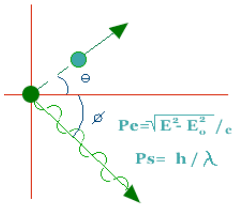
The dispersive optical model as an interface between ab initio calculations and experiment

FRIB
6/20/2018

Washington University in St. Louis



Wim Dickhoff
Bob Charity
Lee Sobotka
Hossein Mahzoon (Ph.D.2015)
Mack Atkinson
Natalya Calleya
Michael Keim
Blake Bordelon

- Motivation
- Green's functions/propagator method
  - vehicle for ab initio calculations —> matter
  - as a framework to link data at positive and negative energy (and to generate predictions for exotic nuclei)

-> dispersive optical model (DOM <- Claude Mahaux)

- Recent DOM extension to non-local potentials
- Revisit (e,e'p) data from NIKHEF & outlook (p,pN)
- Neutron skin in ^{48}Ca (importance of total xsections)
- Preliminary ^{208}Pb results
- Outlook for transfer reactions
- Conclusions

Recent DOM review:
WD, Bob Charity, Hossein Mahzoon
J. Phys. G: Nucl. Part. Phys. 44 (2017) 033001

Motivation

- Rare isotope physics requires a **much** stronger link between nuclear reactions and nuclear structure descriptions

- We need an ab initio approach for optical potentials —> optical potentials must therefore become **nonlocal** and **dispersive**

- Current status to extract structure information from nuclear reactions involving strongly interacting probes **unsatisfactory**

- Intermediate step: dispersive optical model as originally proposed by Claude Mahaux —> recent **extensions** discussed here

Problems with ab initio optical potentials

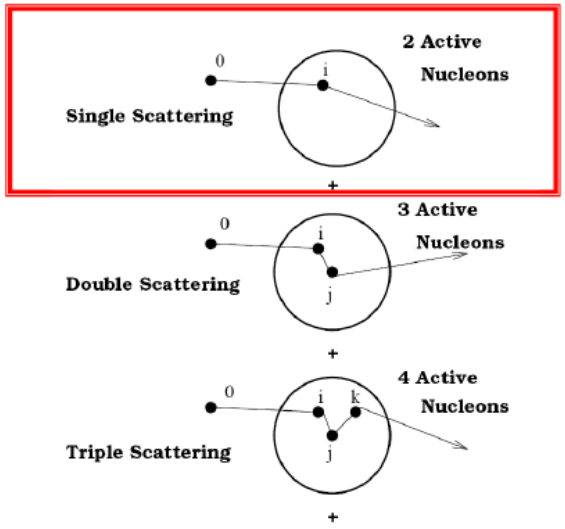
- angular momentum constraints (illustrated here)
- configuration space & density of low-lying states

PHYSICAL REVIEW C **95**, 024315 (2017)

Optical potential from first principles

J. Rotureau,[1,2] P. Danielewicz,[1,3] G. Hagen,[4,5] F. M. Nunes,[1,3] and T. Papenbrock[4,5]

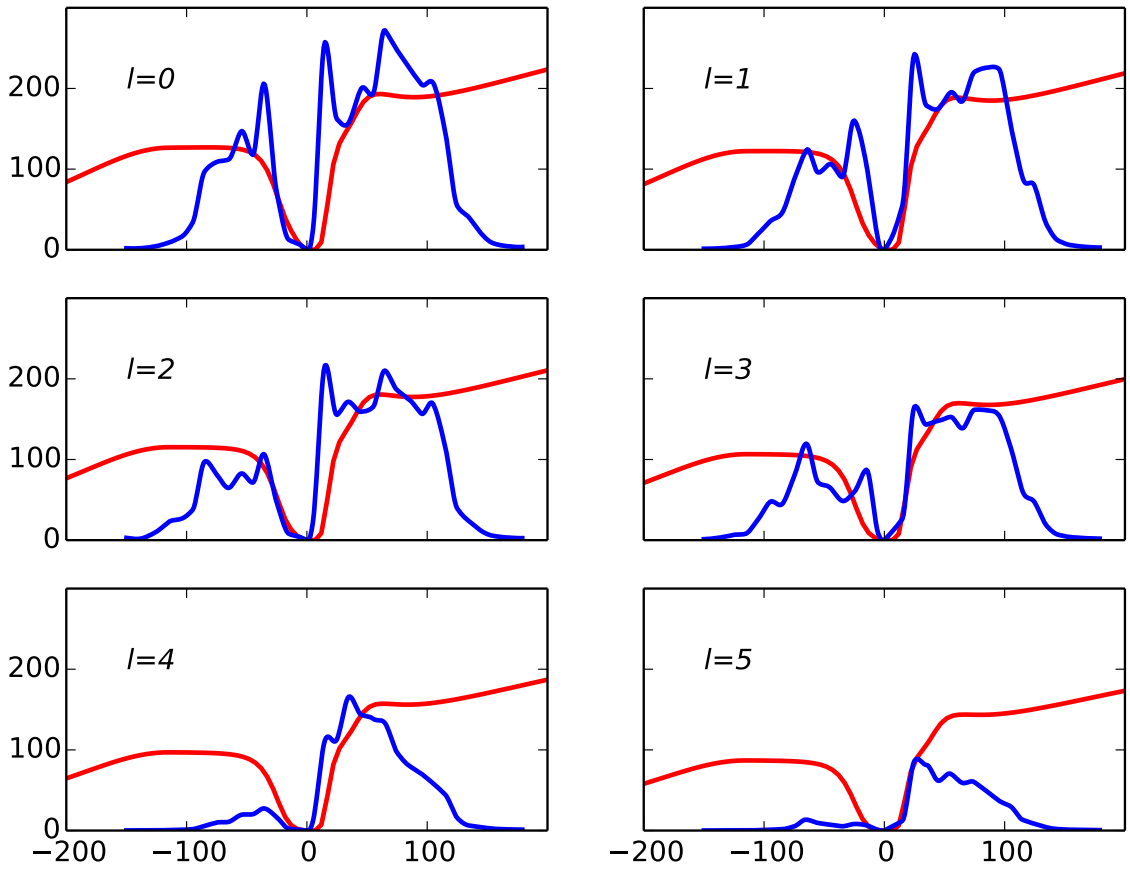
- multiple scattering T x rho cannot be systematically improved



- consistency requires simultaneous description of particle removal which determines the density

Comparison with ab initio FRPA calculation

- Volume integrals of imaginary part of nonlocal ab initio (FRPA) self-energy compared with DOM result for ^{40}Ca

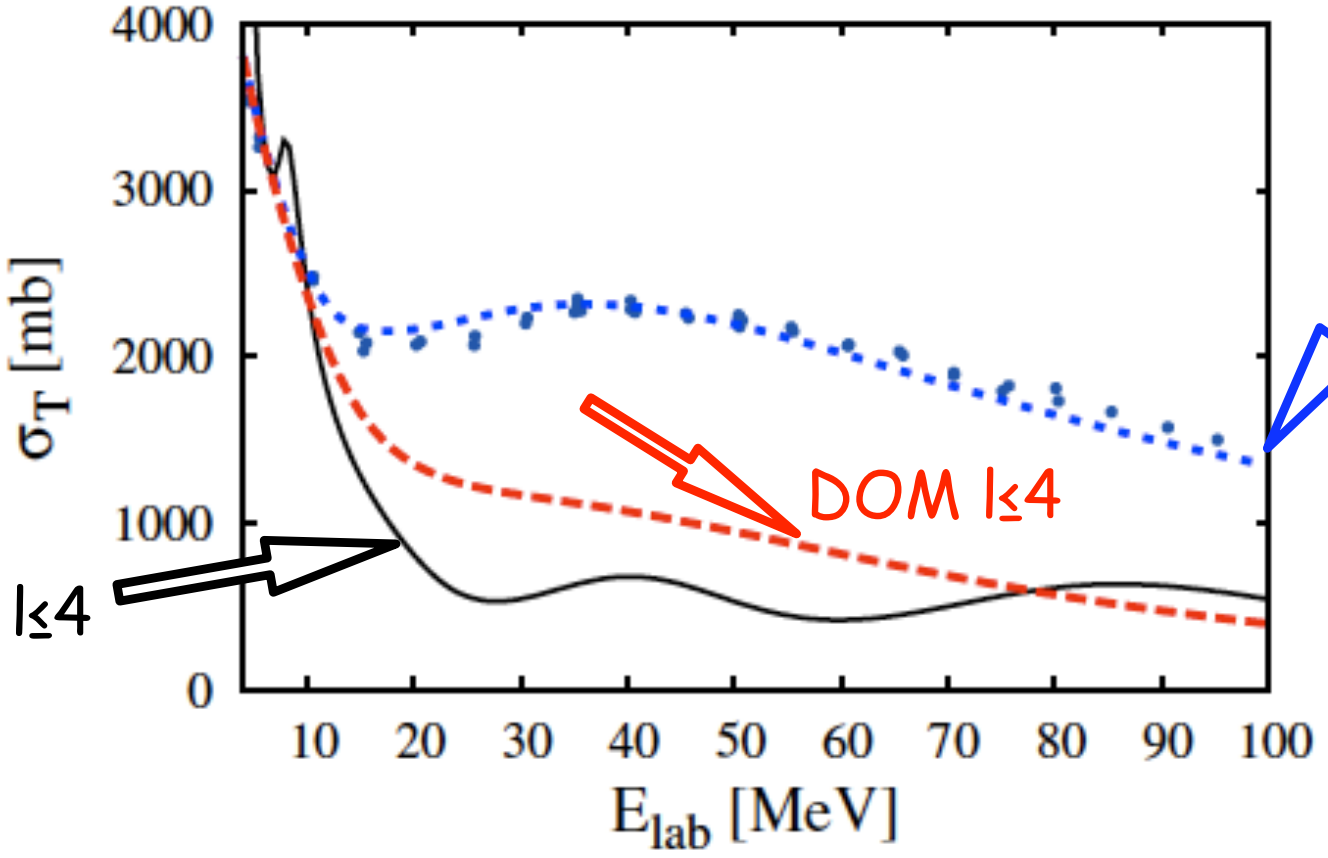


- Ab initio

S. J. Waldecker, C. Barbieri and W. H. Dickhoff
Microscopic self-energy calculations and dispersive-optical-model potentials.
Phys. Rev. C84, 034616 (2011), 1-11.

Ab initio calculation of elastic scattering n+^{40}Ca

- Dussan, Waldecker, Müther, Polls, WD PRC84, 044319 (2011)
- Also generates high-momentum nucleons below the Fermi energy
- ONLY treatment of short-range and tensor correlations



DOM & data

DOM l≤4

CDBonn l≤4

Propagator / Green's function

- Lehmann representation

$$G_{\ell j}(k,k';E) = \sum_m \frac{\langle \Psi_0^A |\, a_{k\ell j}\, | \Psi_m^{A+1}\rangle \langle \Psi_m^{A+1} |\, a^\dagger_{k'\ell j}\, | \Psi_0^A\rangle}{E - (E_m^{A+1} - E_0^A) + i\eta} + \sum_n \frac{\langle \Psi_0^A |\, a^\dagger_{k'\ell j}\, | \Psi_n^{A-1}\rangle \langle \Psi_n^{A-1} |\, a_{k\ell j}\, | \Psi_0^A\rangle}{E - (E_0^A - E_n^{A-1}) - i\eta}$$

- Any other single-particle basis can be used & continuum integrals implied
- Overlap functions --> numerator
- Corresponding eigenvalues --> denominator
- Spectral function

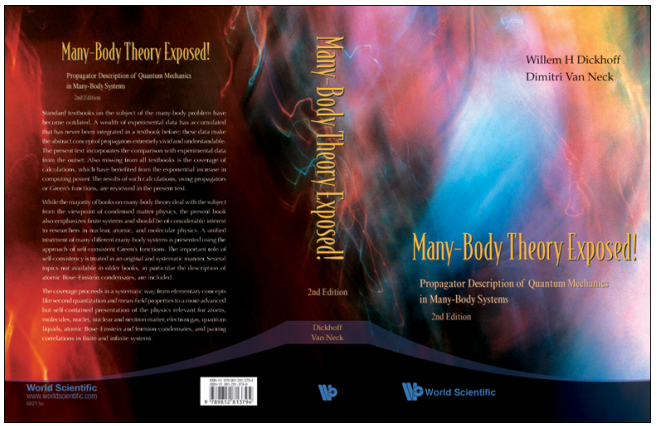
$$S_{\ell j}(k;E) = \frac{1}{\pi}\,\mathrm{Im}\; G_{\ell j}(k,k;E) \qquad E \le \varepsilon_F^-$$

$$= \sum_n \left| \langle \Psi_n^{A-1} |\, a_{k\ell j}\, | \Psi_0^A\rangle \right|^2 \delta(E - (E_0^A - E_n^{A-1}))$$

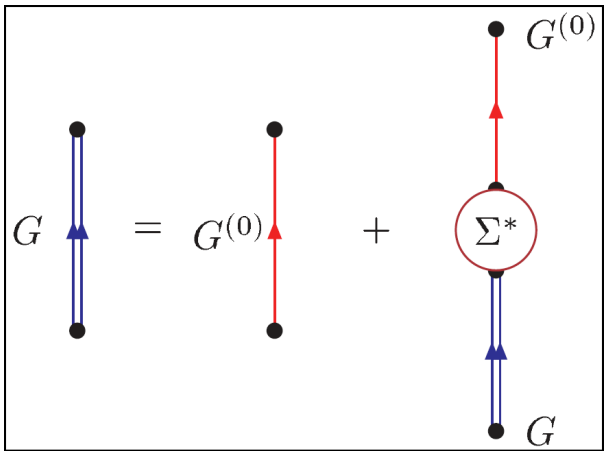
- Spectral strength in the continuum

$$S_{\ell j}(E) = \int_0^\infty dk\; k^2\; S_{\ell j}(k;E)$$

- Discrete transitions $\sqrt{S^n_{\ell j}}\;\phi^n_{\ell j}(k) = \langle \Psi_n^{A-1} |\, a_{k\ell j}\, | \Psi_0^A\rangle$
- Positive energy —> see later



Propagator from Dyson Equation and "experiment"



Equivalent to …

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

Self-energy: non-local, energy-dependent potential

With energy dependence: spectroscopic factors < 1

⇒ as extracted from (e,e'p) reaction

$$\frac{k^2}{2m}\phi_{\ell j}^n(k) + \int dq\ q^2\ \Sigma_{\ell j}^*(k,q;E_n^-)\ \phi_{\ell j}^n(q) = E_n^-\ \phi_{\ell j}^n(k)$$

Spectroscopic factor $\quad S_{\ell j}^n = \int dk\ k^2\ \left|\langle \Psi_n^{A-1}|\, a_{k\ell j}\, |\Psi_0^A\rangle\right|^2 < 1$

Dyson equation also yields $\left[\chi_{\ell j}^{elE}(r)\right]^* = \langle \Psi_{elE}^{A+1}|\, a_{r\ell j}^\dagger\, |\Psi_0^A\rangle$ for positive energies

Elastic scattering wave function for protons or neutrons

Dyson equation therefore provides:

Link between scattering and structure data from **dispersion relations**

Propagator in principle generates

- Elastic scattering cross sections for p and n
- Including all polarization observables
- Total cross sections for n
- Reaction cross sections for p and n
- Overlap functions for adding p or n to bound states in Z+1 or N+1
- Plus normalization --> spectroscopic factor
- Overlap function for removing p or n with normalization
- Hole spectral function including high-momentum description
- One-body density matrix; occupation numbers; natural orbits
- Charge density
- Neutron distribution
- p and n distorted waves
- Contribution to the energy of the ground state from V_{NN}

Dispersive optical potential <--> nucleon self-energy

- e.g. Bell and Squires --> elastic T-matrix = reducible self-energy
- e.g. Mahaux and Sartor Adv. Nucl. Phys. **20**, 1 (1991)
  - relate dynamic (energy-dependent) real part to imaginary part
  - employ subtracted dispersion relation
  - contributions from the hole (structure) and particle (reaction) domain

General dispersion relation for self-energy:

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

Calculated at the Fermi energy $\varepsilon_F = \frac{1}{2}\left\{(E_0^{A+1} - E_0^A) + (E_0^A - E_0^{A-1})\right\}$

$$\mathrm{Re}\ \Sigma(\varepsilon_F) = \Sigma^{HF} - \frac{1}{\pi}\mathcal{P}\int_{E_T^+}^{\infty} dE' \frac{\mathrm{Im}\ \Sigma(E')}{\varepsilon_F - E'} + \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{E_T^-} dE' \frac{\mathrm{Im}\ \Sigma(E')}{\varepsilon_F - E'}$$

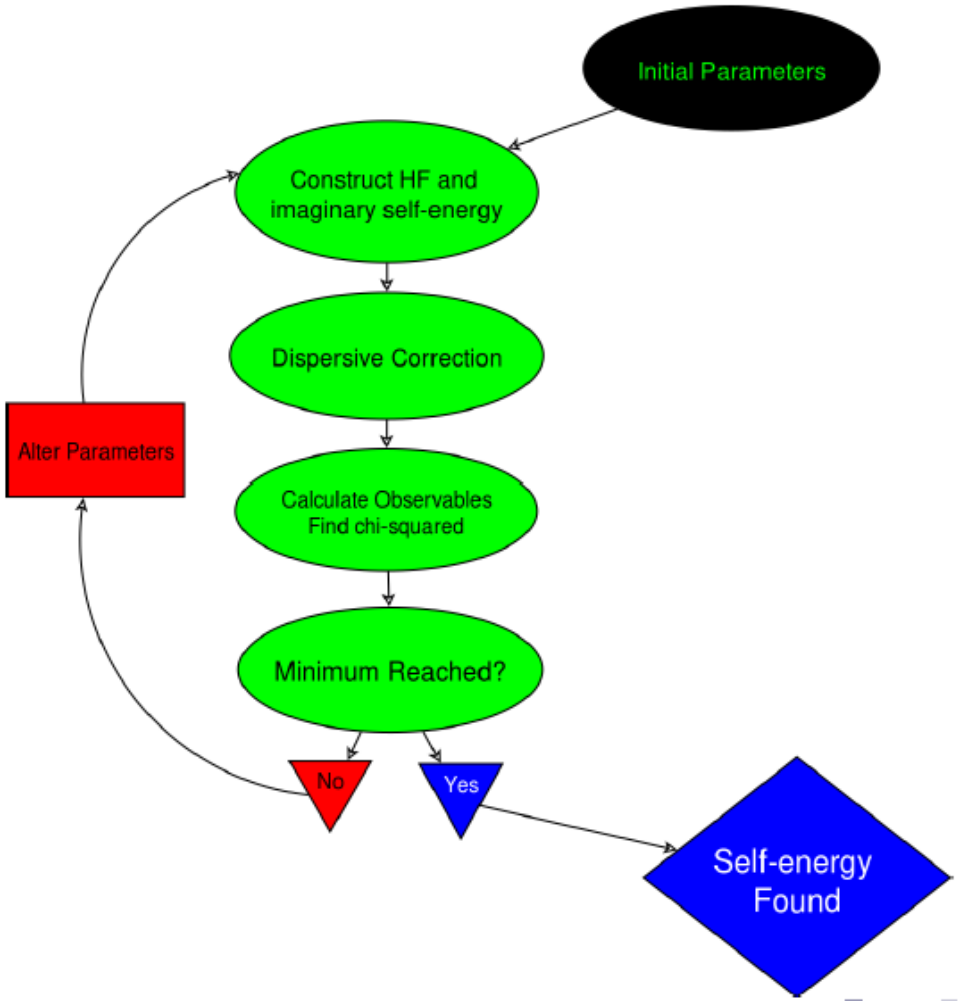
Subtract

$$\mathrm{Re}\ \Sigma(E) = \mathrm{Re}\ \widetilde{\Sigma^{HF}}(\varepsilon_F)$$

$$- \frac{1}{\pi}(\varepsilon_F - E)\mathcal{P}\int_{E_T^+}^{\infty} dE' \frac{\mathrm{Im}\ \Sigma(E')}{(E - E')(\varepsilon_F - E')} + \frac{1}{\pi}(\varepsilon_F - E)\mathcal{P}\int_{-\infty}^{E_T^-} dE' \frac{\mathrm{Im}\ \Sigma(E')}{(E - E')(\varepsilon_F - E')}$$

Functional form and fitting

- Choice of potentials based on empirical knowledge
- Volume absorption —> WS
- Surface absorption —> WS'
- Coulomb
- Spin-orbit
- Hartree-Fock —> WS & WS'
- non-locality —> Gaussian
- E-dependence imaginary part <—> some theory
- Many parameters have canonical values



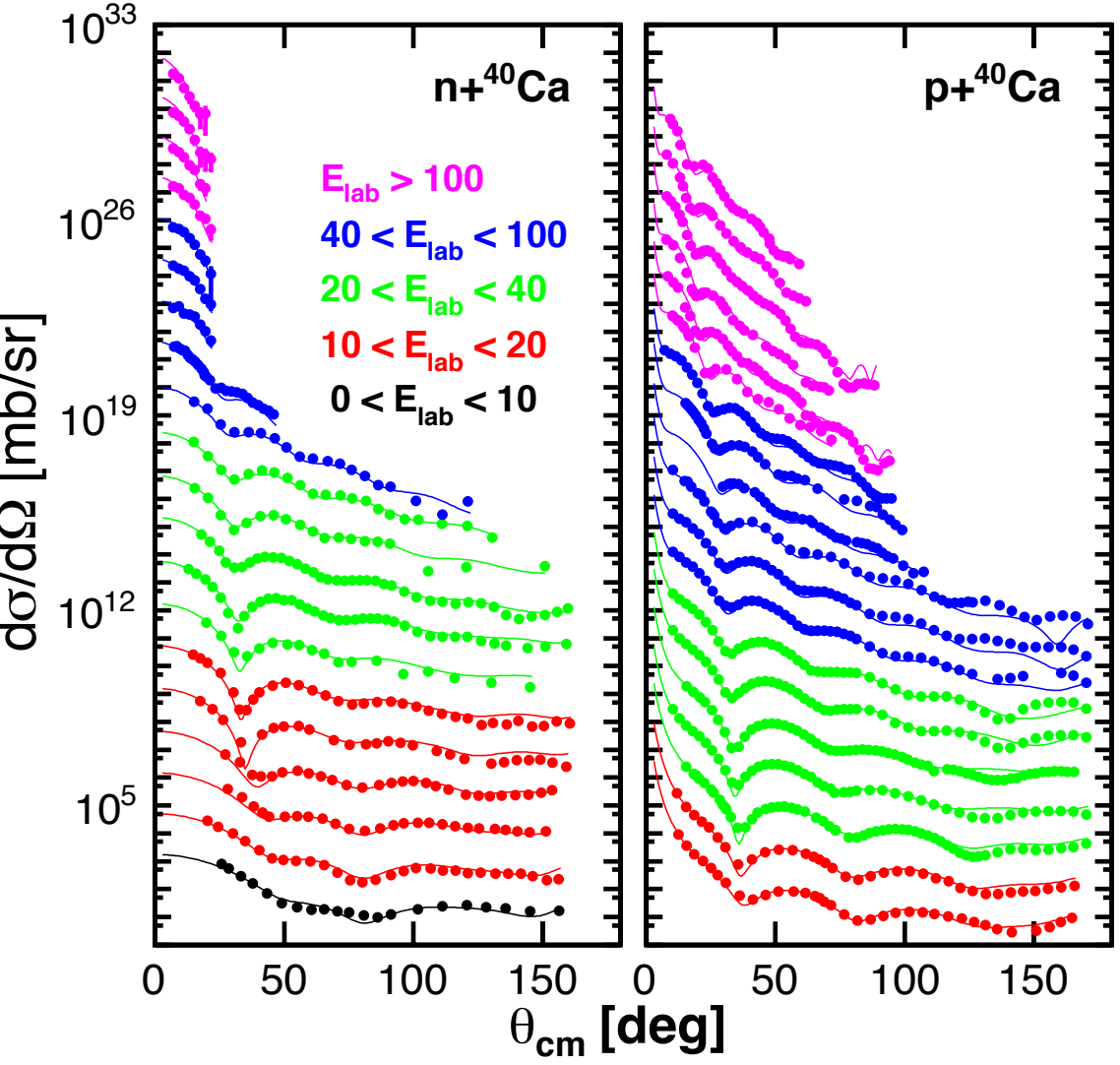
Nonlocal DOM implementation PRL112,162503(2014)

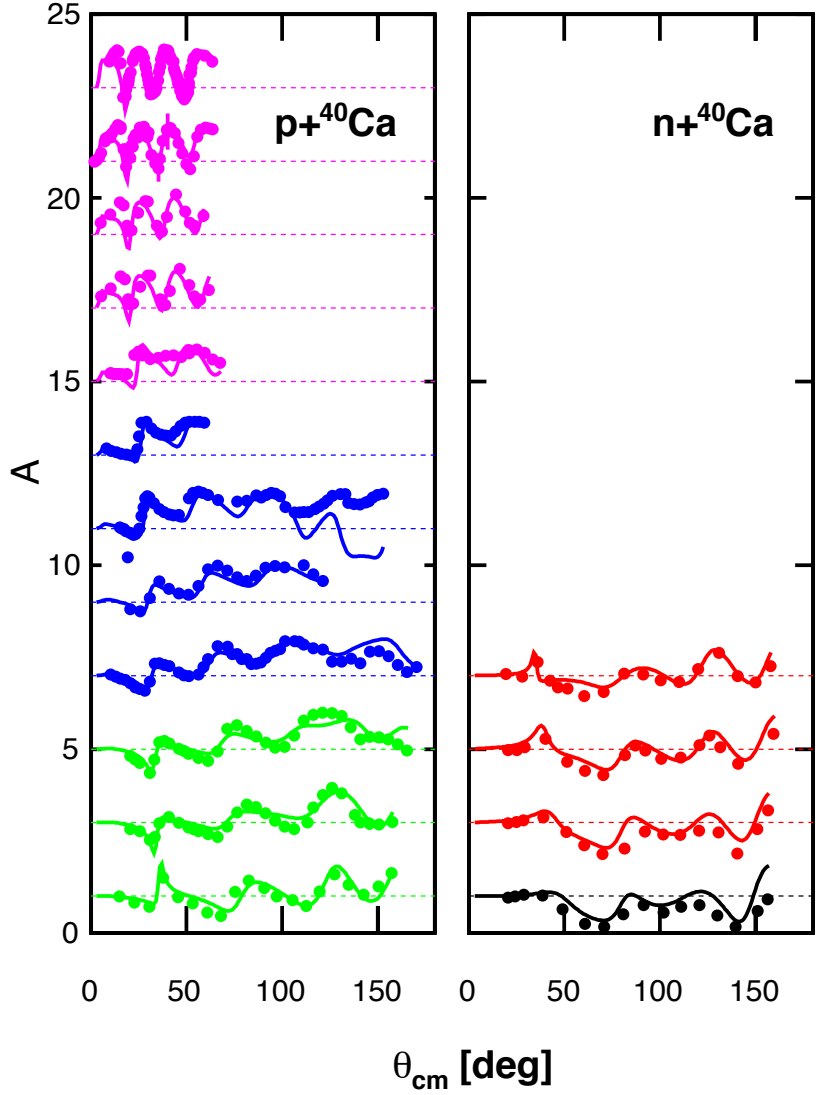
- Particle number --> **nonlocal** imaginary part
- Ab initio FRPA & SRC --> different nonlocal properties above and below the Fermi energy Phys. Rev. C84, 034616 (2011) & Phys. Rev.C84, 044319 (2011)
- Include charge density in fit
- Describe high-momentum nucleons <--> (e,e'p) data from JLab

Implications

- Changes the description of hadronic reactions because interior nucleon wave functions depend on non-locality
- Consistency test of interpretation (e,e'p) reaction (see later)

Differential cross sections and analyzing powers



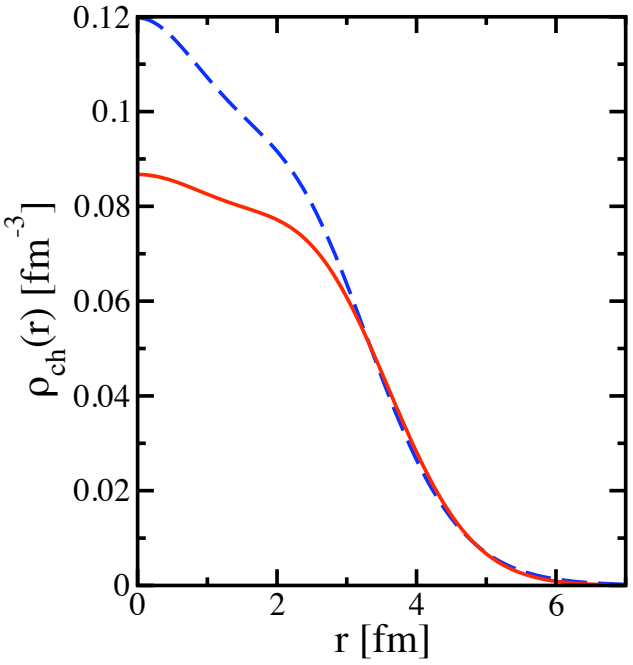


Critical experimental data—> charge density

Local version

radius correct…

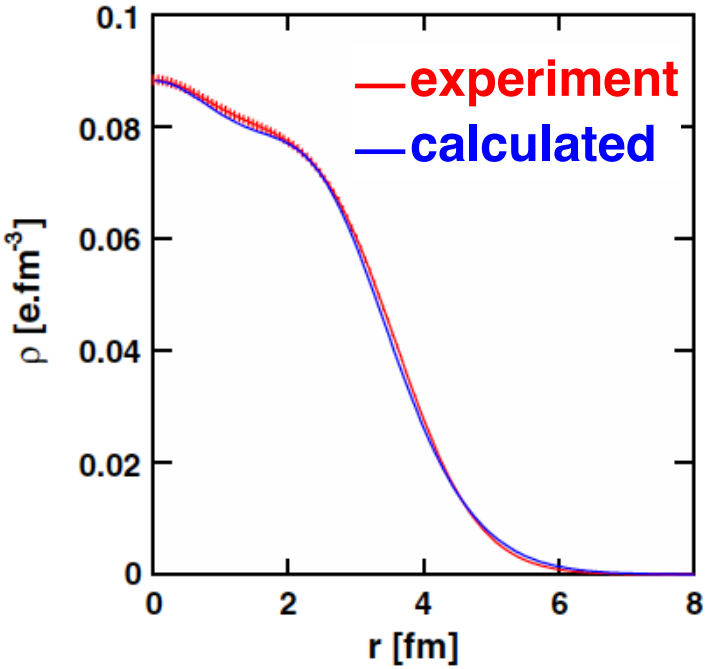
PRC82, 054306 (2010)



Charge density ^{40}Ca

Non-locality essential

PRL 112,162503(2014)



High-momentum nucleons —> JLab can also be described —> E/A

Do elastic scattering data tell us about correlations?

- Scattering T-matrix (neutrons)

$$\Sigma_{\ell j}(k,k';E) = \Sigma^*_{\ell j}(k,k';E) + \int dq q^2 \Sigma^*_{\ell j}(k,q;E) G^{(0)}(q;E) \Sigma_{\ell j}(q,k';E)$$

- Free propagator $\quad G^{(0)}(q;E) = \dfrac{1}{E - \hbar^2 q^2/2m + i\eta}$

- Propagator

$$G_{\ell j}(k,k';E) = \frac{\delta(k-k')}{k^2} G^{(0)}(k;E) + G^{(0)}(k;E) \Sigma_{\ell j}(k,k';E) G^{(0)}(k;E)$$

- Spectral representation

$$G^p_{\ell j}(k,k';E) = \sum_n \frac{\phi^{n+}_{\ell j}(k) \left[\phi^{n+}_{\ell j}(k')\right]^*}{E - E^{*A+1}_n + i\eta} + \sum_c \int_{T_c}^{\infty} dE' \, \frac{\chi^{cE'}_{\ell j}(k) \left[\chi^{cE'}_{\ell j}(k')\right]^*}{E - E' + i\eta}$$

- Spectral density for $E > 0$

$$S^p_{\ell j}(k,k';E) = \frac{i}{2\pi}\left[G^p_{\ell j}(k,k';E^+) - G^p_{\ell j}(k,k';E^-)\right] = \sum_c \chi^{cE}_{\ell j}(k) \left[\chi^{cE}_{\ell j}(k')\right]^*$$

- Coordinate space $\quad S^p_{\ell j}(r,r';E) = \sum_c \chi^{cE}_{\ell j}(r) \left[\chi^{cE}_{\ell j}(r')\right]^*$

- Elastic scattering also explicitly available

$$\chi^{elE}_{\ell j}(r) = \left[\frac{2mk_0}{\pi\hbar^2}\right]^{1/2} \left\{ j_\ell(k_0 r) + \int dk k^2 j_\ell(kr) G^{(0)}(k;E) \Sigma_{\ell j}(k,k_0;E) \right\}$$

Determine location of bound-state strength

- Fold spectral function with bound state wave function

$$S^{n+}_{\ell j}(E) = \int dr\ r^2 \int dr'\ r'^2 \phi^{n-}_{\ell j}(r) S^{p}_{\ell j}(r, r'; E) \phi^{n-}_{\ell j}(r')$$

- —> Addition probability of bound orbit
- Also removal probability

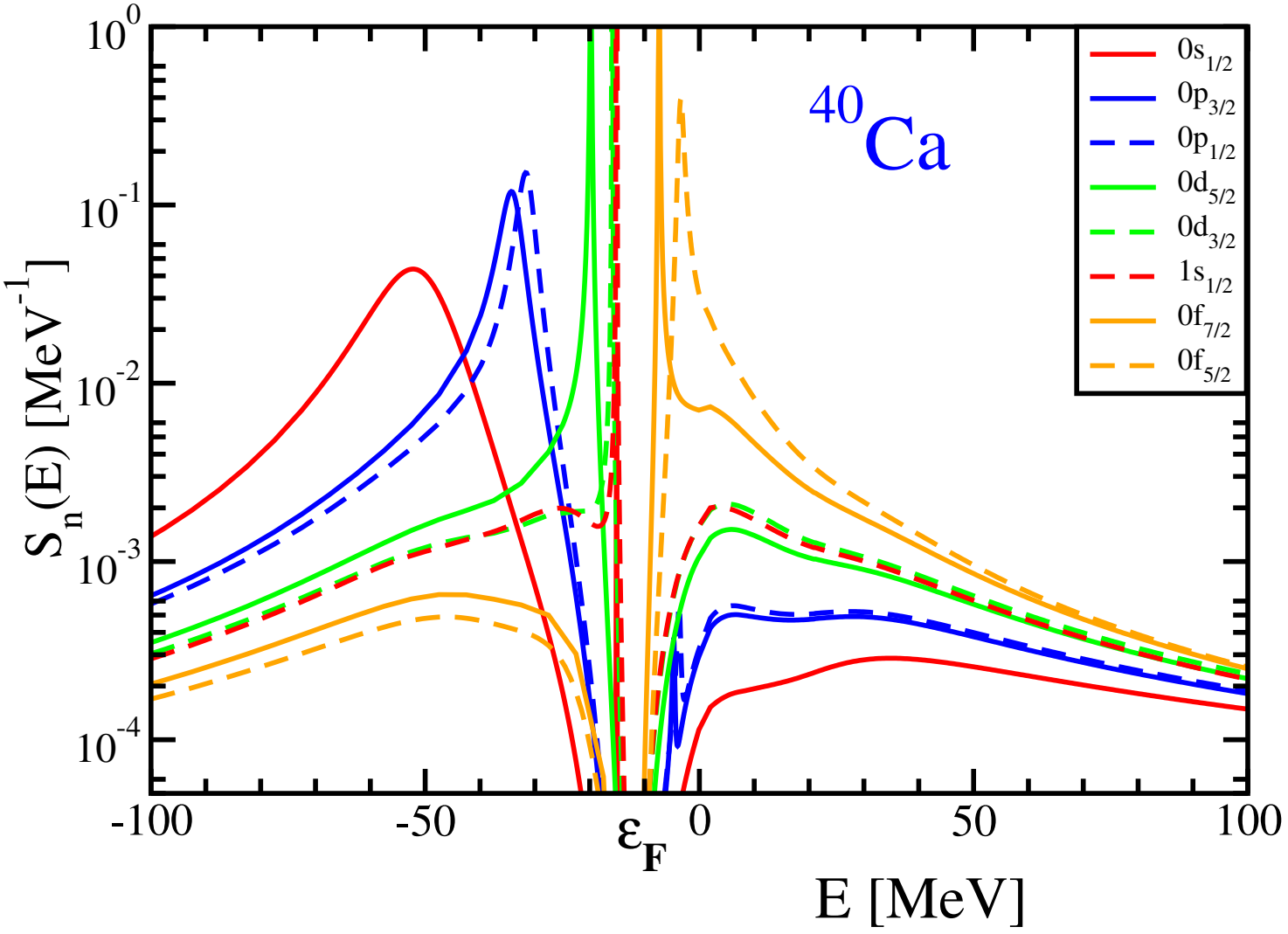
$$S^{n-}_{\ell j}(E) = \int dr r^2 \int dr' r'^2 \phi^{n-}_{\ell j}(r) S^{h}_{\ell j}(r, r'; E) \phi^{n-}_{\ell j}(r')$$

- Overlap function $\sqrt{S^{n}_{\ell j}}\phi^{n-}_{\ell j}(r) = \langle \Psi^{A-1}_{n} | \, a_{r\ell j} \, | \Psi^{A}_{0} \rangle$

- Sum rule $1 = n_{n\ell j} + d_{n\ell j} = \int_{-\infty}^{\varepsilon_F} dE\ S^{n-}_{\ell j}(E) + \int_{\varepsilon_F}^{\infty} dE\ S^{n-}_{\ell j}(E)$

Spectral function for bound states

- [0,200] MeV —> constrained by elastic scattering data



Emptiness constrained!

PRC90, 061603(R) (2014)

Quantitatively

- Orbit closer to the continuum —> more strength in the continuum
- Note "particle" orbits
- Drip-line nuclei have valence orbits very near the continuum

Table 1: Occupation and depletion numbers for bound orbits in ^{40}Ca. $d_{nlj}[0, 200]$ depletion numbers have been integrated from 0 to 200 MeV. The fraction of the sum rule that is exhausted, is illustrated by $n_{n\ell j} + d_{n\ell j}[\varepsilon_F, 200]$. Last column $d_{nlj}[0, 200]$ depletion numbers for the CDBonn calculation.

orbit	$n_{n\ell j}$ DOM	$d_{n\ell j}[0, 200]$ DOM	$n_{n\ell j} + d_{n\ell j}[\varepsilon_F, 200]$ DOM	$d_{n\ell j}[0, 200]$ CDBonn
$0s_{1/2}$	0.926	0.032	0.958	0.035
$0p_{3/2}$	0.914	0.047	0.961	0.036
$1p_{1/2}$	0.906	0.051	0.957	0.038
$0d_{5/2}$	0.883	0.081	0.964	0.040
$1s_{1/2}$	0.871	0.091	0.962	0.038
$0d_{3/2}$	0.859	0.097	0.966	0.041
$0f_{7/2}$	0.046	0.202	0.970	0.034
$0f_{5/2}$	0.036	0.320	0.947	0.036

PRC90, 061603(R) (2014)

Another look at (e,e'p) data

- collaboration with Louk Lapikás and Henk Blok from NIKHEF
- Data published at E_p = 100 MeV Kramer thesis NIKHEF for $^{40}Ca(e,e'p)^{39}K$
  Phys. Lett. B227, 199 (1989)
  Results: $S(d_{3/2})$=0.65 and $S(s_{1/2})$=0.51
- More data at 70 and 135 MeV (only in a conference paper)
- What do these spectroscopic factor numbers really represent?
  - Assume DWIA for the reaction description
    - Use kinematics (momentum transfer parallel to initial proton momentum) favoring simplest part of the excitation operator (no two-body current) & sufficient energy for the knocked out proton
  - Overlap function:
    - WS with radius adjusted to shape of cross section
    - Depth adjusted to separation energy
  - Distorted proton wave from standard local non-dispersive "global optical potential"
  - Fit normalization of overlap function to data -> spectroscopic factor

Why go back there?

Removal probability for valence protons from NIKHEF data

L. Lapikás, Nucl. Phys. A553,297c (1993)

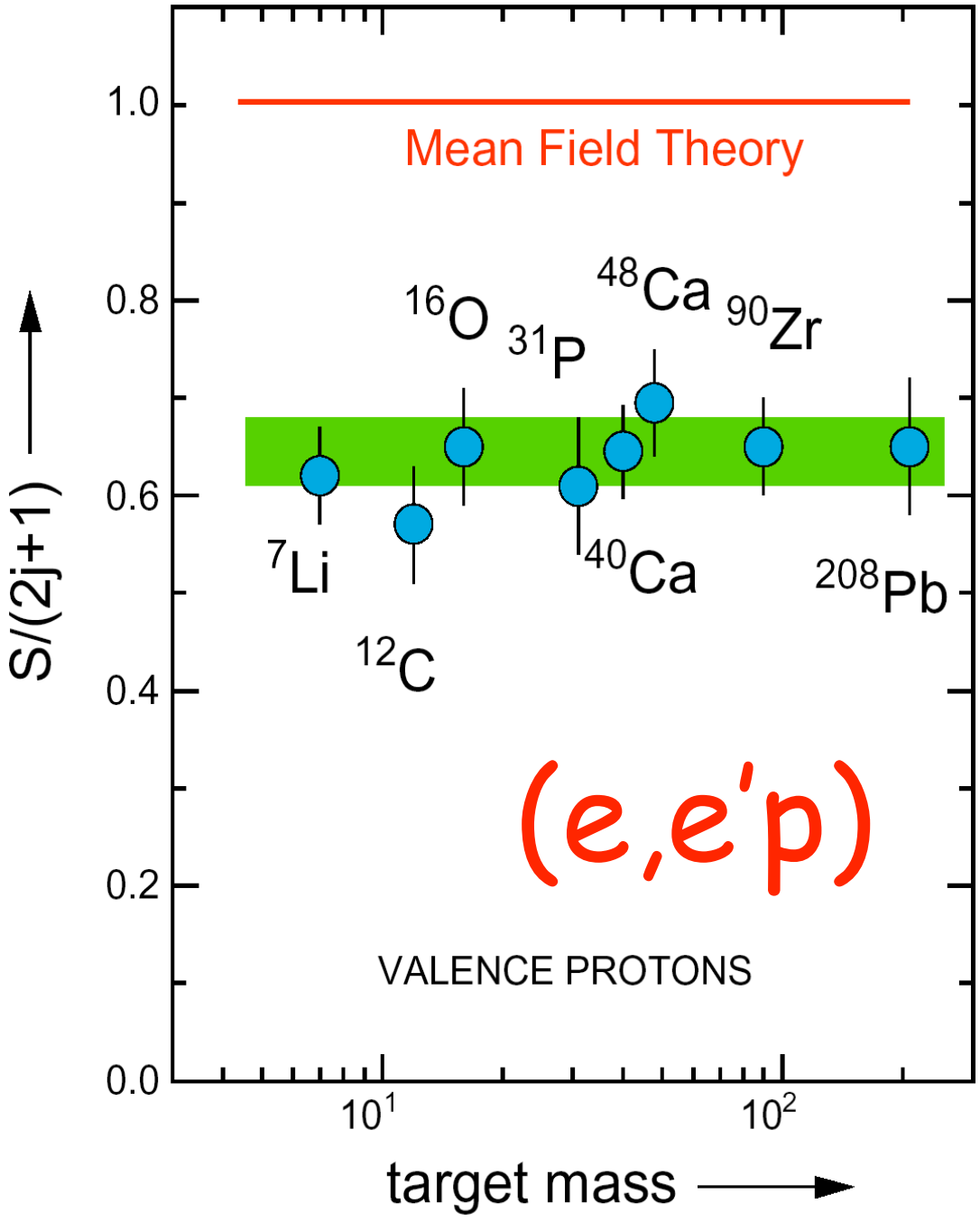
S ≈ 0.65 for valence protons

Reduction ⇒ both SRC and LRC

Weak probe but propagation in the nucleus of removed proton using standard optical potentials to generate distorted wave --> associated uncertainty ~ 5-15%

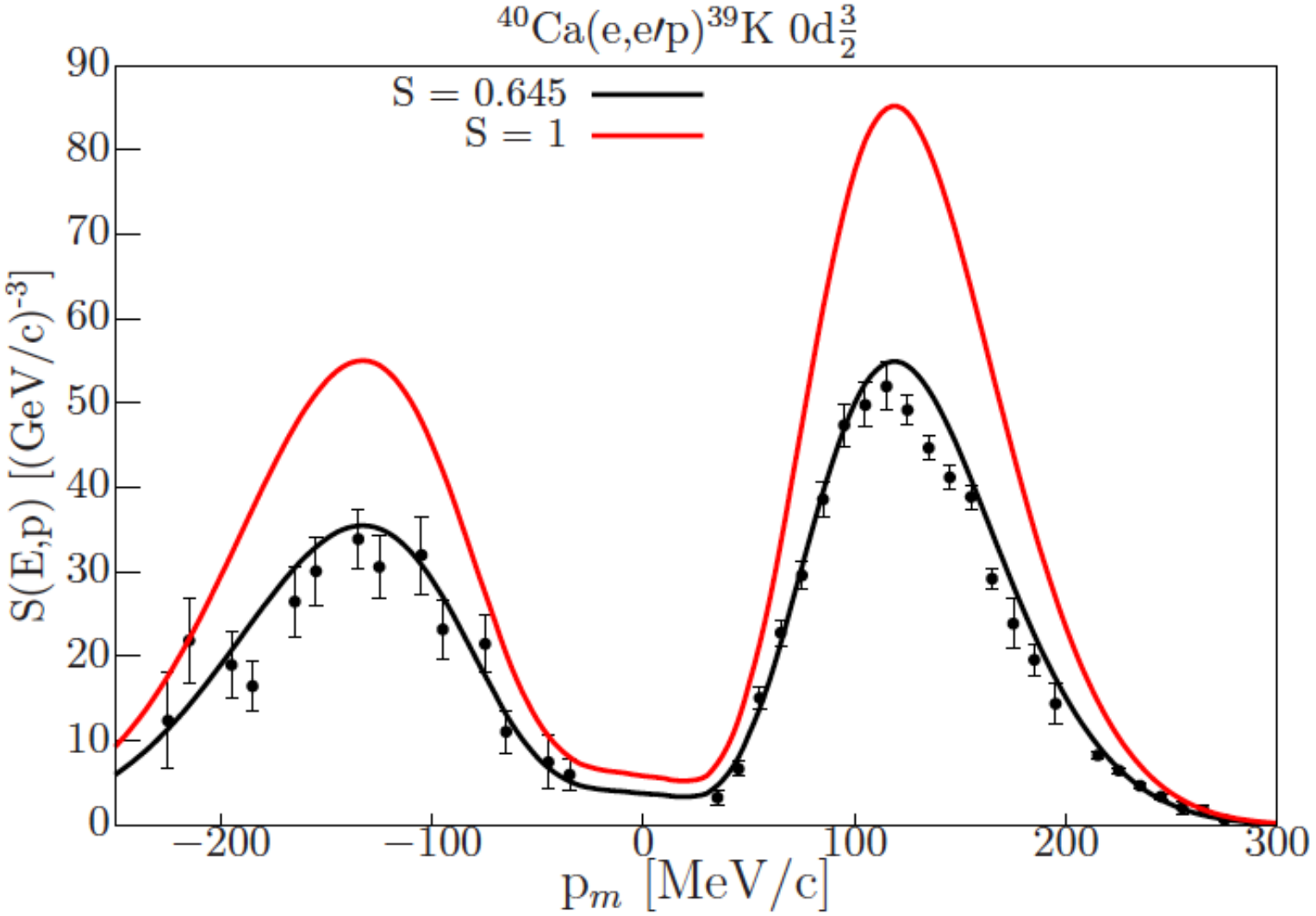
Why: details of the interior scattering wave function uncertain since non-locality is not constrained (so far.....)

but now available for ^{40}Ca!



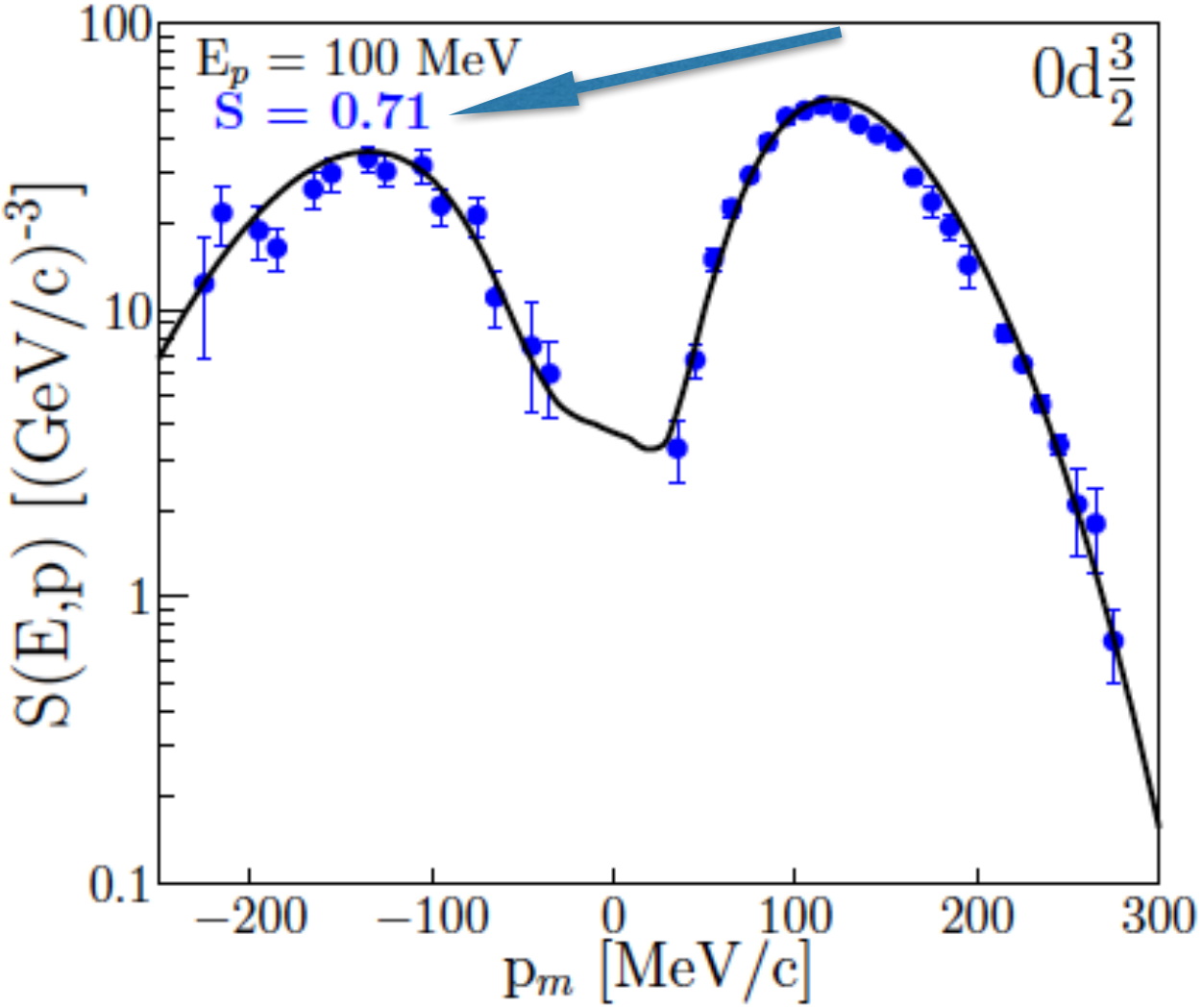
NIKHEF analysis PLB227,199(1989)

- Schwandt et al. (1981) optical potential
- BSW from adjusted WS



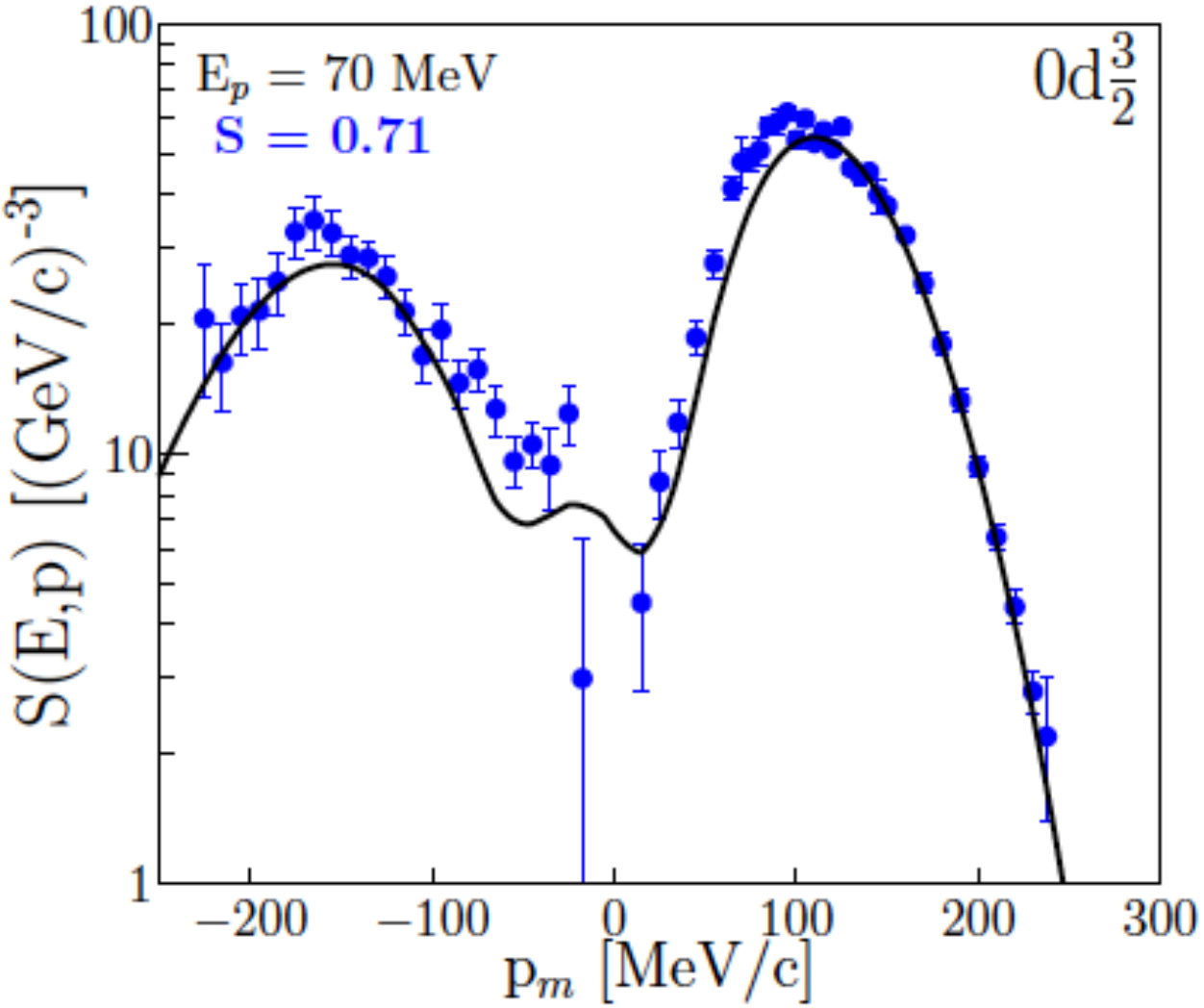
NIKHEF data PLB227,199(1989)

- NIKHEF: $S(d_{3/2})=0.65\pm0.06$
- Only DOM ingredients



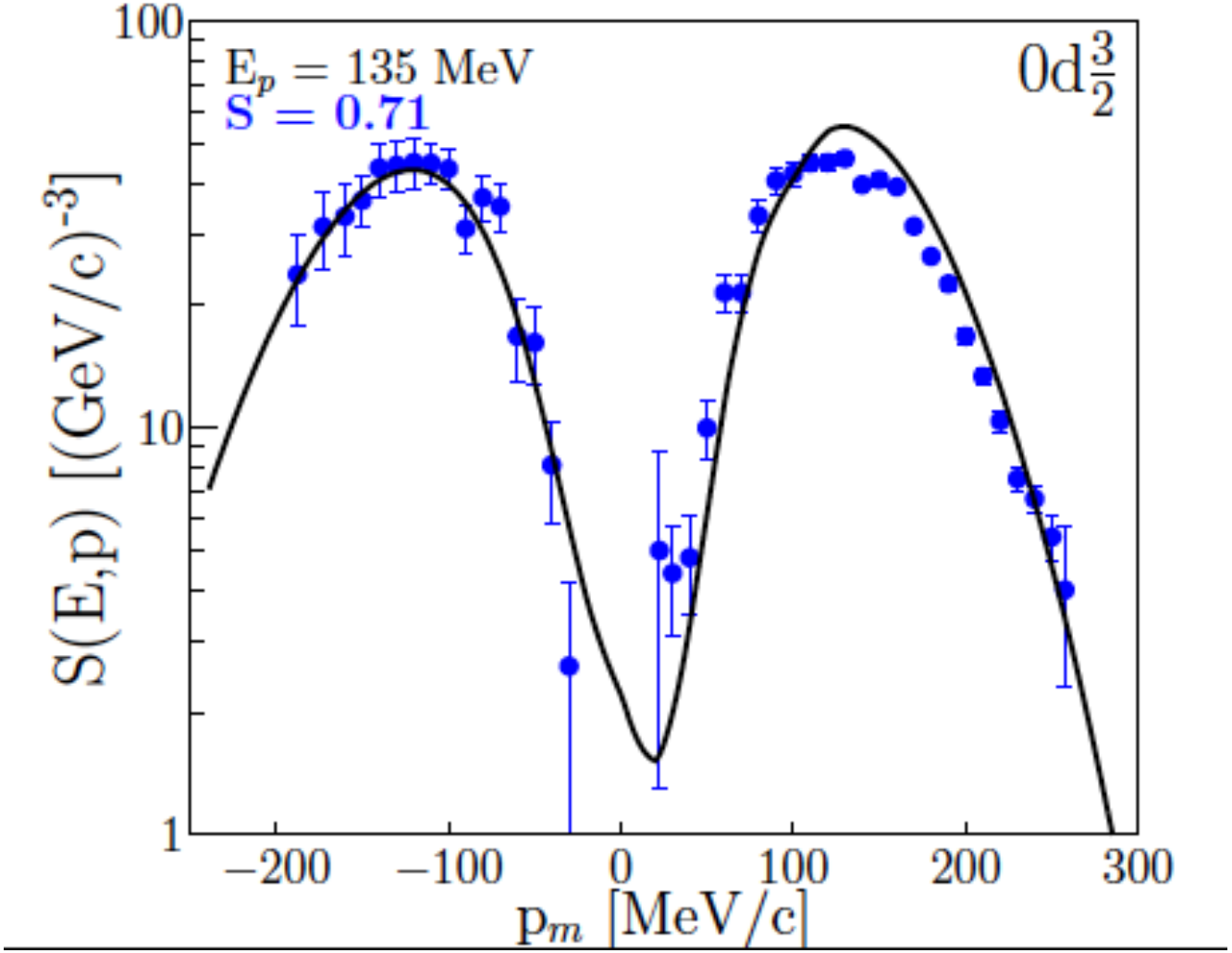
NIKHEF data unpublished

- Only DOM ingredients
- DWEEPY code C. Giusti



NIKHEF data unpublished

- Only DOM ingredients

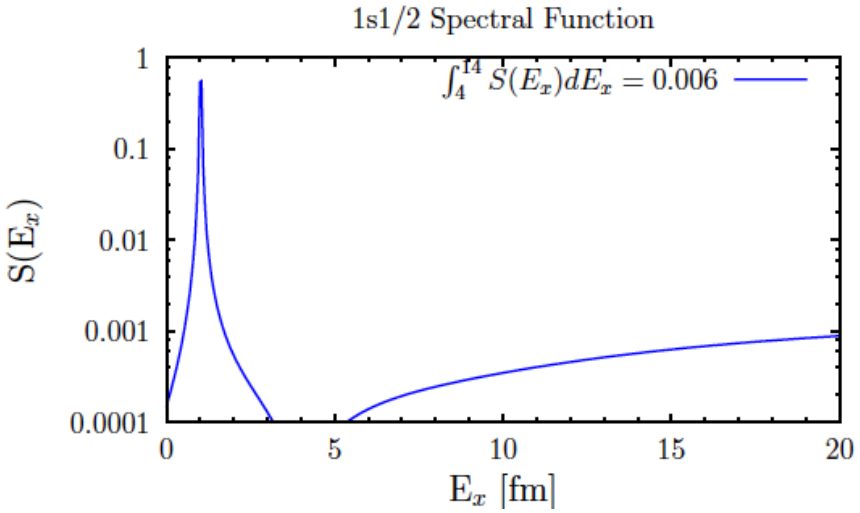


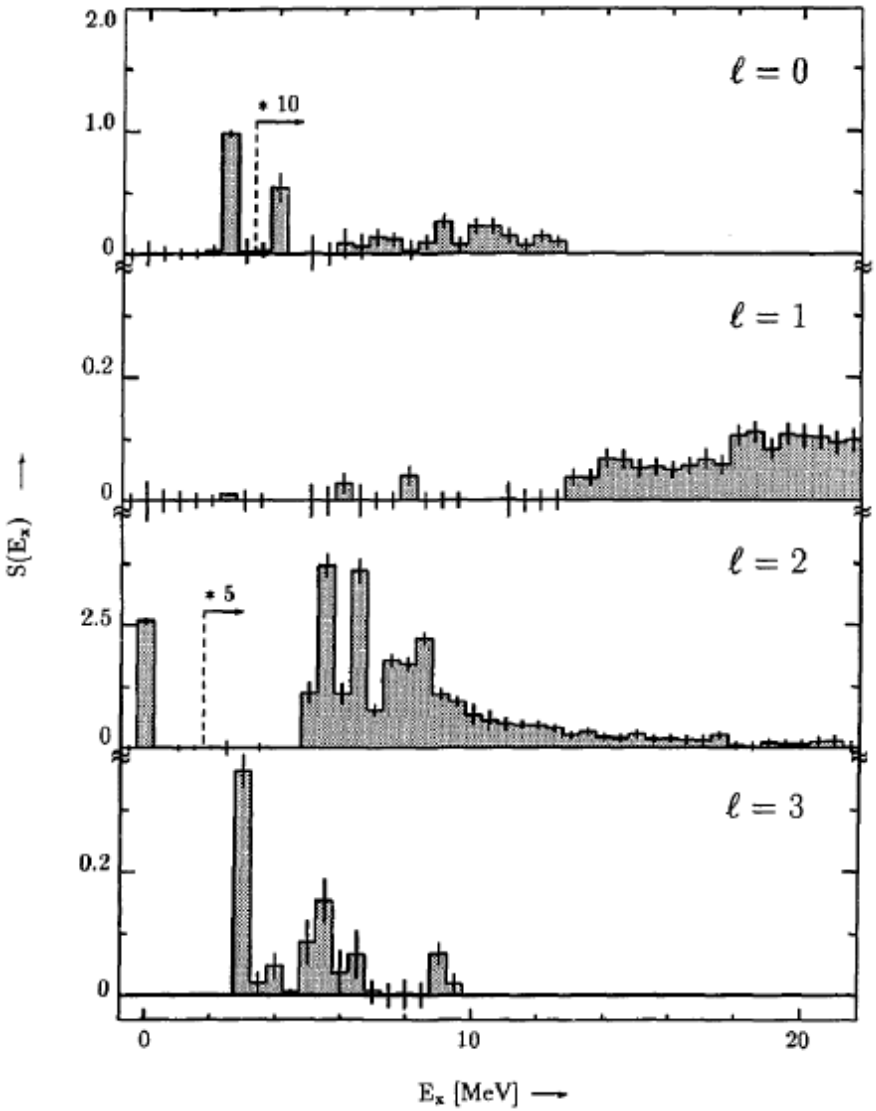
- at this energy DWIA may no longer be the whole story

Thesis G. J. Kramer (1990)

- $s_{1/2}$ strength fragmented

- Not yet included in DOM

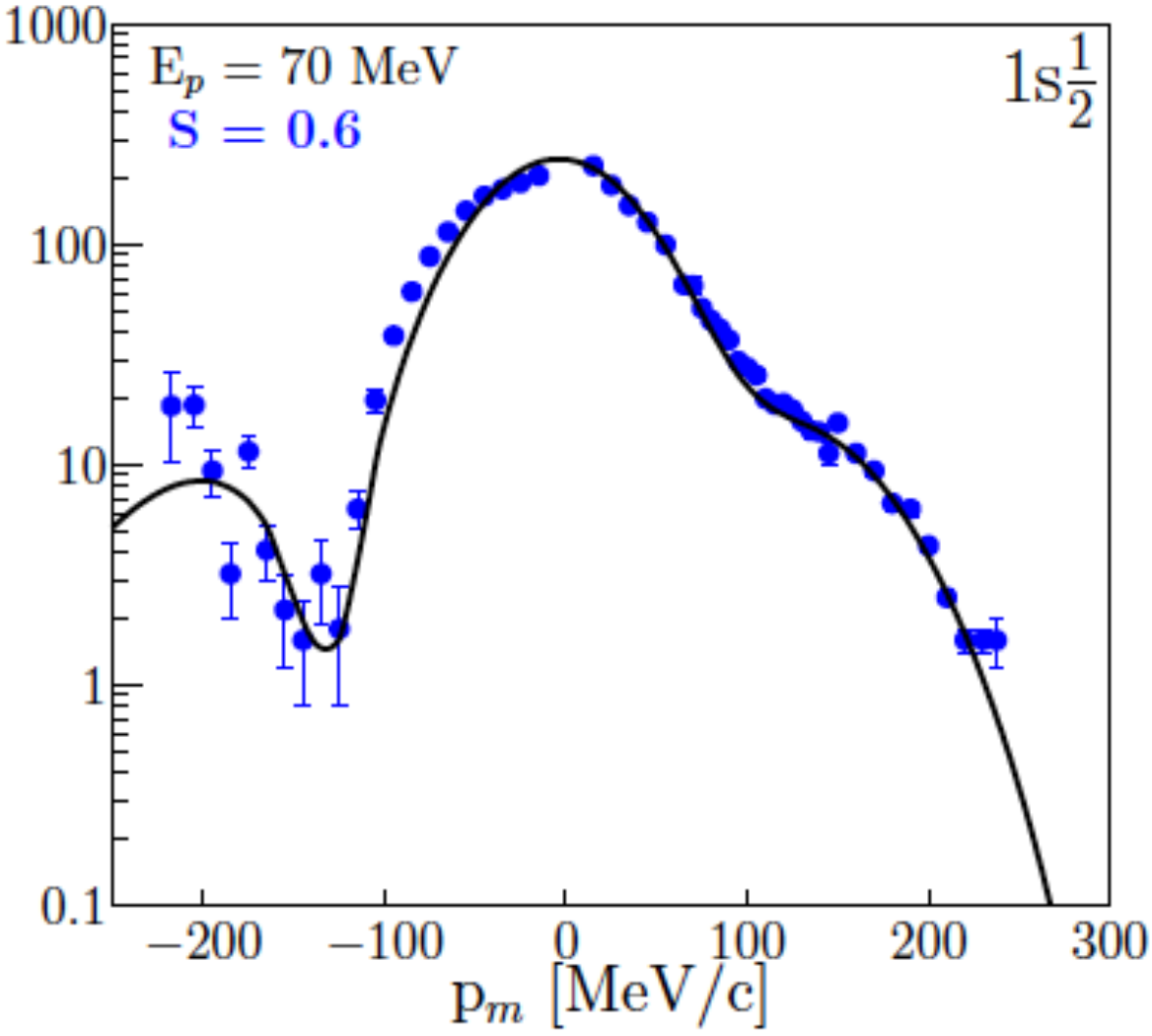




- Corrects DOM spectroscopic factor to 0.62

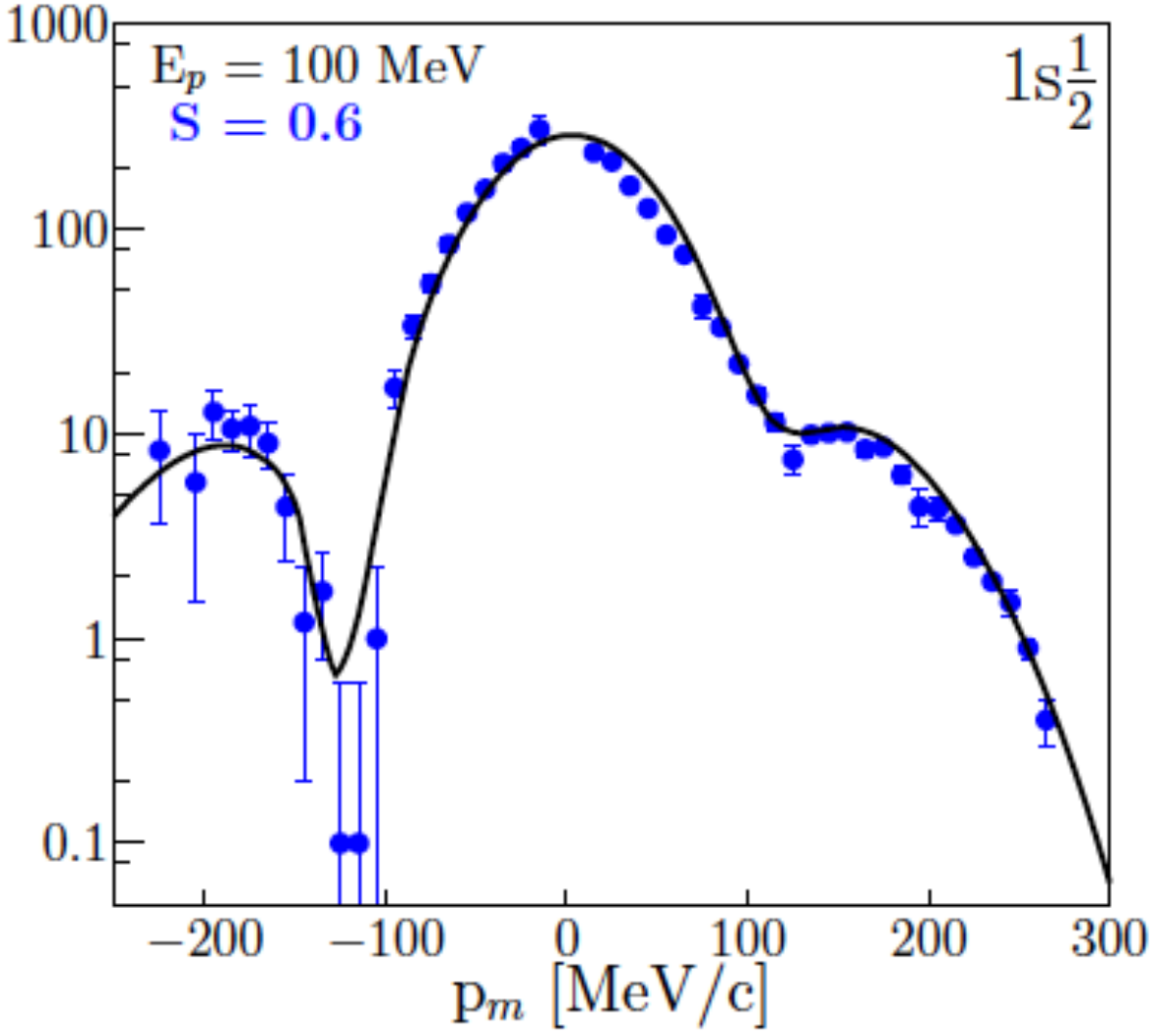
NIKHEF data unpublished

- Only DOM ingredients



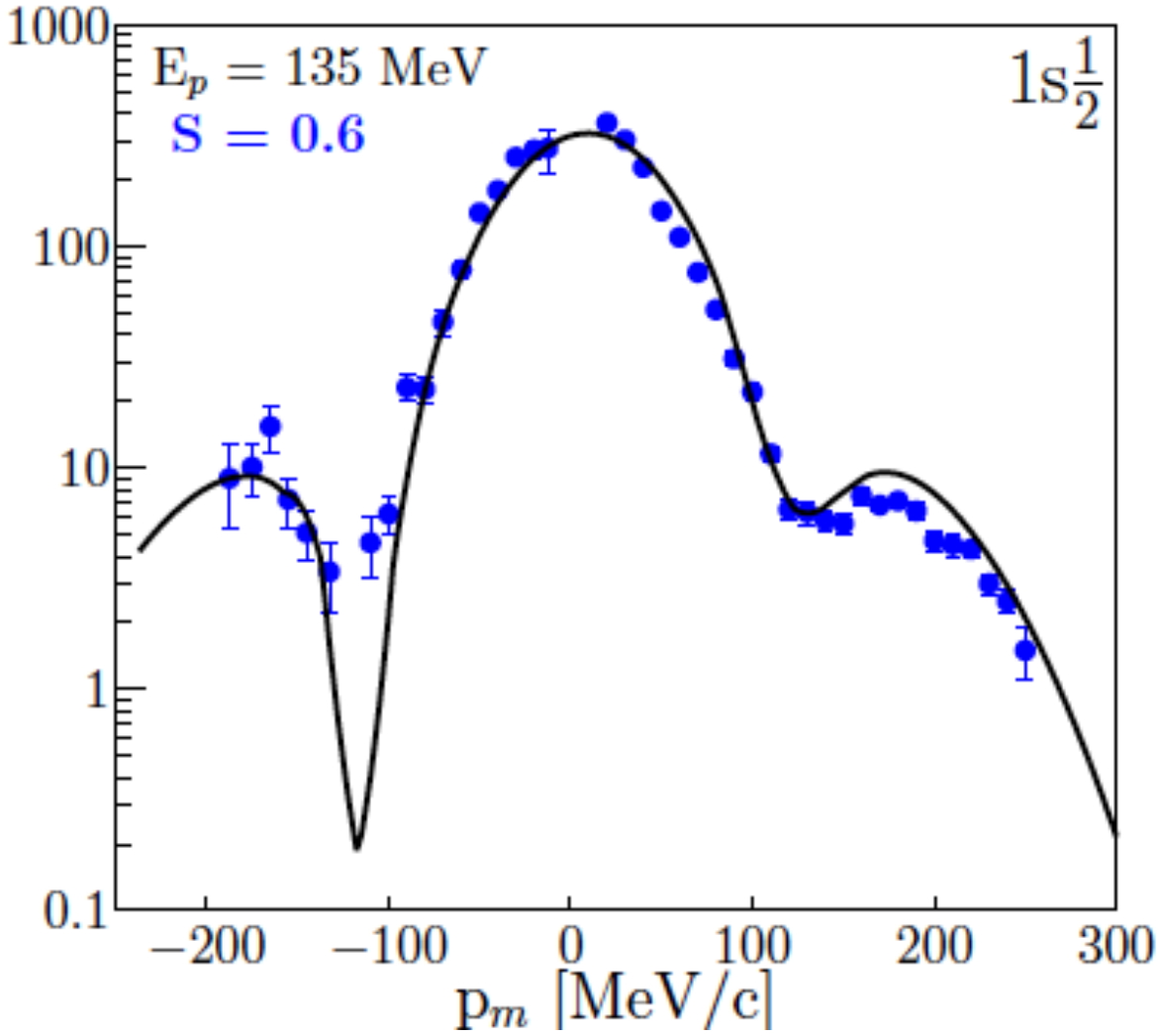
NIKHEF data PLB227,199(1989)

- NIKHEF: $S(s_{1/2})=0.51\pm0.05$



NIKHEF data unpublished

- Only DOM ingredients



Message

- Nonlocal dispersive potentials yield consistent input

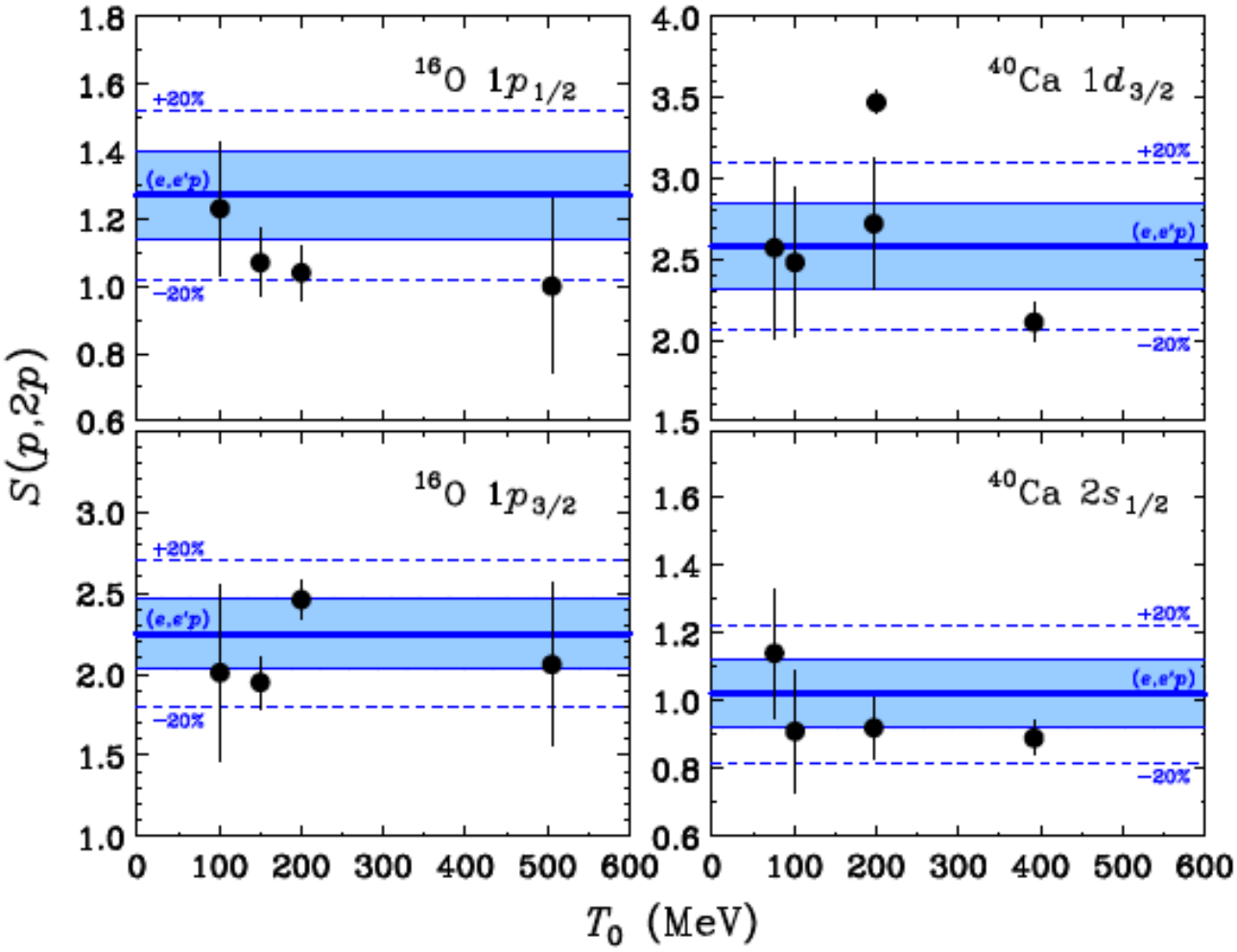
- Constraints from other data generate spectroscopic factors $S(d_{3/2})=0.71$ in ^{40}Ca for ground state transition
- Experimental $s_{1/2}$ strength distribution: 2.5 MeV —> $S(s_{1/2})=0.62$

- NIKHEF 0.65±0.06 and 0.51±0.05, respectively (local)
- Implications for transfer reactions significant

- (p,2p) reaction for stable targets can be constrained and then extended to unstable ones
- Consistent with inelastic electron scattering data

Project (p,pN) with Ogata et al.

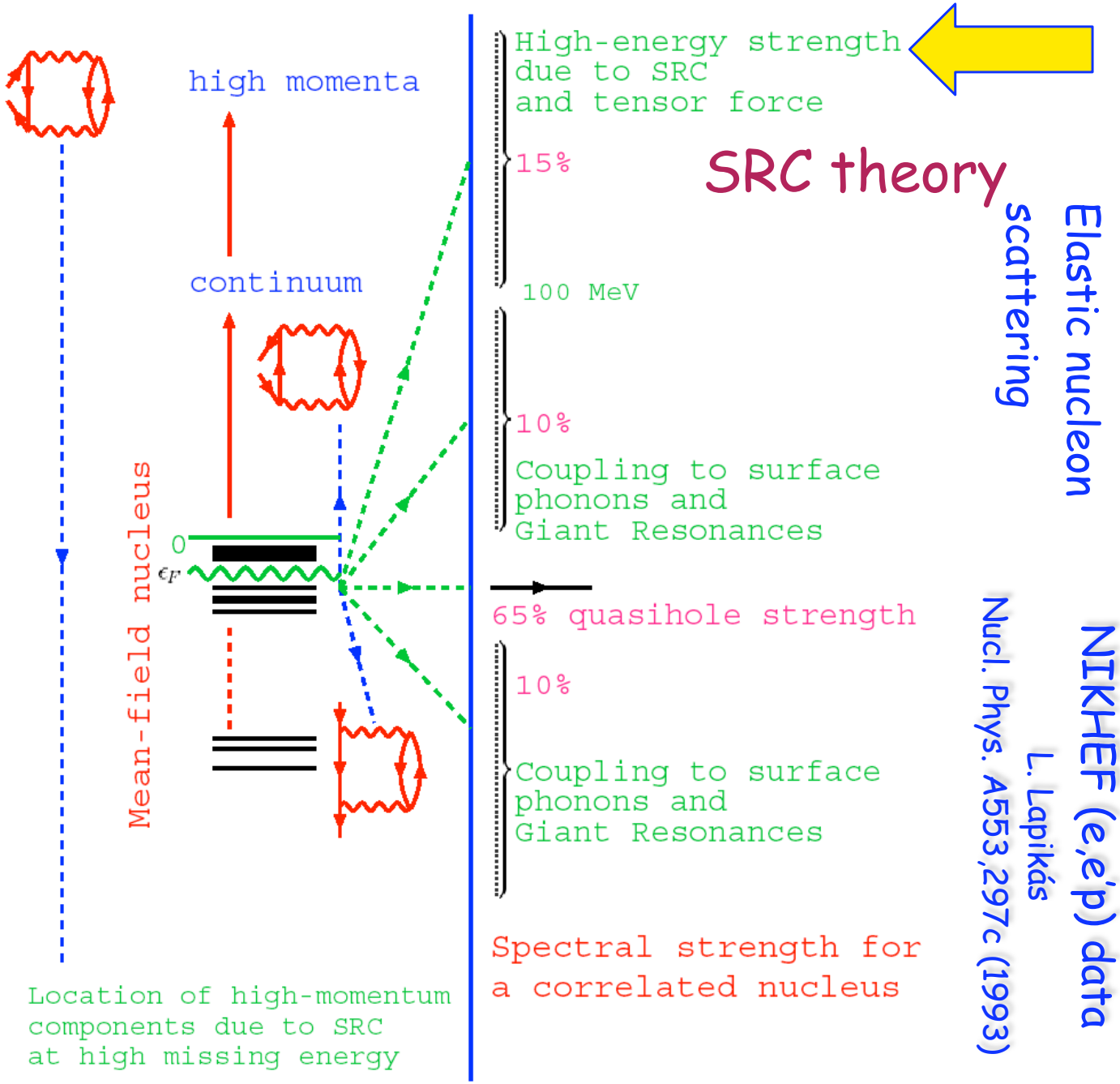
- Distorted waves and overlap from DOM
- Can gauge interaction (beyond free T-matrix)
- Can predict results for exotic nuclei using DOM extrapolations



Reviewed in Prog. Part. Nucl. Phys. 52 (2004) 377-496

Location of single-particle strength in closed-shell (stable) nuclei

For example: protons in ^{208}Pb



SRC

JLab E97-006

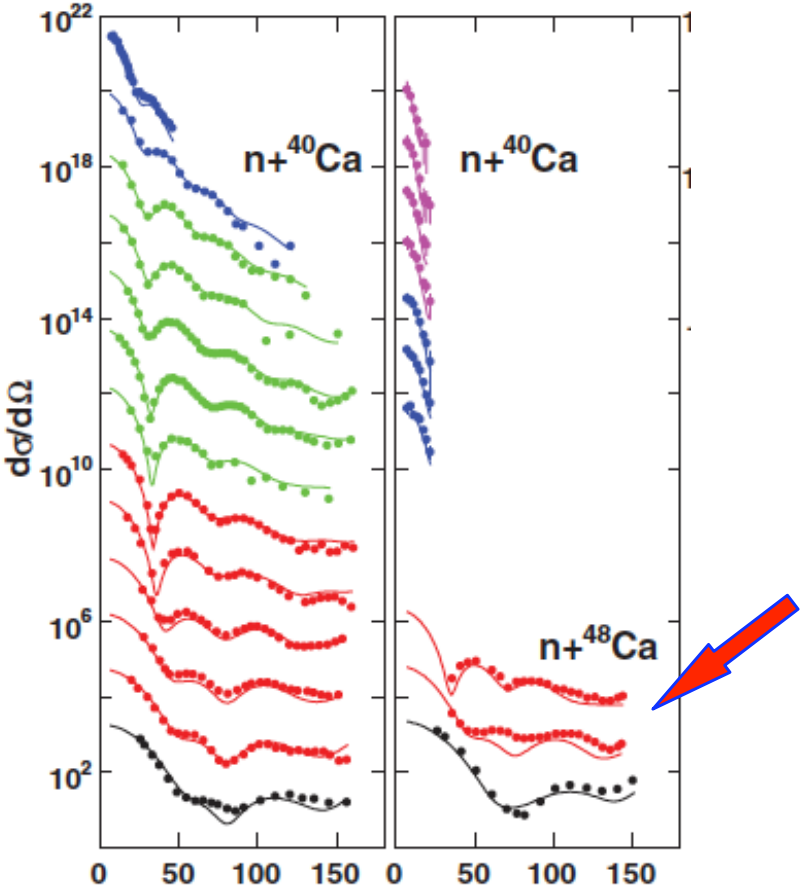
Phys. Rev. Lett. 93, 182501 (2004) D. Rohe et al.

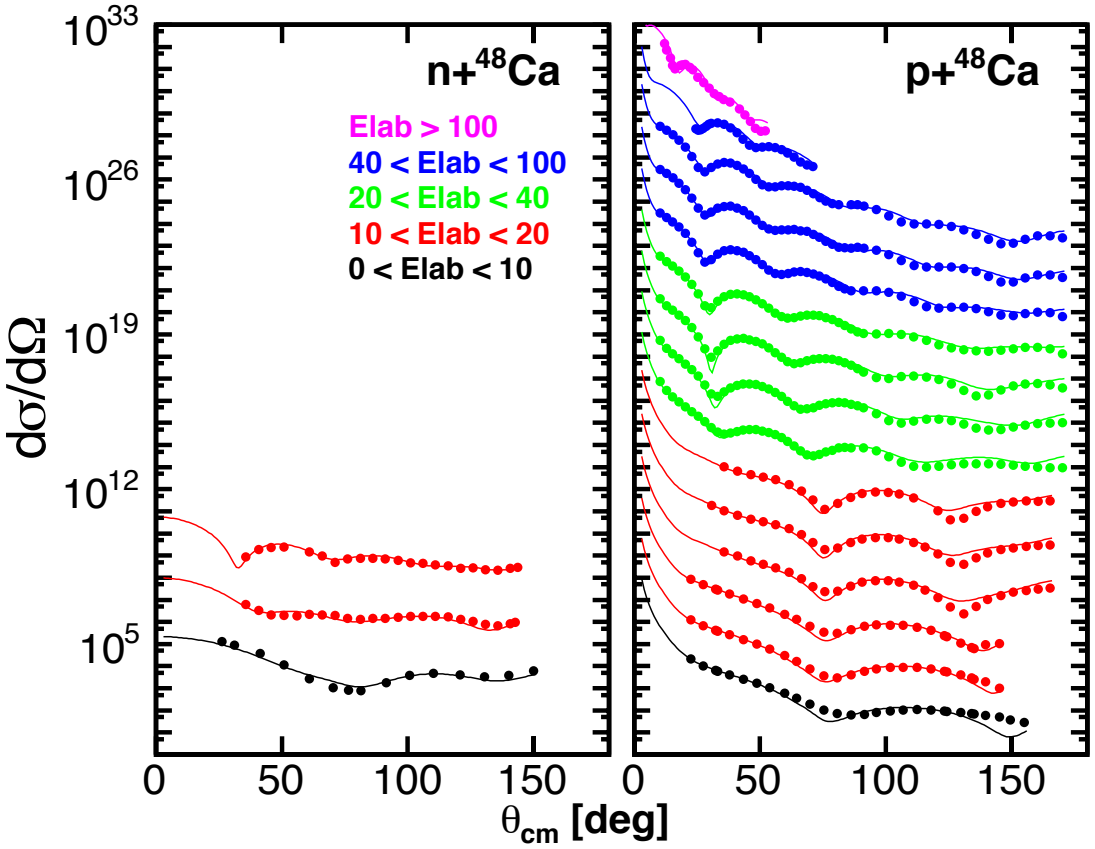
DOM results for ^{48}Ca

- Change of proton properties when 8 neutrons are added to ^{40}Ca?
- Change of neutron properties?
- Can hard to measure quantities be indirectly constrained?

What about neutrons?

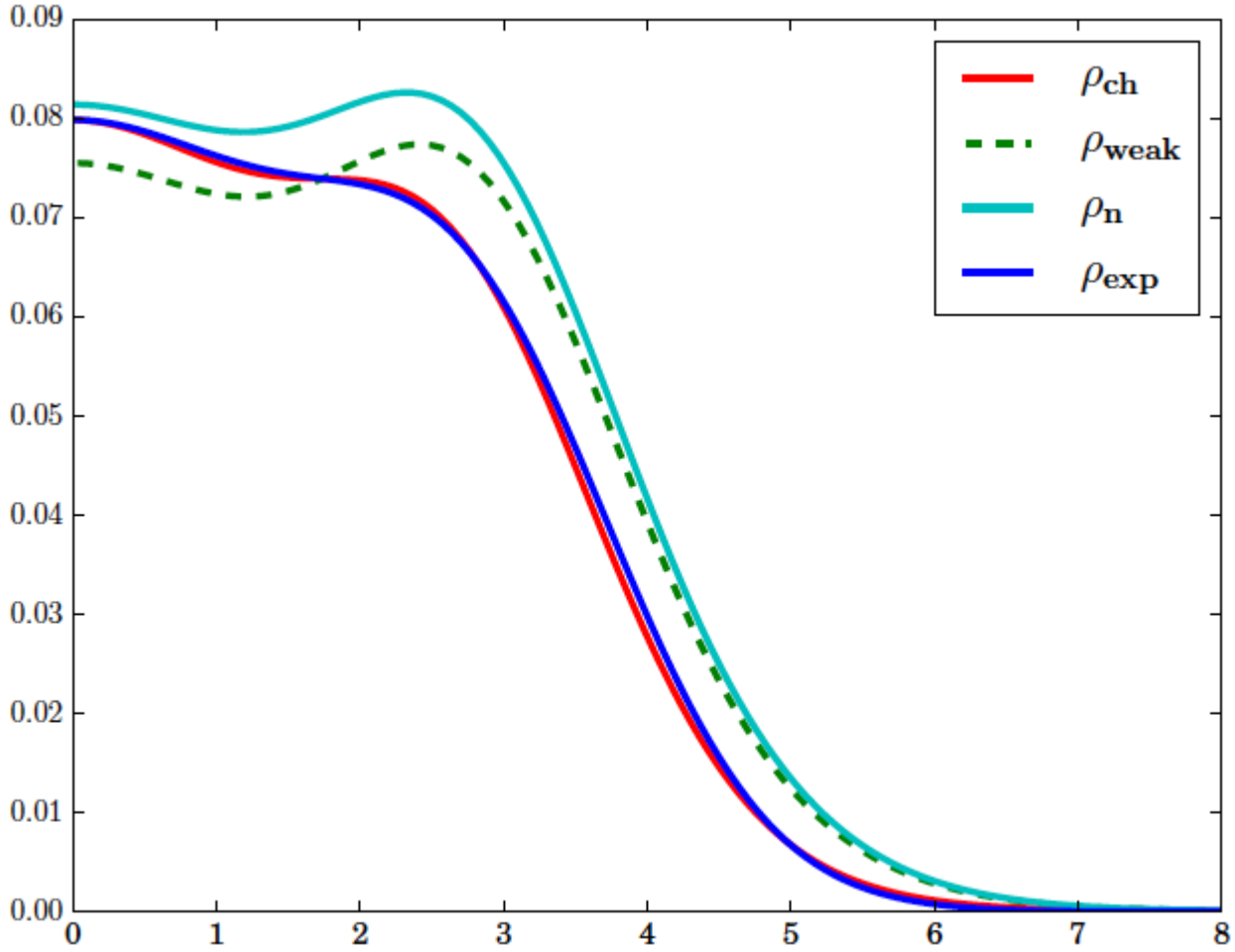
- ^{48}Ca —> charge density has been measured
- Recent neutron elastic scattering **data** —> PRC83,064605(2011)
- Local DOM **OLD** Nonlocal DOM **NEW**





Results ^{48}Ca

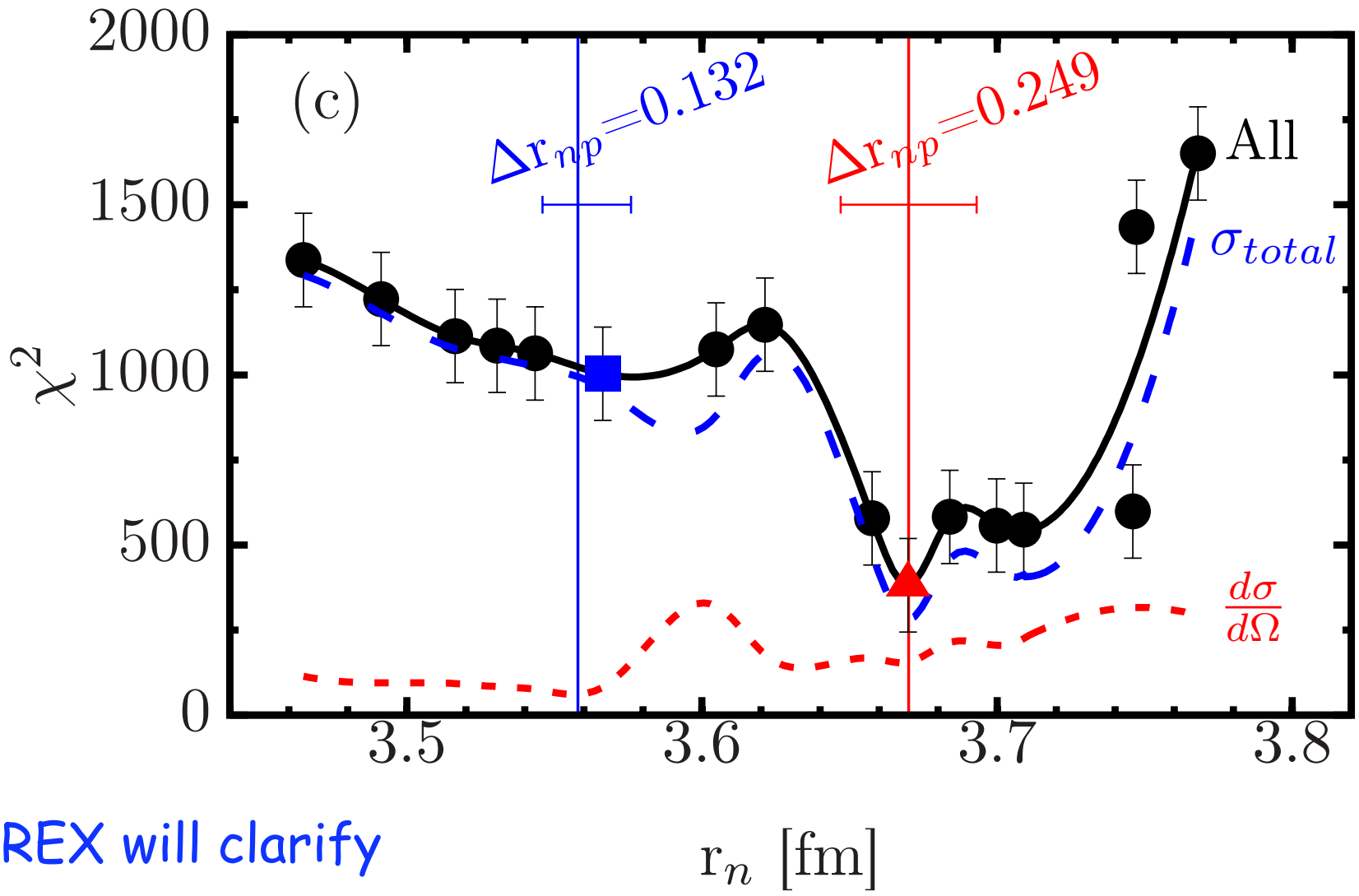
- Density distributions
- DOM —> neutron distribution —> R_n-R_p



r [fm]

Comparison with small neutron skin

- Data sensitivity and error

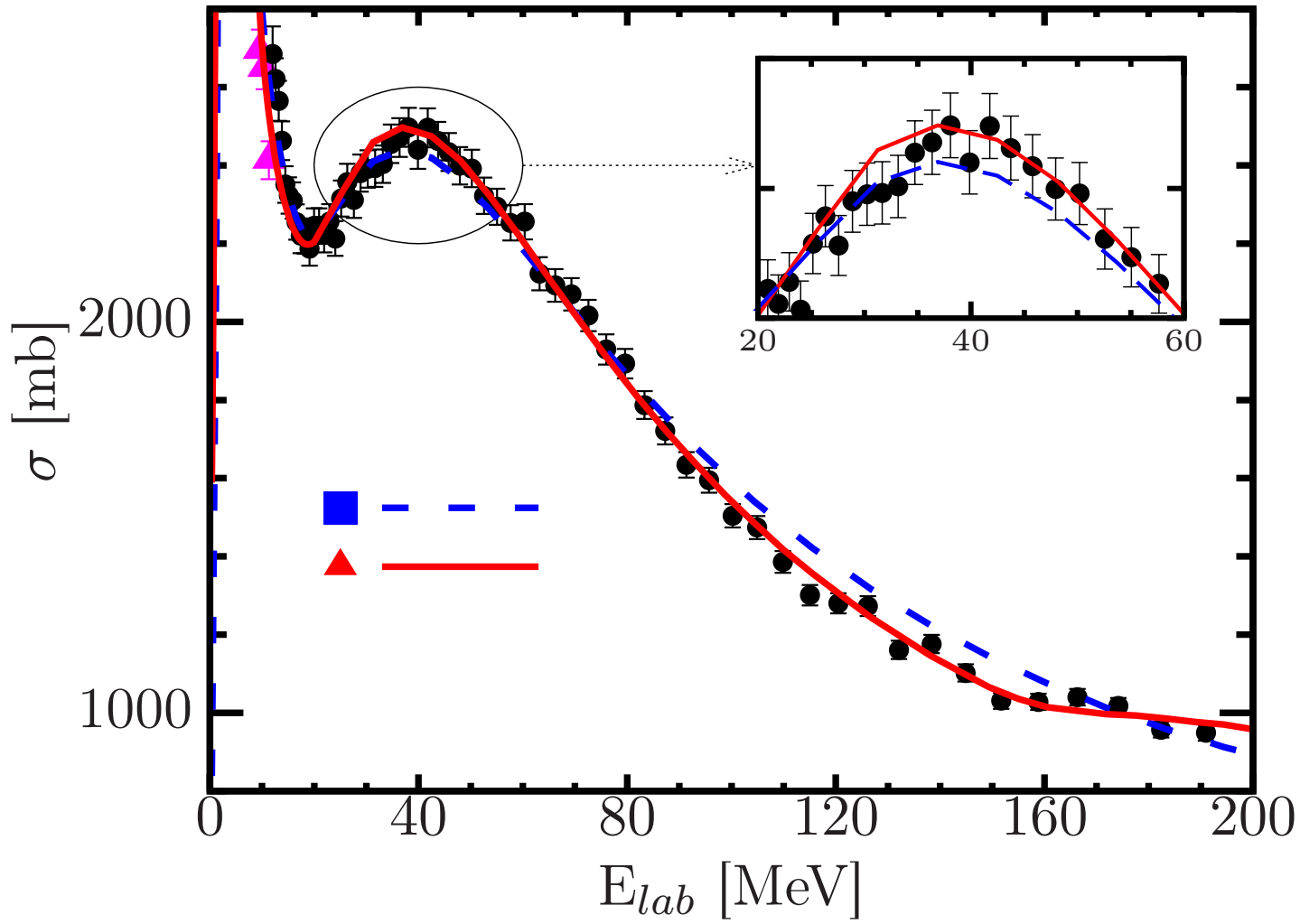


- CREX will clarify

--> drip line

Constraining the neutron radius

- Using total neutron cross sections



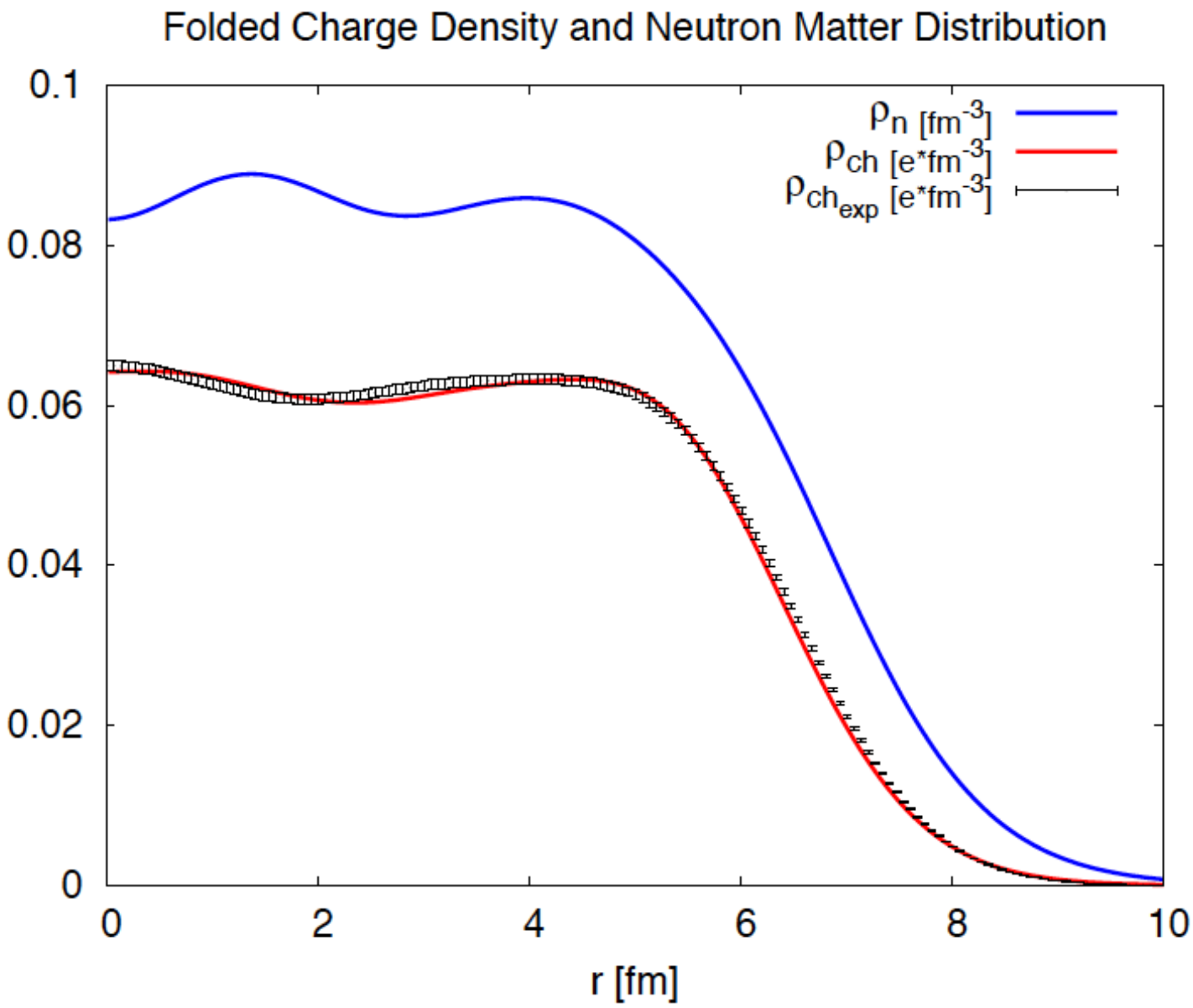
- M.H. Mahzoon, M.C. Atkinson, R.J. Charity, W.D.

  Phys. Rev. Lett. **119**, 222503 (2017)

--> drip line

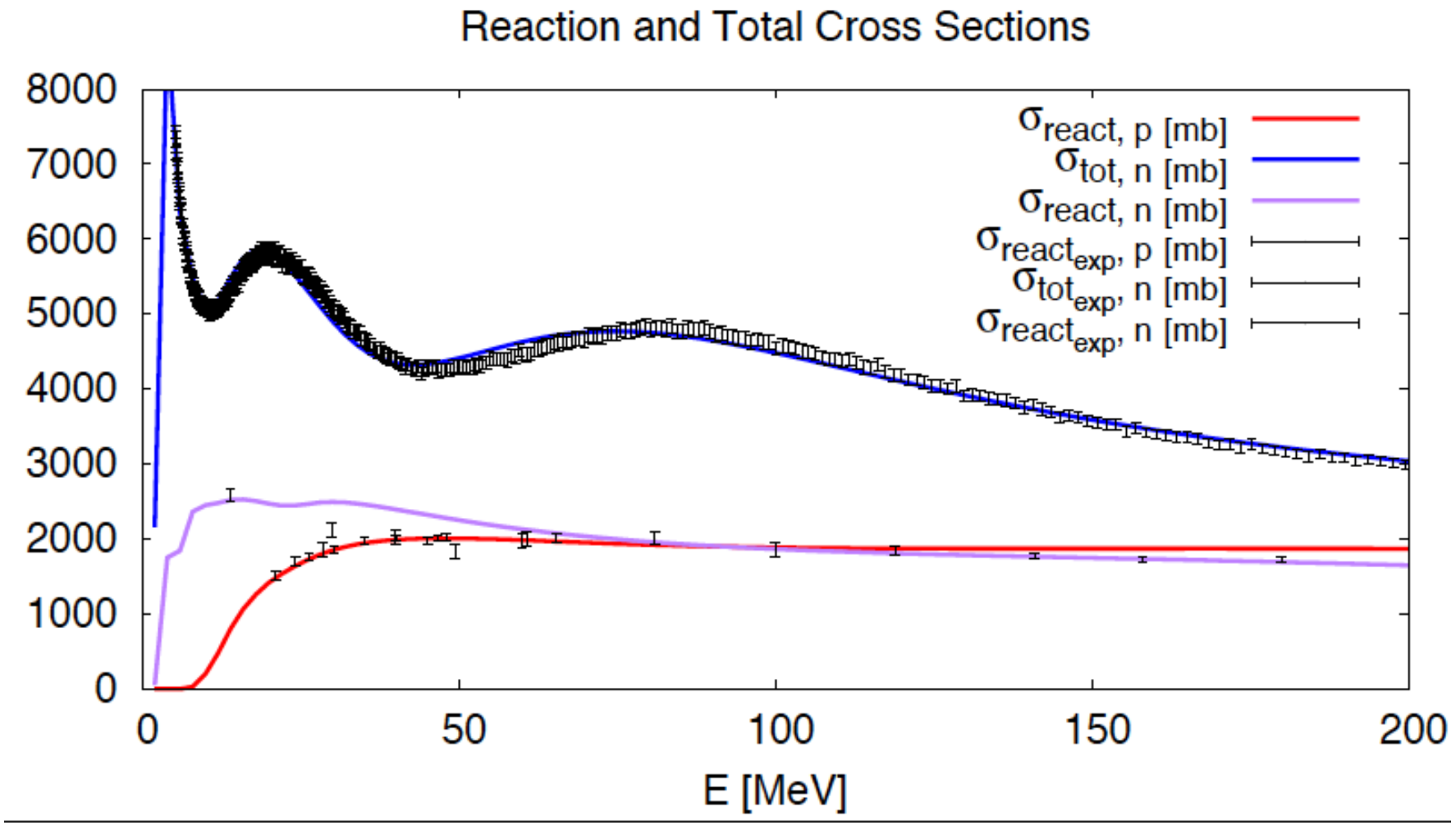
^{208}Pb Charge density and neutron skin

- Possible to get a good charge density (preliminary)



^{208}Pb (not finished)

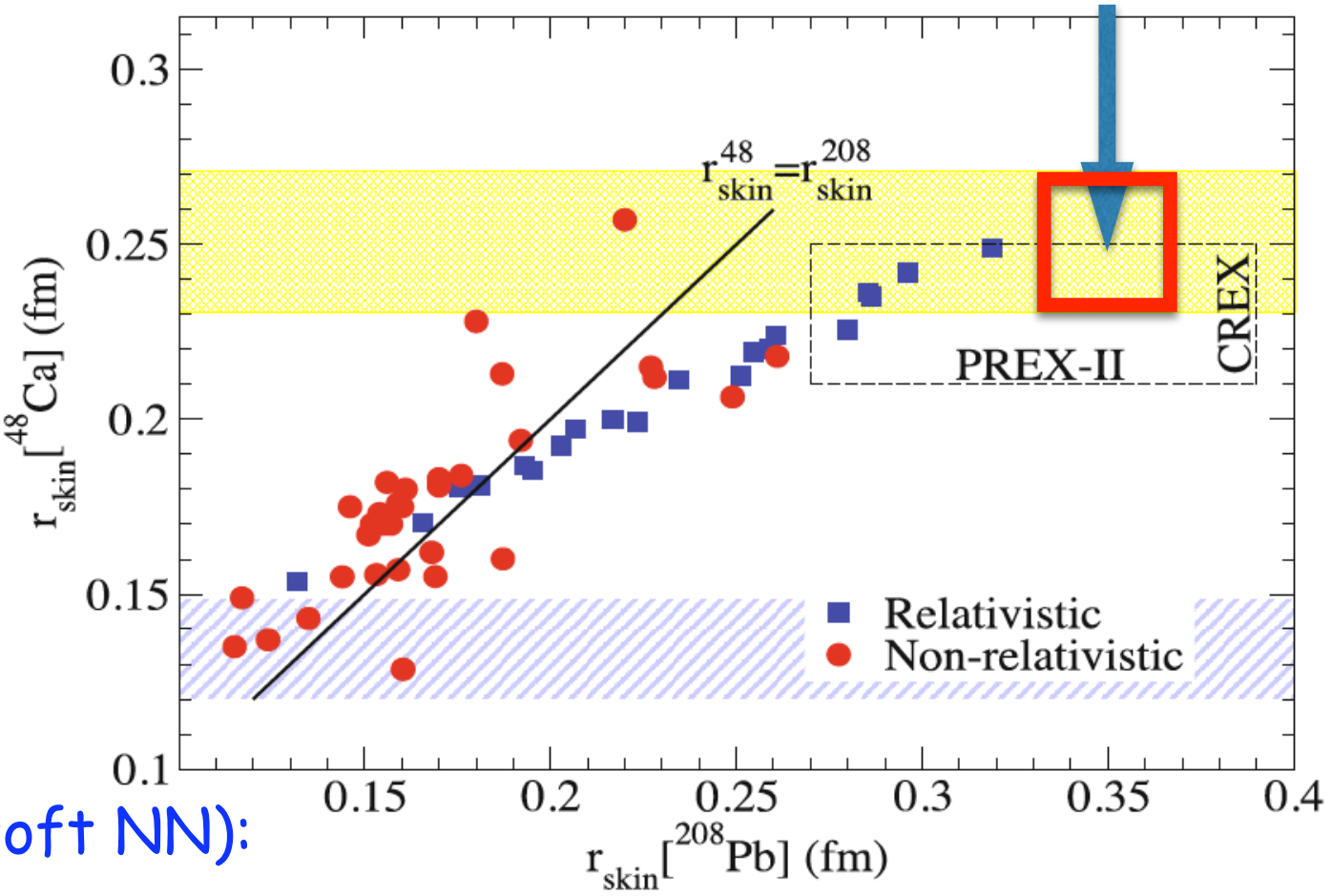
- Total neutron cross sections and proton reaction cross section



Comparison of neutron skin with other calculations and future experiments…

- Figure adapted from

C.J. Horowitz, K.S. Kumar, and R. Michaels, Eur. Phys. J. A (2014)



- Ab initio (soft NN):

G. Hagen et al., Nature Phys. 12, 186 (2016)

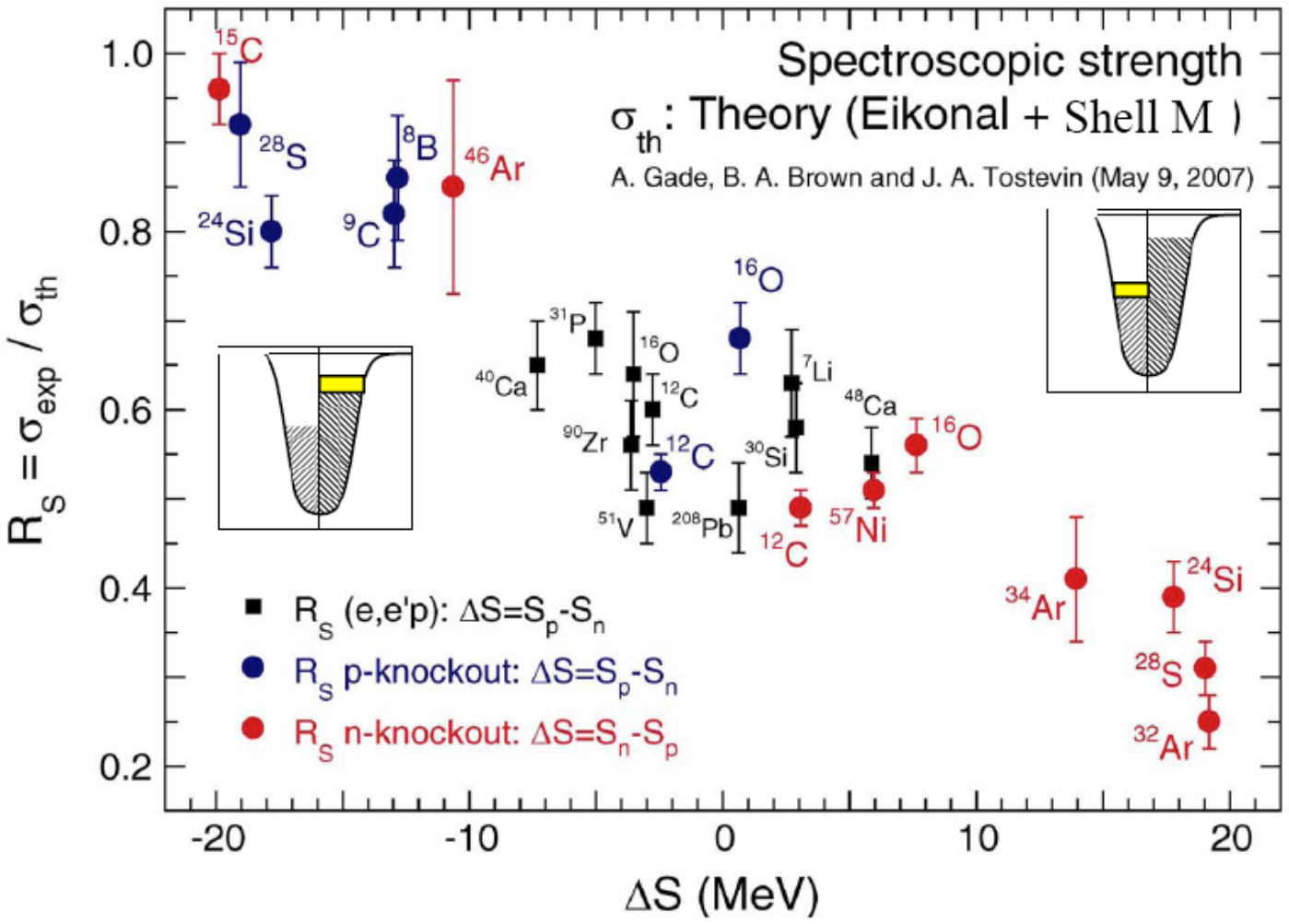
--> drip line

What about spectroscopic factors?

- Automatically generated from DOM potential
- DOM results consistent with (e,e'p) data but ~ 0.7 for ^{40}Ca
- N-Z dependence -> ^{48}Ca
- What about ^{208}Pb?
- Future predictions must include pairing considerations for open shells

Gade et al. Phys Rev C77, 044396 (2008)

Deeply-bound systems



$R_S \neq$ not spectroscopic factor

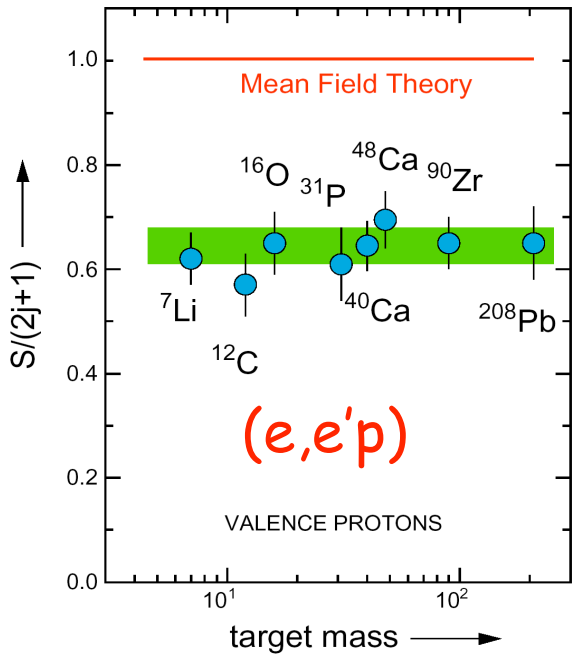
Reduction w.r.t. shell model

neutrons more correlated with increasing proton number and accompanying increasing separation energy & vice versa

⇒ Spectroscopic factors become very small; way too small?

Linking nuclear reactions and nuclear structure —> DOM

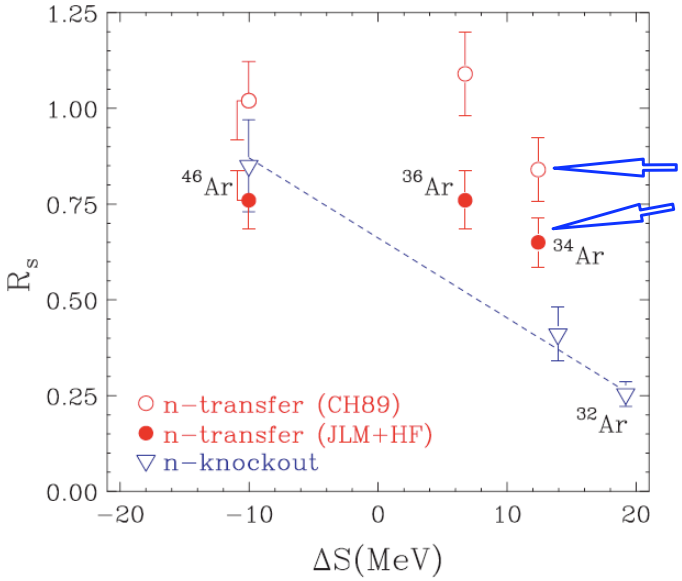
Correlations from nuclear reactions



In (e,e'p) proton still has to get out of the nucleus —> optical potential

Nucl. Phys. A553,297c (1993)

Appears more or less consistent with DOM analysis!

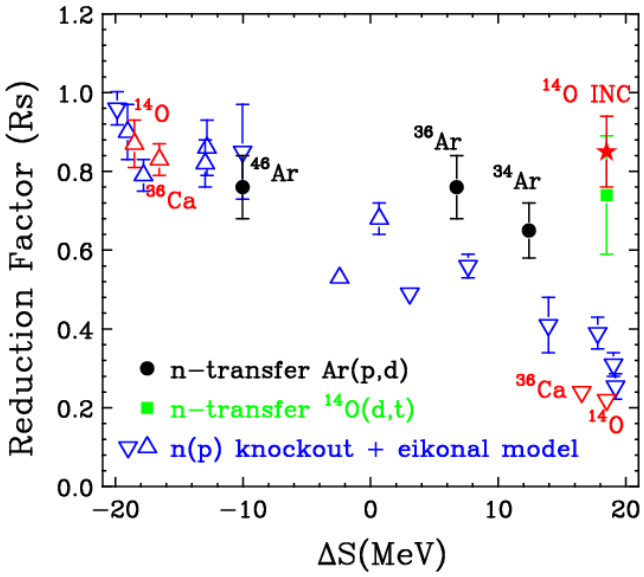


Different optical potentials --> different reduction factors for transfer reactions

Spectroscopic factors > 1 ???

PRL 93, 042501 (2004) HI

PRL 104, 112701 (2010) Transfer



Recent summary —> Jenny Lee

Different reactions different results???

Transfer reactions and the drip line

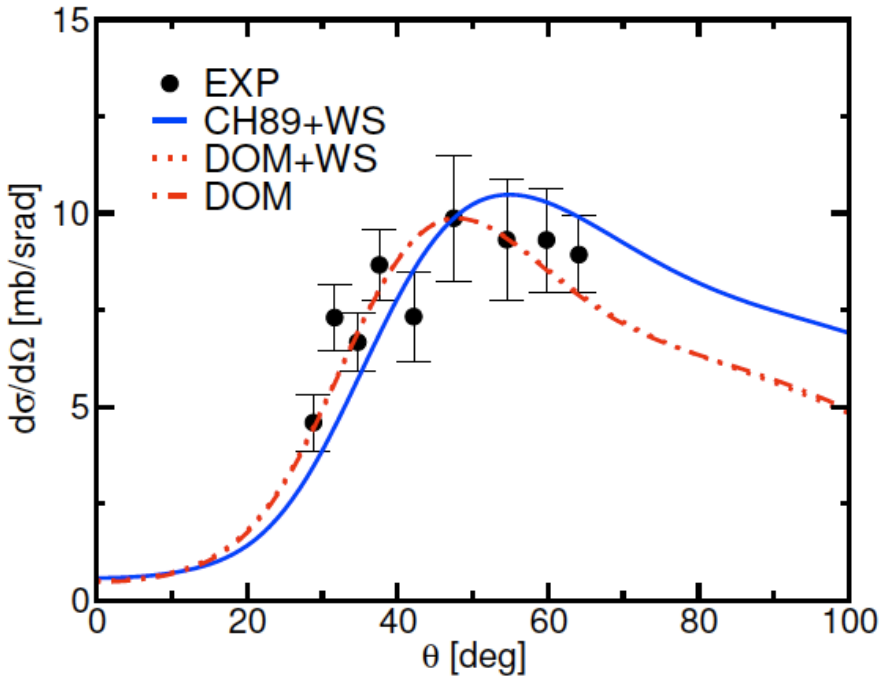
^{132}Sn(d,p)

How does it work when the potentials are extrapolated?

- Ingredients from local DOM
  - Overlap function
  - p and n optical potential
- Reaction model ADWA (Ron Johnson)
- MSU-WashU:--> N. B. Nguyen, S. J. Waldecker, F. M. Nuñes, R. J. Charity, and W. H. Dickhoff
- ^{40,48}Ca,^{132}Sn,^{208}Pb(d,p)

Phys. Rev. C84, 044611 (2011), 1-9

- Data: K.L. Jones et al., Nature 465, 454 (2010)
- E_d = 9.46 MeV ^{132}Sn(d,p)^{133}Sn
  - CH89+ws --> $S_{1f7/2}$ =1.1
  - DOM --> $S_{1f7/2}$ =0.72



Recent effort

Eur. Phys. J. A (2017) **53**: 178
DOI 10.1140/epja/i2017-12371-9

THE EUROPEAN PHYSICAL JOURNAL A

Regular Article – Theoretical Physics

Toward a complete theory for predicting inclusive deuteron breakup away from stability

G. Potel[1,a], G. Perdikakis[1,2,3,b], B.V. Carlson[4,c], M.C. Atkinson[5], W.H. Dickhoff[5], J.E. Escher[6], M.S. Hussein[4,7,8], J. Lei[9,d], W. Li[1], A.O. Macchiavelli[10], A.M. Moro[9], F.M. Nunes[1,11], S.D. Pain[12], and J. Rotureau[1]

- State of the art inclusive (d,p)
- Employs local DOM potentials constrained for ^{40}Ca and ^{48}Ca and extrapolated to ^{60}Ca
- Explores link with (n,γ) process

Why DOM?

- Compare standard optical potential with DOM

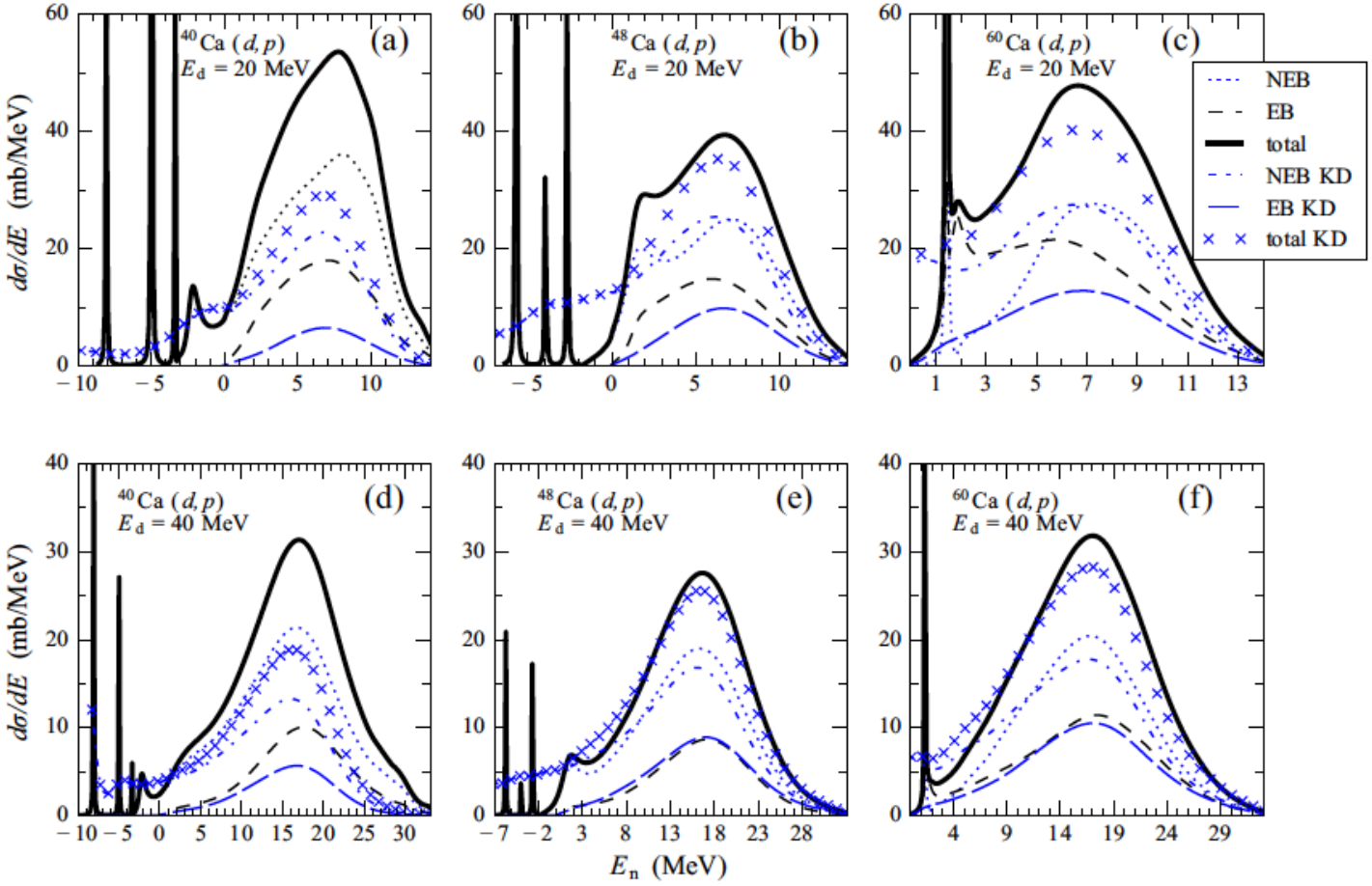


Fig. 8. Comparison of KD phenomenological optical potential and the DOM: elastic breakup (EB) and non-elastic breakup (NEB) proton spectra for the reactions ^{40}Ca(d,p), ^{48}Ca(d,p), and ^{60}Ca(d,p), at $E_d = 20$ MeV and $E_d = 40$ MeV.

- Current effort: implement nonlocal potentials and apply also to (p,d) together with Gregory Potel

Program to improve the description of the deuteron

- Present
  - Local potentials
  - Non dispersive

Collaboration with Gregory Potel

- Approach motivated by DOM for nucleons
  - p-n propagator in the medium
  - Fold with deuteron wave function
  - Directly generates deuteron elastic cross section
  - Distorted wave can be constructed
  - Use NN interaction + correction adjusted to data for p-n interaction in the medium and in-medium p and n (DOM)
  - Can start with real correction extend to dispersive one

Ongoing work

- ^{208}Pb fit —> neutron skin prediction
- ^{48}Ca(e,e'p)
- ^{112}Sn and ^{124}Sn total neutron cross sections being analyzed
- ^{64}Ni measurement of total neutron cross section just completed
- Local then nonlocal fit to Sn, and Ni isotopes
- Integrate DOM ingredients with (d,p) - (n,γ) surrogate- and (p,d) codes
- Insert correlated Hartree-Fock contribution from realistic NN interactions in DOM self-energy—> tensor force included in mean field
- Extrapolations to the respective drip lines becoming available necessitating inclusion of pairing in the DOM
- Analyze energy density as a function of density and nucleon asymmetry
- **Ab initio optical potential calculations initiated CC and Green's function method**

Conclusions

- It is possible to link nuclear reactions and nuclear structure
- Vehicle: **nonlocal** version of **Dispersive Optical Model** (Green's function method) as developed by Mahaux in a local version
- Interface between theory and experiment
- Can be used as input for analyzing nuclear reactions
- Can predict properties of exotic nuclei
- Can describe ground-state properties
  - charge density & momentum distribution
  - spectral properties including high-momentum Jefferson Lab data
- Elastic scattering determines depletion of bound orbitals
- Outlook: reanalyze many reactions with nonlocal potentials...
- For $N \geqslant Z$ sensitive to properties of neutrons —> weak charge prediction, **large neutron skin**, perhaps more...