spectroscopic factors

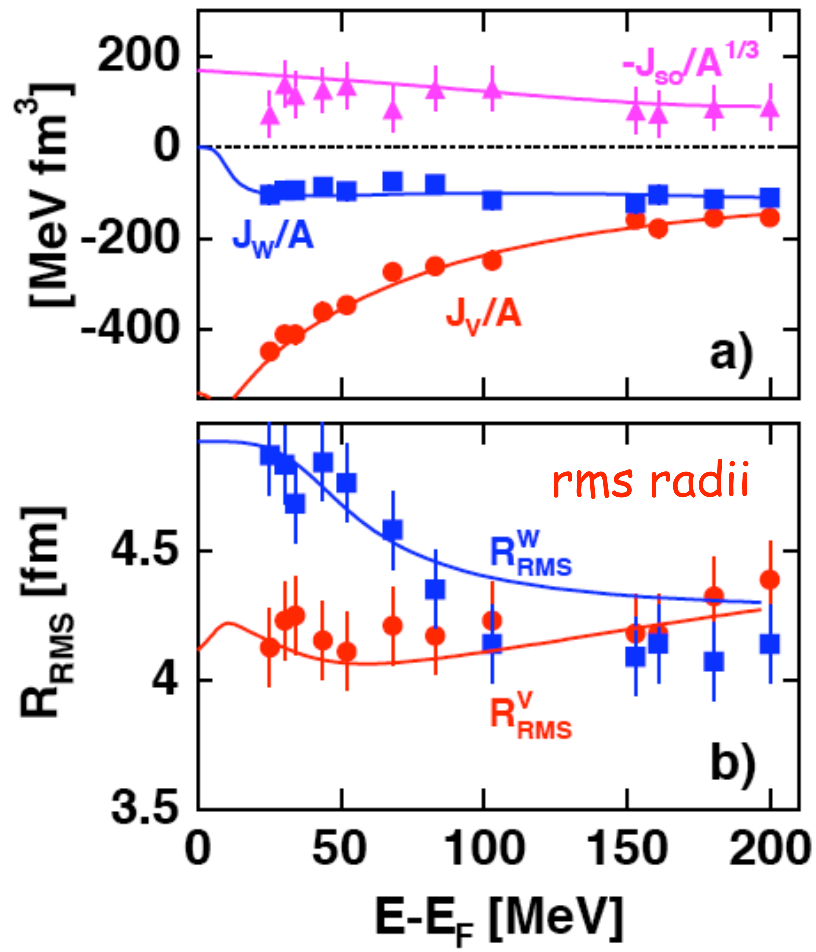
widths of strength distribution

Potentials

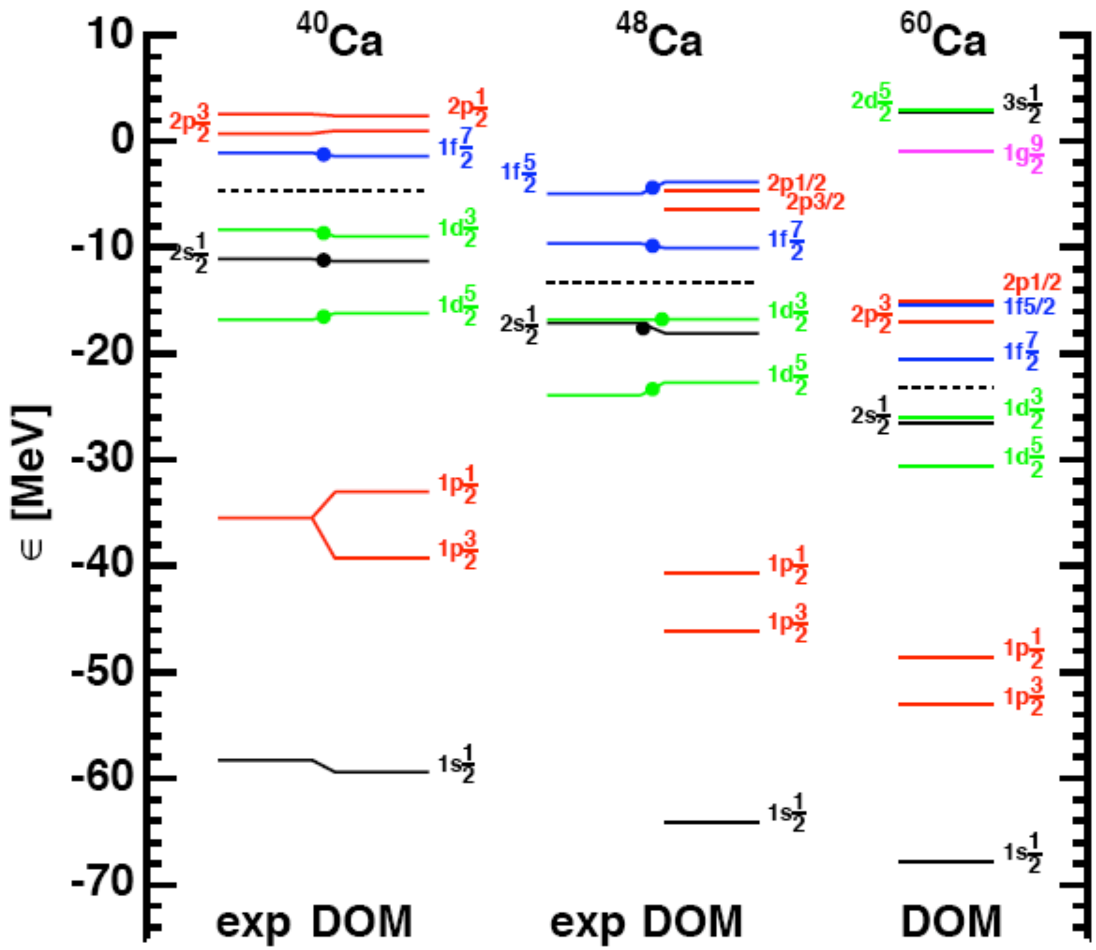
Surface potential strengthens
with increasing asymmetry
for protons



Volume integrals



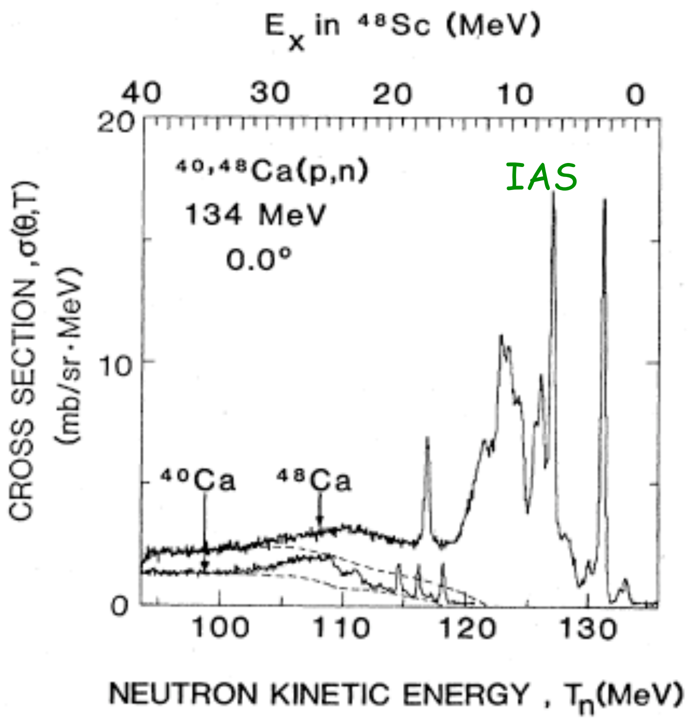
Proton single-particle structure and asymmetry



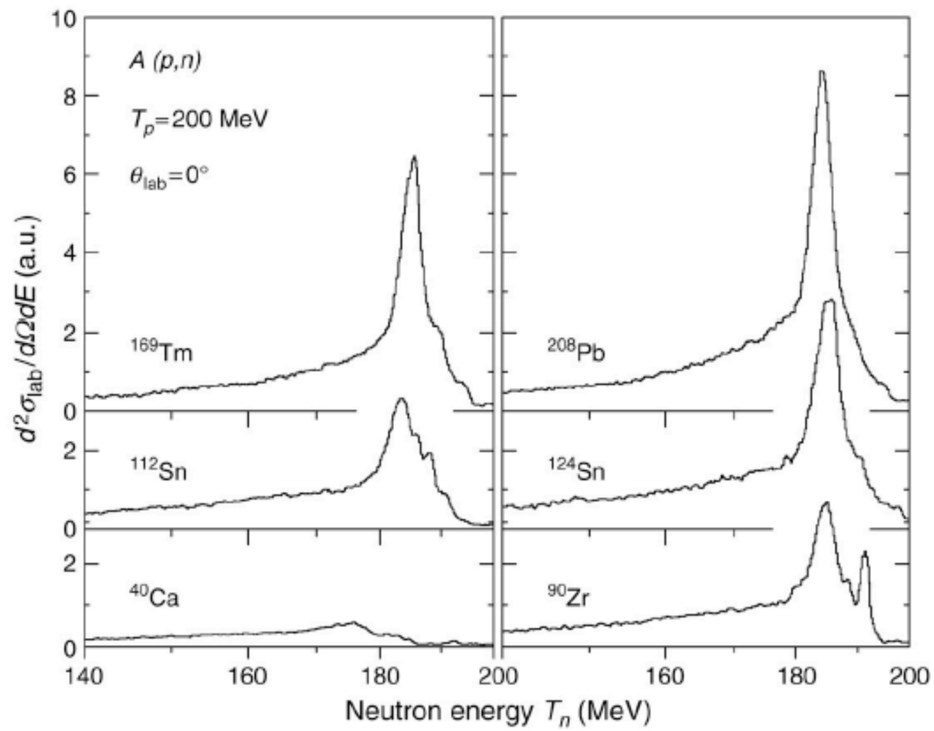
Pairing of protons due to *pn* correlations?!

Increased correlations with increasing asymmetry!

What's the physics? GT resonance?



PRC31,1161(1985)

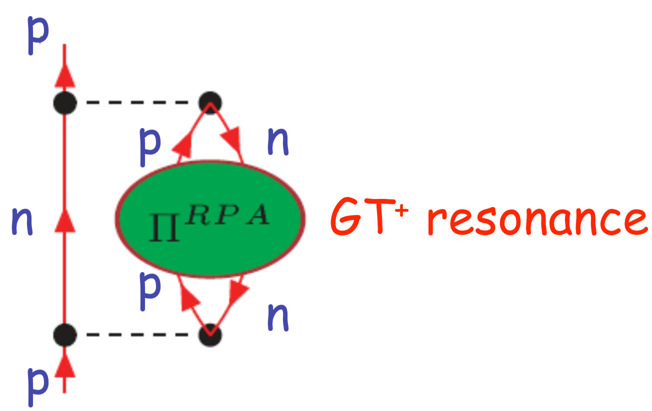


NPA369,258(1981)

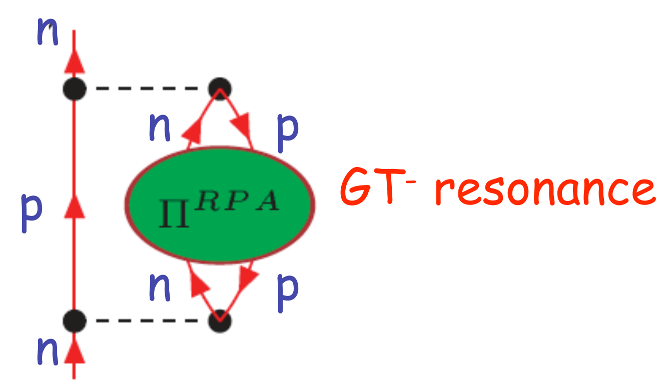
Influence of Gamow-Teller Giant Resonance or $\sigma_1.\sigma_2\ \tau_1.\tau_2$ (& tensor force) ph interaction

Sum rule for strength: $S(\beta^{+}) - S(\beta^{-}) = 3(N-Z)$

For N>Z only p affected



For Z>N only n affected



Related issue:
Change in magic numbers with increasing asymmetry
e.g. Otsuka et al., Phys. Rev. Lett. 95, 232502 (2005)

Extrapolation in δ

Naïve: $p/n \Rightarrow D_1 \Rightarrow \pm (N-Z)/A$

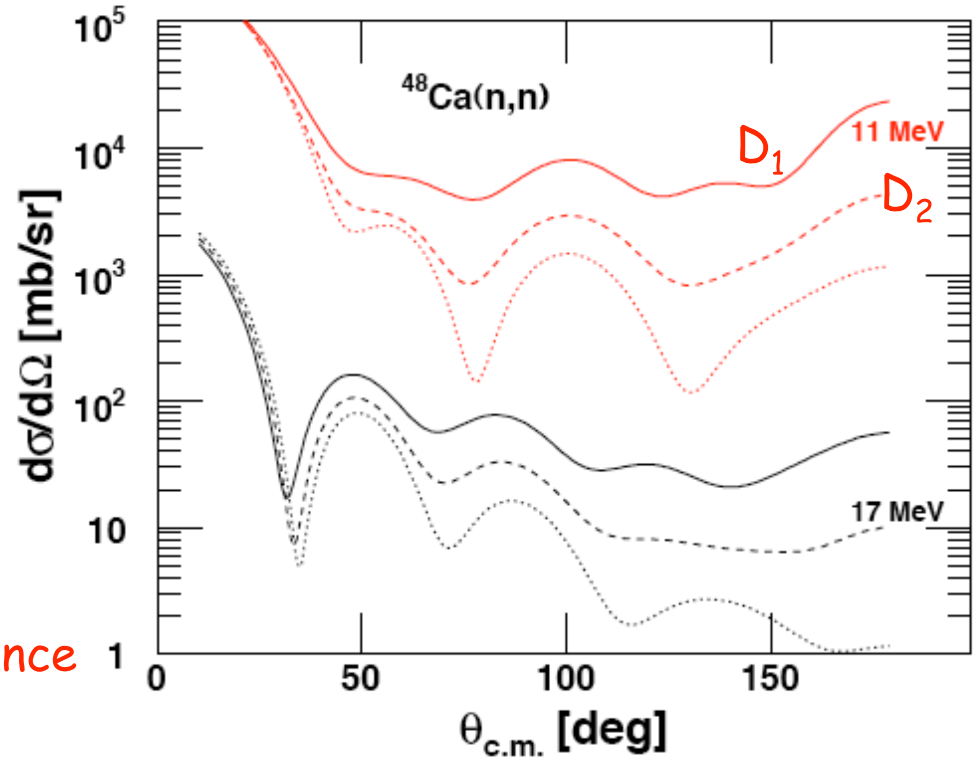
Cannot be extrapolated for n

Less naïve:

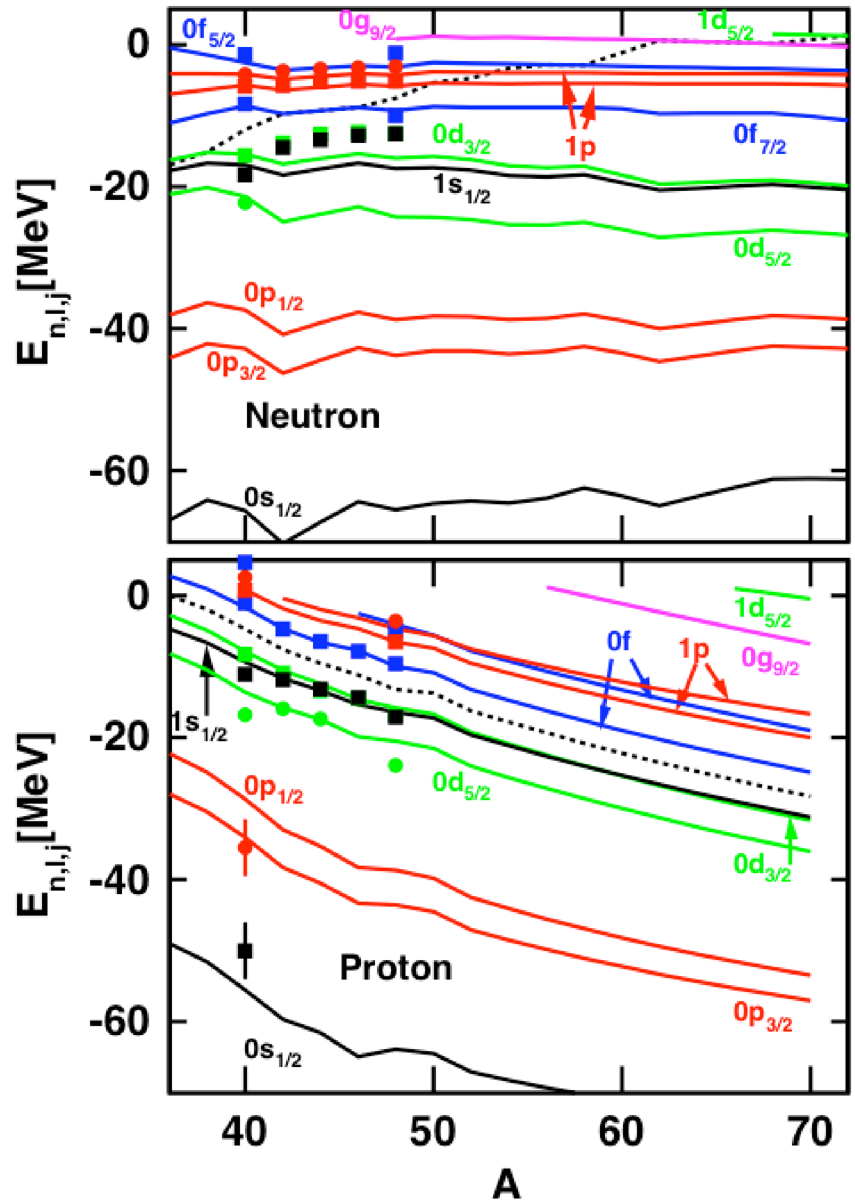
$D_2 \Rightarrow p \Rightarrow +(N-Z)/A$
$D_2 \Rightarrow n \Rightarrow 0$

Emphasizes coupling to GT resonance
Consistent with n+^{A}Mo data

Need n+^{48}Ca elastic scattering data!!!

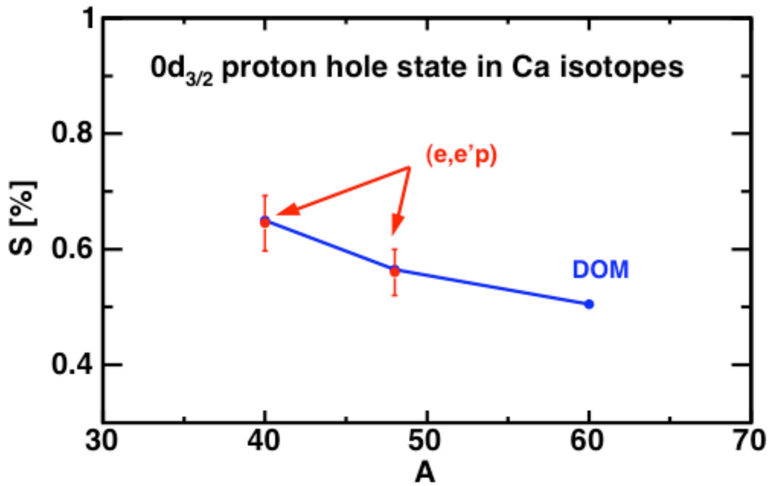


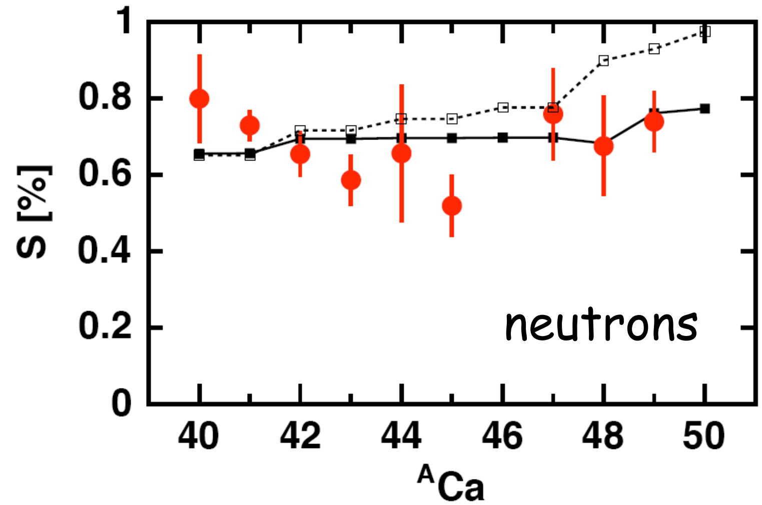
Extrapolation for large N of sp levels

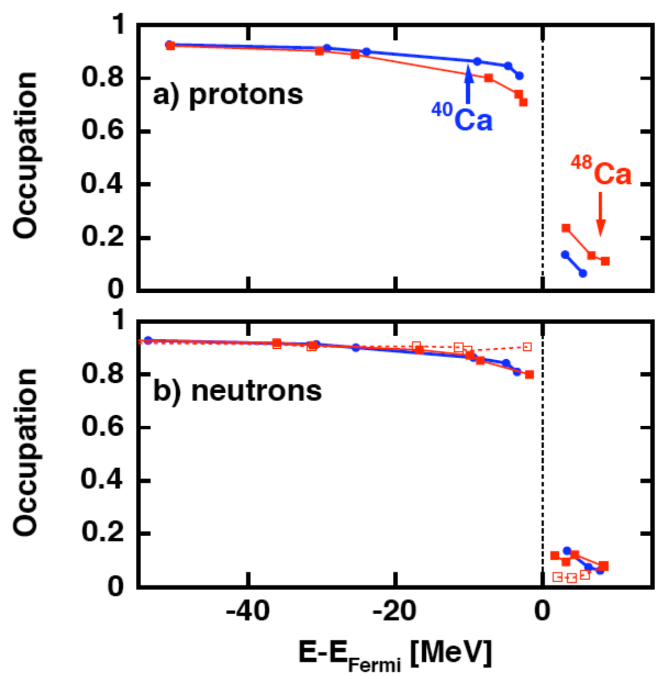


Old ^{48}Ca(p,pn) data
J.W.Watson et al.
Phys. Rev. C26,961 (1982)
~ consistent with DOM

Spectroscopic factors as a function of δ





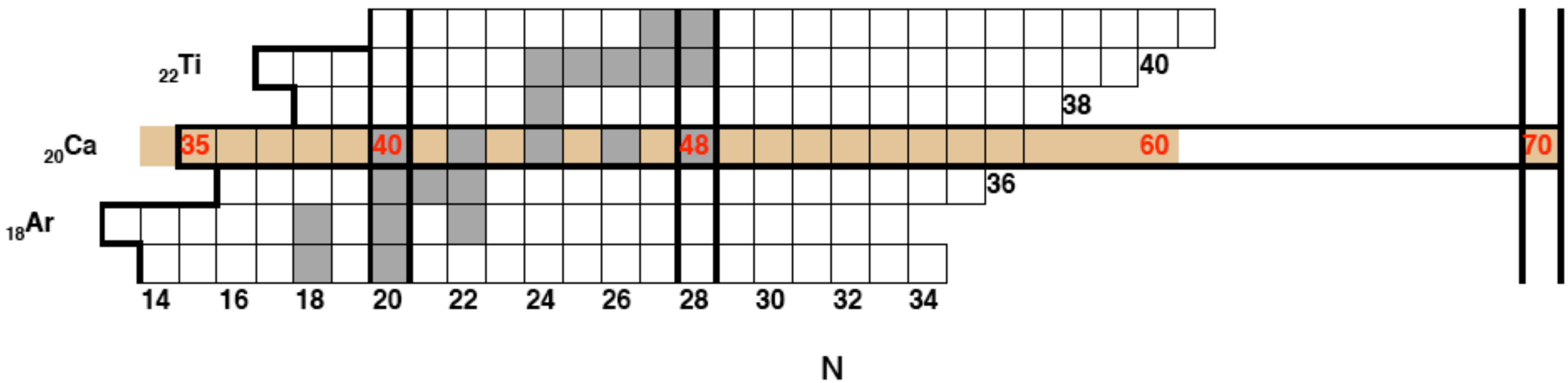


Occupation numbers

Protons more correlated with δ

Neutrons not much change

Driplines



Proton dripline wrong by 1

Neutron dripline more complicated:

^{60}Ca and ^{70}Ca particle bound
Intermediate isotopes unbound
Reef?

Outlook

- Explore the Gamow-Teller connection
    - link with excited states
- More experimental information from elastic nucleon scattering is important!
    - lots of informative experiments to be done with radioactive beams
- Neutron experiments on ^{48}Ca and ^{48}Ca(p,d) in the ^{47}Ca continuum
- Data-driven extrapolations to the neutron dripline

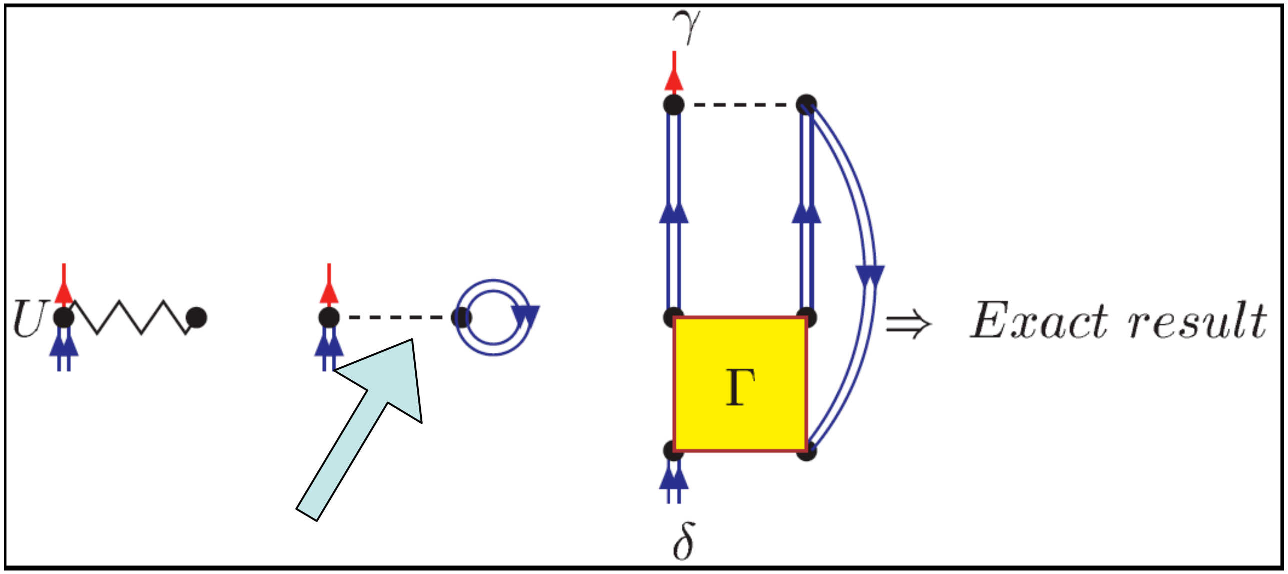
- More DOM analysis
- Exact solution of the Dyson equation with nonlocal potentials (in progress)
- Employ information of nucleon self-energy to generate functionals for

QP-DFT = Quasi-Particle Density Functional Theory (Van Neck et al. $\Rightarrow$ PRA)

DFT that includes a correct description of QP properties!!

Inclusion of V_{NN} (or parts of it)

Self-energy



Requires one-body density matrix
Already "determined" from experiment
Can take explicit realistic tensor force V_T
Refit to data
Useful for asymmetry dependence!

See also
Otsuka, Matsuo, and Abe,
PRL97, 162501 (2006)

Improvements in progress

Replace treatment of nonlocality in terms of local equivalent but energy-dependent potential by explicitly nonlocal potential

$\Rightarrow$ Necessary for exact solution of Dyson equation

- Yields complete spectral density as a function of energy OK
- Yields one-body density OK
- Yields natural orbits OK
- Yields charge density OK
- Yields neutron density OK
- Data for charge density can be included in fit
- Data for (e,e'p) cross sections near E_F can be included in fit
- High-momentum components can be included (Jlab data)
- E/A can be calculated/ used as constraint $\Rightarrow$ TNI
- NN Tensor force can be included explicitly
- Generate functionals for QP-DFT

Exact solution of Dyson equation

Coordinate space technique employed for atoms can be employed to solve Dyson equation including any true nonlocality (Van Neck)

Yields

$$S_h(\alpha,\beta;E)=\sum_n \left\langle \Psi_0^N \left| a_\beta^\dagger \right| \Psi_n^{N-1} \right\rangle \left\langle \Psi_n^{N-1} \left| a_\alpha \right| \Psi_0^N \right\rangle \delta\left(E-\left(E_0^N - E_n^{N-1}\right)\right)$$

spectral density (spectral function for $\alpha = \beta$) and therefore

$$n(\beta,\alpha)=\int_{-\infty}^{\varepsilon_F^-} dE\, S_h(\alpha,\beta;E)=\sum_n \left\langle \Psi_0^N \left| a_\beta^\dagger \right| \Psi_n^{N-1} \right\rangle \left\langle \Psi_n^{N-1} \left| a_\alpha \right| \Psi_0^N \right\rangle = \left\langle \Psi_0^N \left| a_\beta^\dagger a_\alpha \right| \Psi_0^N \right\rangle$$

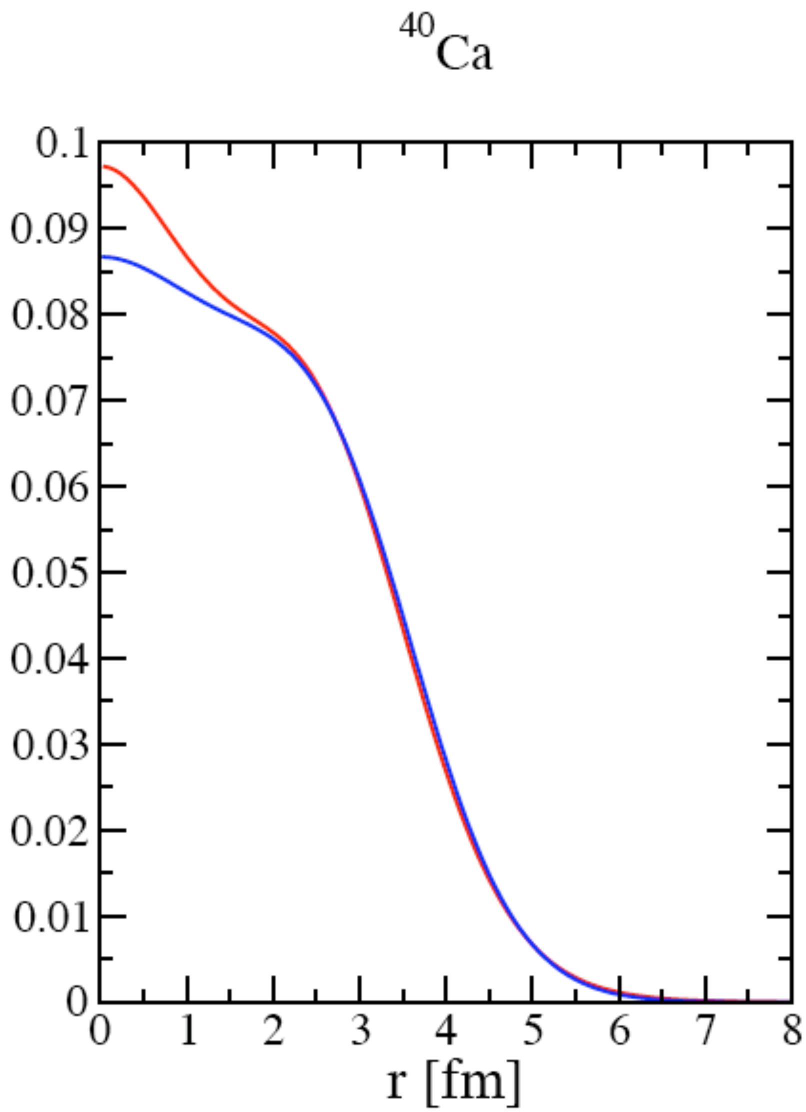
the one-body density matrix including occupation numbers ($\alpha = \beta$), charge density, *etc.* and last but not least

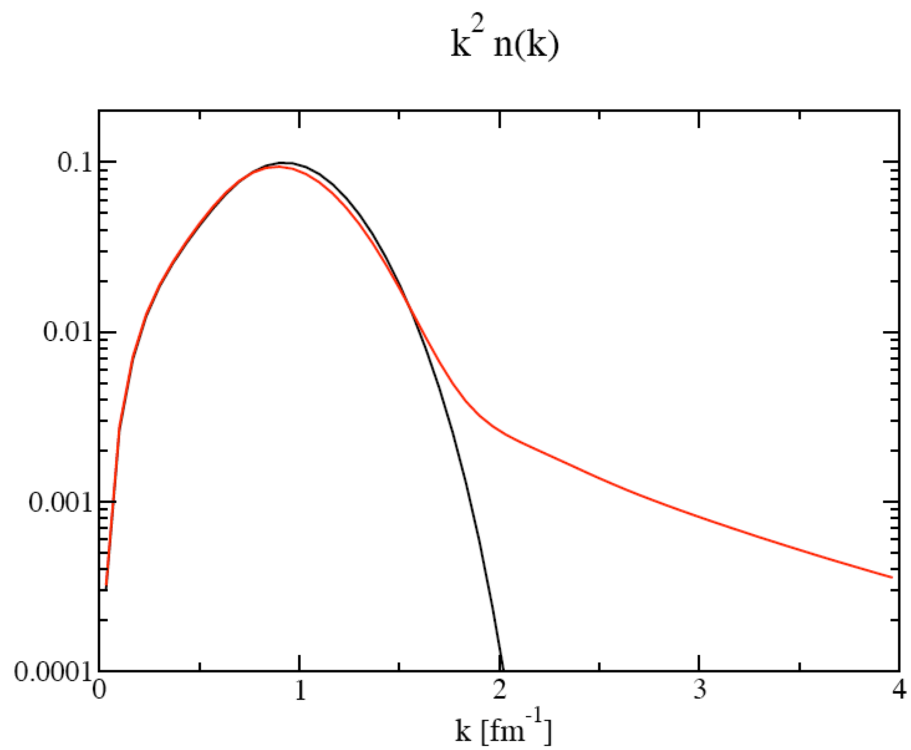
$$E_0^N = \frac{1}{2}\left(\sum_{\alpha,\beta}\langle\alpha|T|\beta\rangle n(\alpha,\beta)+\sum_\alpha \int_{-\infty}^{\varepsilon_F^-} dE\, E\, S_h(\alpha;E)\right)$$

$$=\frac{1}{2}\left(\sum_{\ell j}\int_0^\infty dk\, k^2(2j+1)\frac{\hbar^2 k^2}{2m} n_{\ell j}(k)+\sum_{\ell j}(2j+1)\int_0^\infty dk\, k^2 \int_{-\infty}^{\varepsilon_F^-} dE\, E\, S_{\ell j}(k;E)\right)$$

the ground state energy $\Rightarrow$ useful constraints (includes also Z & N)

Charge density & High-momentum components





Only 2% high-momentum strength
⇒ Modify self-energy to include more
high-momentum strength
Consistent with theoretical experience
and Jlab data!

Summary

- Proton sp properties in stable closed-shell nuclei understood (mostly)

Study of N≠ Z nuclei based on DOM framework and experimental data

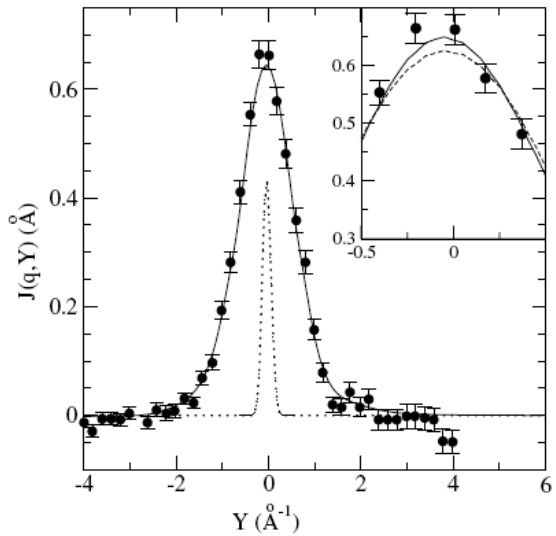
- Description of huge amounts of data
- Sensible extrapolations to systems with large asymmetry
- More data necessary to improve/pin down extrapolation
- More theory

Predictions

- N≠ Z p more correlated while n similar (for N>Z) and vice versa
- Proton closed-shells with N>>Z ⇒ may favor pp pairing
- Neutron dripline may be more complicated (reef)

Deep-inelastic neutron scattering off quantum liquids

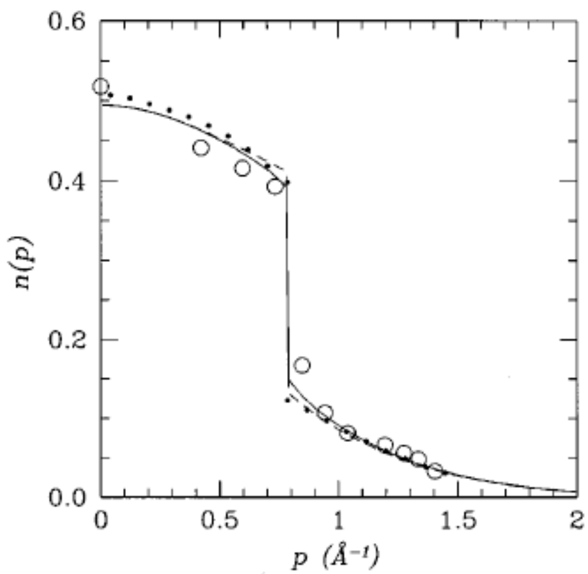
Liquid ^{3}He



Response at 19.4 Å^{-1}
Probe: neutrons
R.T. Azuah et al., J. Low Temp. Phys. **101**, 951 (1995)

Theory: Monte Carlo n(k) & FSE (ρ_2) beyond IA
F. Mazzanti et al., Phys. Rev. Lett. **92**, 085301 (2004)

$$J(Y) = \frac{1}{2\pi^2 \rho} \int_{|Y|}^{\infty} dk\, k\, n(k)$$ IA result



$$Y = \frac{m\omega}{q} - \frac{q}{2}$$ scaling variable

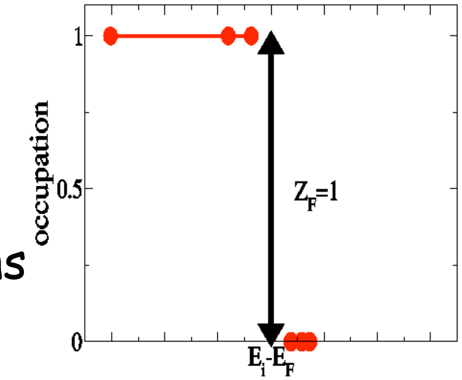
Momentum distribution liquid ^{3}He

S. Moroni et al., Phys. Rev. B**55**, 1040 (1997)
Comparison of DMC, GFMC, and VMC & HNC

Correlations in ...

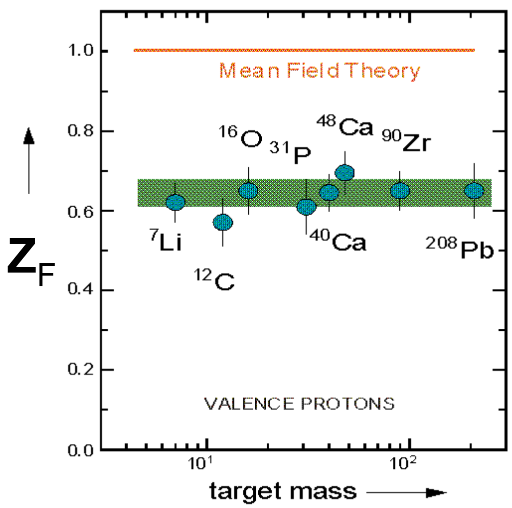
Atoms

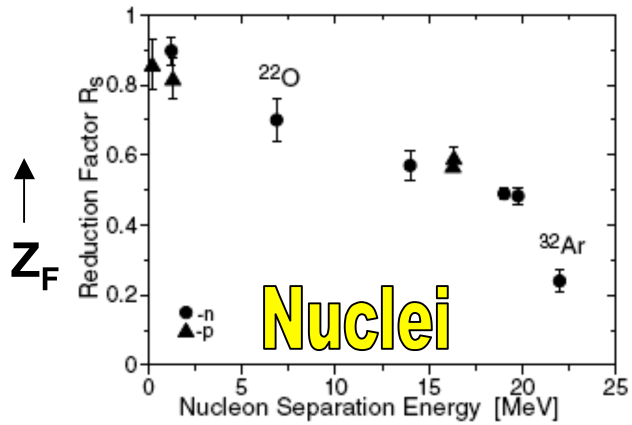
weak correlations



electrons in Ne
Data from (e,2e)

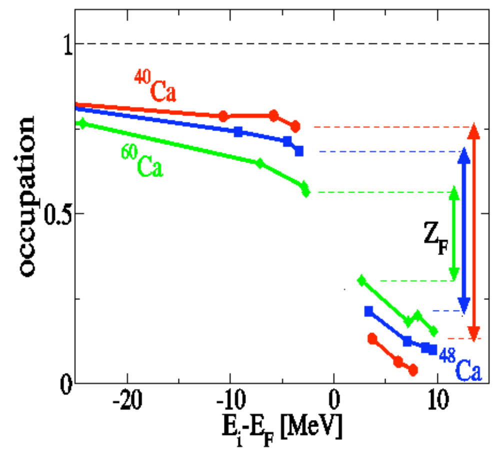
(e,e'p)





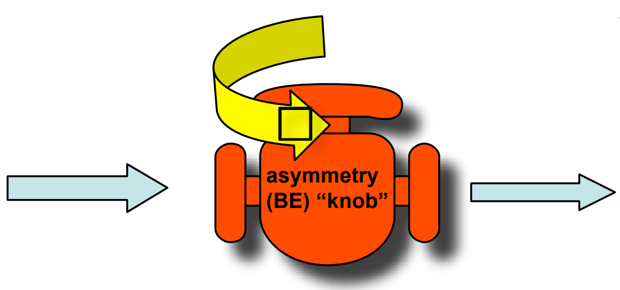
Neutron-proton asymmetry

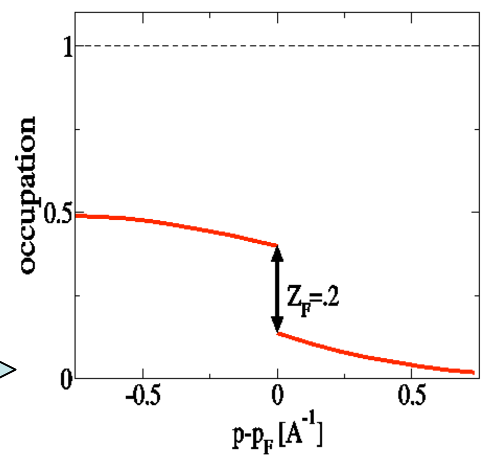
DOM



protons in stable
closed-shell nuclei

protons in Ca





Liquid 3He

very strong correlations
Data from (n,n')

New framework to do self-consistent sp theory

Quasiparticle density functional theory ⇒ QP-DFT

D. Van Neck et al., Phys. Rev. A**74**, 042501 (2006)

Ground-state energy and one-body density matrix from self-consistent sp equations that extend the Kohn-Sham scheme.

Based on separating the propagator into a quasiparticle part and a background, expressing only the latter as a functional of the density matrix.
⇒ in addition yields qp energies and overlap functions

Reminder: DFT does not yield removal energies of atoms

Relative deviation [%]

		DFT	HF
He atom	1s	37.4	1.5
Ne atom	2p	38.7	6.8
Ar atom	3p	36.1	2.0

While ground-state energies are closer to exp in DFT than in HF

Can be developed for nuclei from DOM input!

Isospin analysis