The Green's function method as a framework for data-driven extrapolations to the dripline and the extension of the density functional methods

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Green's function method/framework

- F-RPA: V ⇒ self-energy/propagator
- QP-DFT: functionals ⇒
  computationally harder systems
- DOM: data ⇒ self-energy/propagator
  data-driven extrapolations ⇒ drip line
- Outlook

Self-consistent Green's functions

F-RPA incarnation

Faddeev Random Phase Approximation

$V_{NN} \Rightarrow$ data

- Ground state A-particle system
- Excited states for A, A±2 systems RPA
  - Low-lying
  - Giant resonances
  - ± 100 MeV from ε_F
  - A±2 (with ladders outside of configuration space)
- Feedback on sp propagator $\Rightarrow$ A±1 systems Faddeev

Developed for nuclei $\Rightarrow$ Carlo Barbieri thesis WU (2002)

Recent application: Neon atom Phys. Rev. A (2007)

Why atoms?

- DFT extension (QP-DFT) requires accurate self-energy
  in order to construct relevant functionals
- Current atomic electron self-energy and electron
  gas self-energy incompatible

  ADC(3) = *2p1h/2h1p* TDA *vs.* RPA = *GW* self-energy
- Hence F-RPA explore quality for atoms
  can resolve electron-gas conundrum

Self-consistent Green's functions and the energy of the ground state of the electron gas

GW approximation

G self-consistent sp propagator

W screened Coulomb interaction

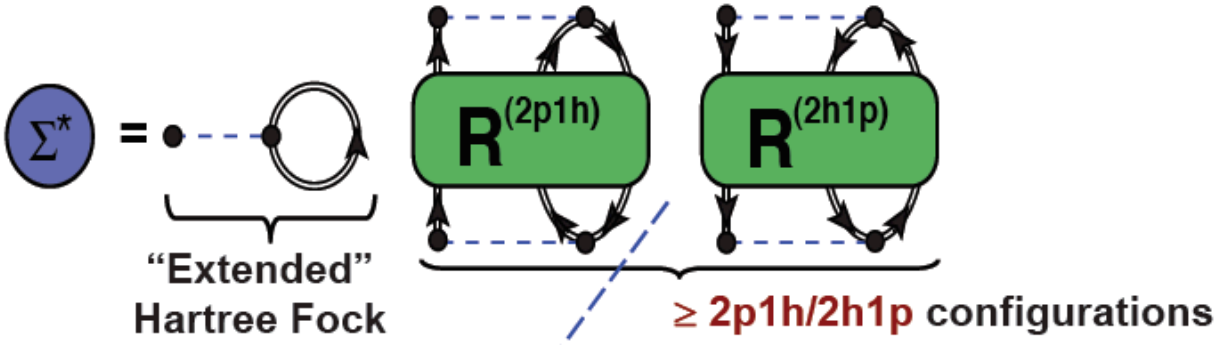
$\Rightarrow$ RPA with dressed sp propagators

Electron gas : -XC energies (Hartrees)

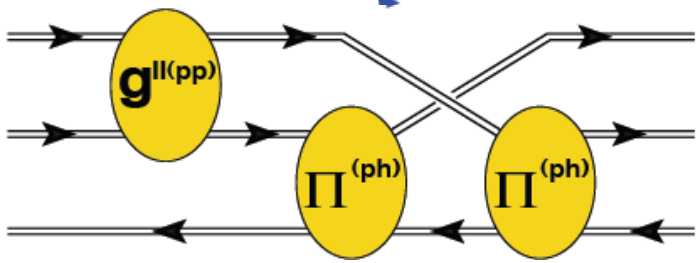
Method	r_s = 1	r_s=2	r_s=4	r_s=5	r_s=10	r_s=20	Reference
QMC	0.5180	0.2742	0.1464	0.1197	0.0644	0.0344	CA80
	0.5144	0.2729	0.1474	0.1199	0.0641	0.0344	OB94;OHB99
GW	0.5160	0.2727	0.1450	0.1185	0.0620	0.032	GG01
		0.2741	0.1465				HB98

Starting point

- Non perturbative expansion of the self-energy:



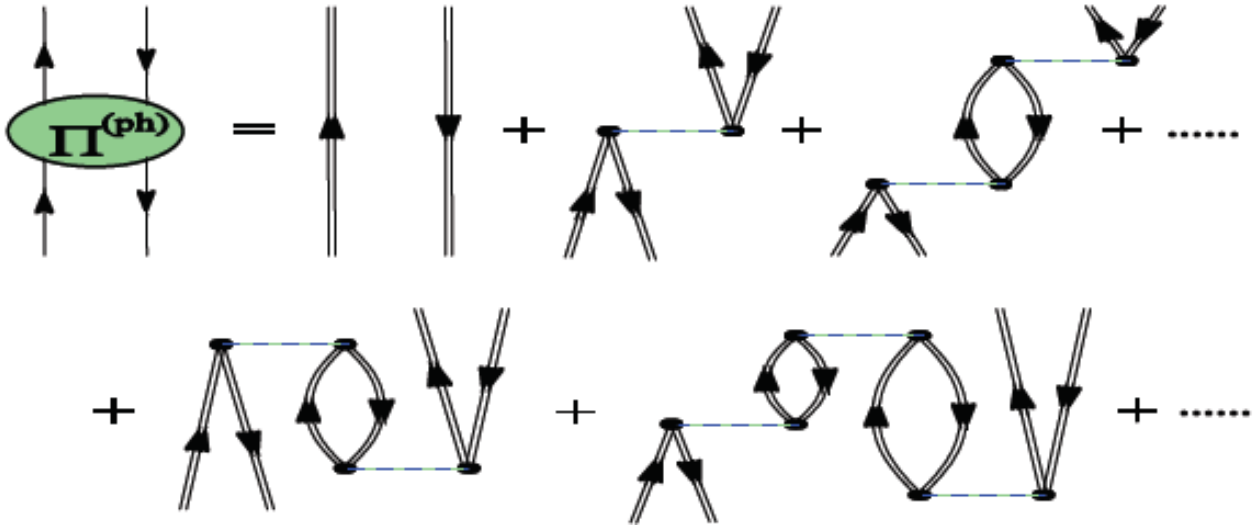
- Explicit correlations enter the "three-particle irreducible" propagators:



- Both pp (ladder) and ph (ring) modes included
- Pauli exchange at 2p1h/2h1p level

Faddeev summation of RPA propagators

Containing *e.g.*

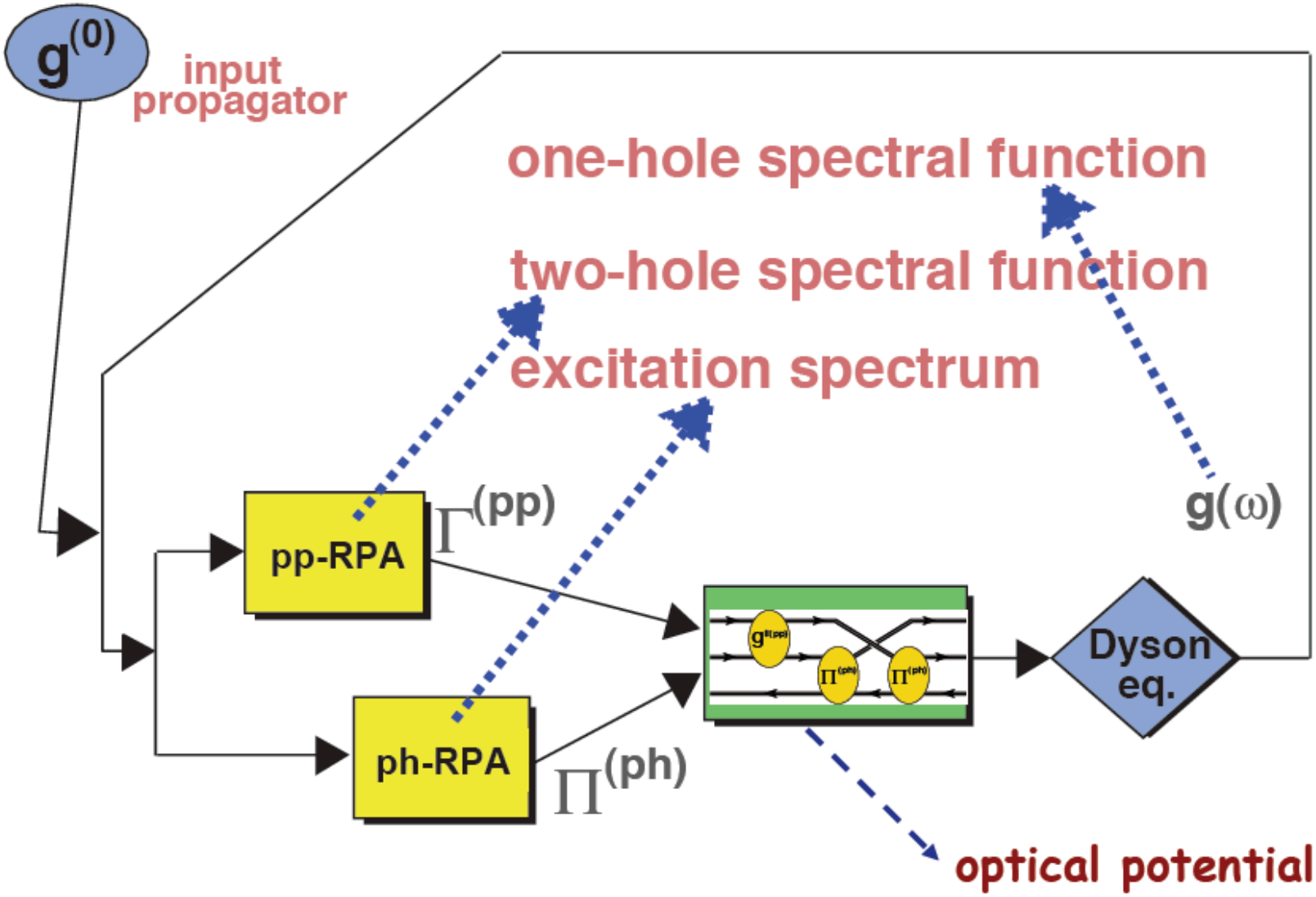


Describing excited states

Essential for the electron gas ⇒ Plasmon

But *GW* yields good total energy not a good self-energy

SCGF ⇔ F-RPA


g(0)
input propagator
one-hole spectral function
two-hole spectral function
excitation spectrum
pp-RPA
Γ(pp)
g(ω)
ph-RPA
Π(ph)
Dyson eq.
optical potential

Application to Neon atom

C. Barbieri, D. Van Neck, and WD, Phys. Rev. A, in press

	F-TDA *	F-RPA	F-TDAc	F-RPAc	Expt.
2p	-0.807	-0.799	-0.808	-0.801 (0.94)	-0.793 (0.92)
2s	-1.802	-1.792	-1.804	-1.795 (0.91)	-1.782 (0.85)
1s	-32.136	-32.097	-32.142	-32.104 (0.81)	-31.70
$E_{\rm tot}$	-128.863	-128.857	-128.883	-128.888	-128.928

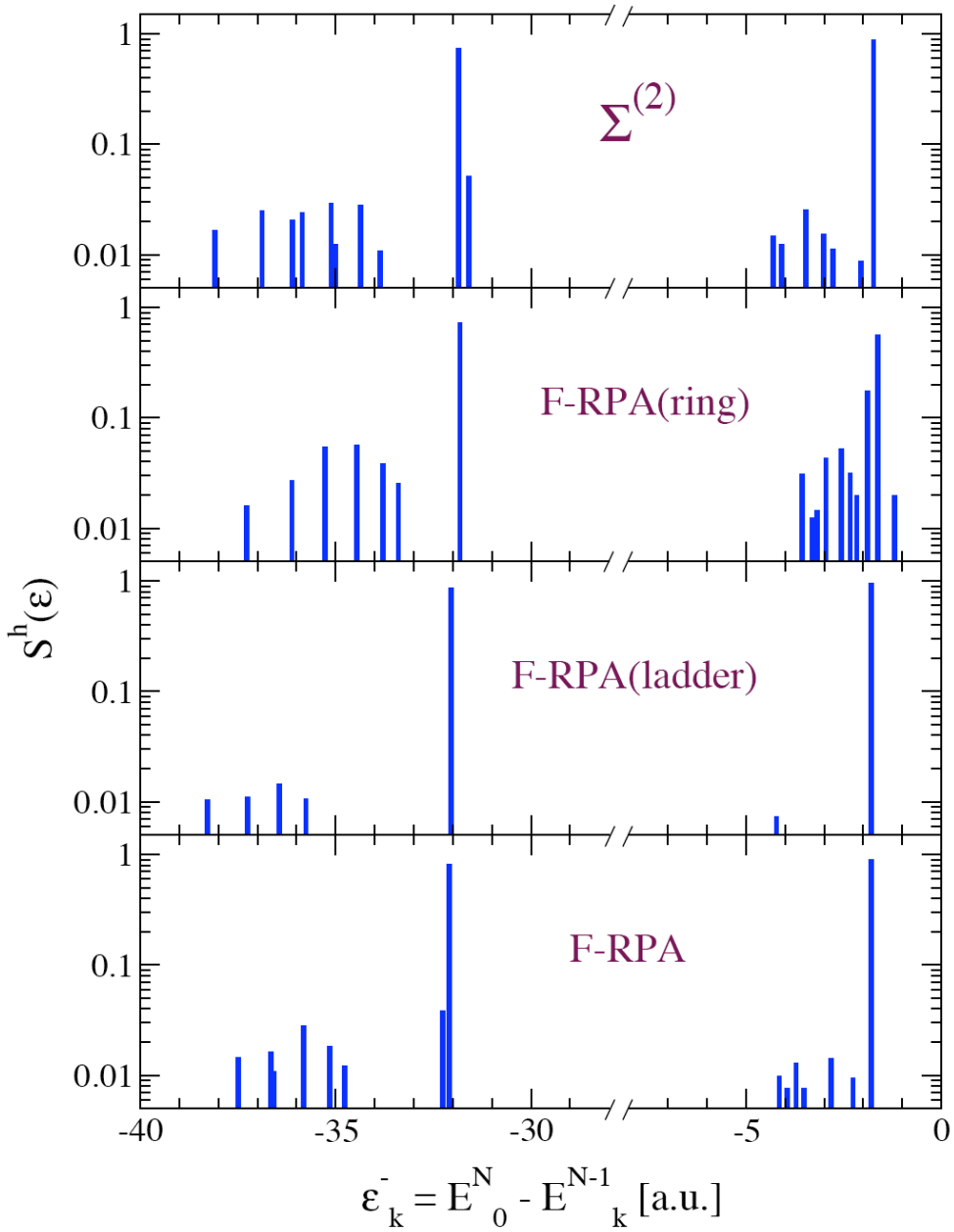
Main peaks in brackets

* Consistent with results from Heidelberg group

Some details

1s and 2s strength
Neon atom

Quasiparticles
easily identified



Analysis

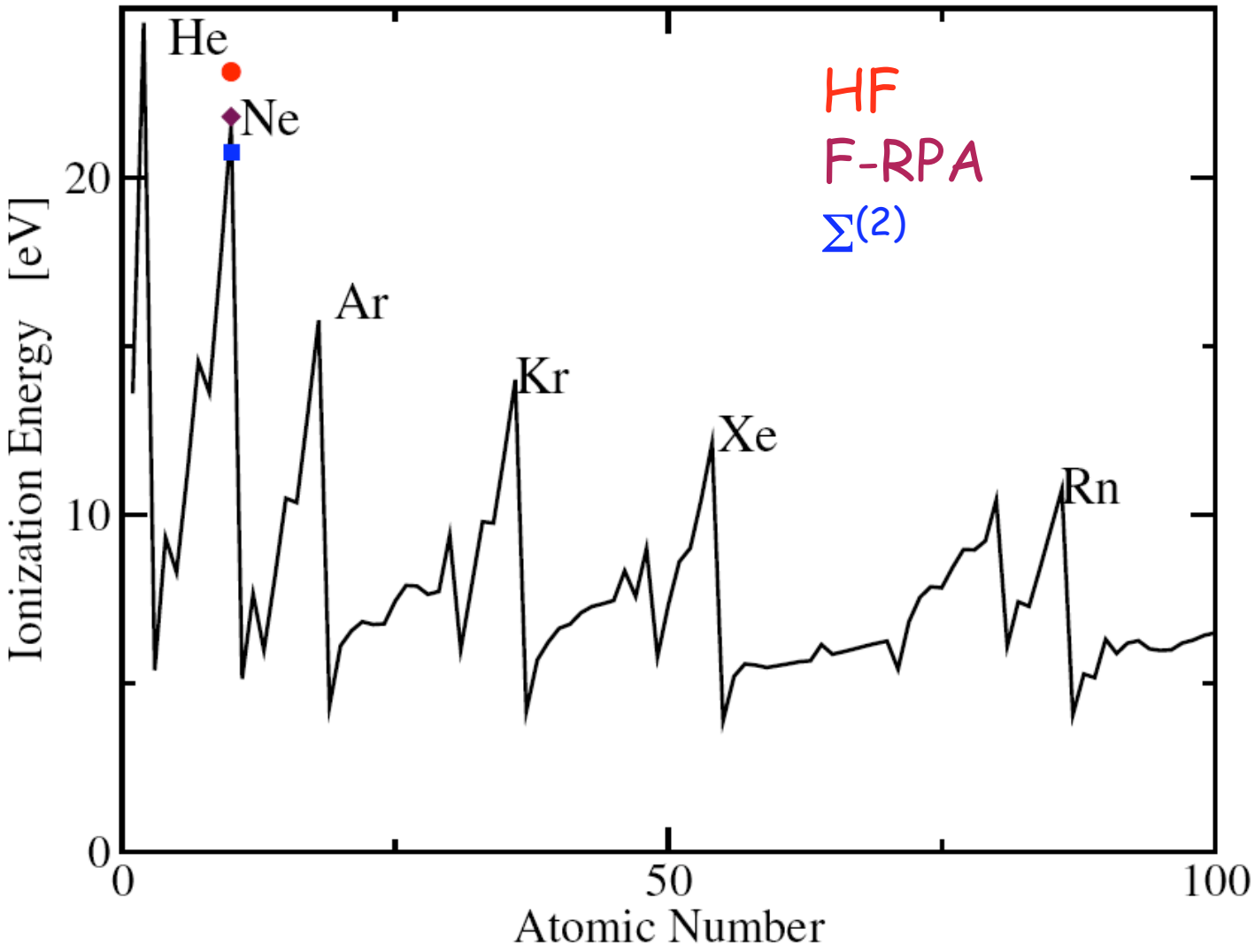
	1s	2s	2p
HF	-32.77 (1.00)	-1.931 (1.00)	-0.850 (1.00)
$\Sigma^{(2)}$	-31.84 (0.74)	-1.736 (0.88)	-0.747 (0.91)
G_0W_0	-31.14 (0.85)	-1.774 (0.91)	-0.801 (0.94)
F-RPA (ring)	-31.82 (0.73)	-1.636 (0.56)	-0.730 (0.80)
F-RPA (ladder)	-32.04 (0.87)	-1.802 (0.95)	-0.781 (0.96)
F-RPA	-32.10 (0.81)	-1.792 (0.91)	-0.799 (0.94)
Exp.	-31.70	-1.782 (0.85)	-0.793 (0.92)

Energies in hartrees (27.2 eV)

Brackets contain strength of largest fragment

Interference!

Periodic table



Quasiparticle density functional theory

QP-DFT

D.Van Neck *et al.* Phys. Rev. A74, 042501(2006)

- Kohn-Sham implementation of density functional theory "as simple" as Hartree-Fock but includes correlations beyond HF while still only solving sp equations (self-consistently)
- DFT not good for near degenerate systems characterized by small particle-hole gaps
- Wave functions not easily interpreted
- Quasiparticles (QPs) are missing from KS-DFT
- Near the Fermi energy QPs describe the physics (Landau)

Motivation ⇒

- Develop sp equations whose solutions correspond to QP orbitals and energies, including the total energy and density matrix of the system (QP-DFT) Dimitri Van Neck, U of Ghent

New framework to do self-consistent sp theory

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

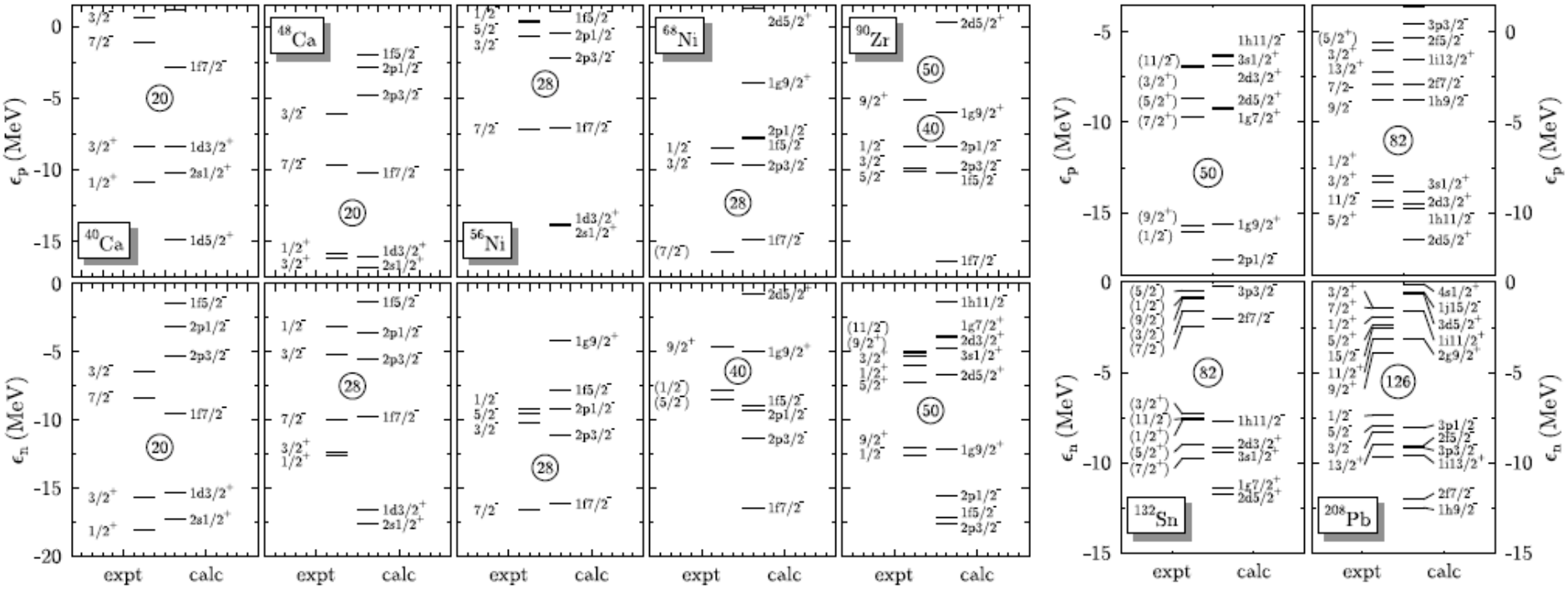
Based on separating the propagator into a quasiparticle part and a background, expressing only the latter as a functional of the density matrix.
⇒ in addition yields qp energies and overlap functions

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

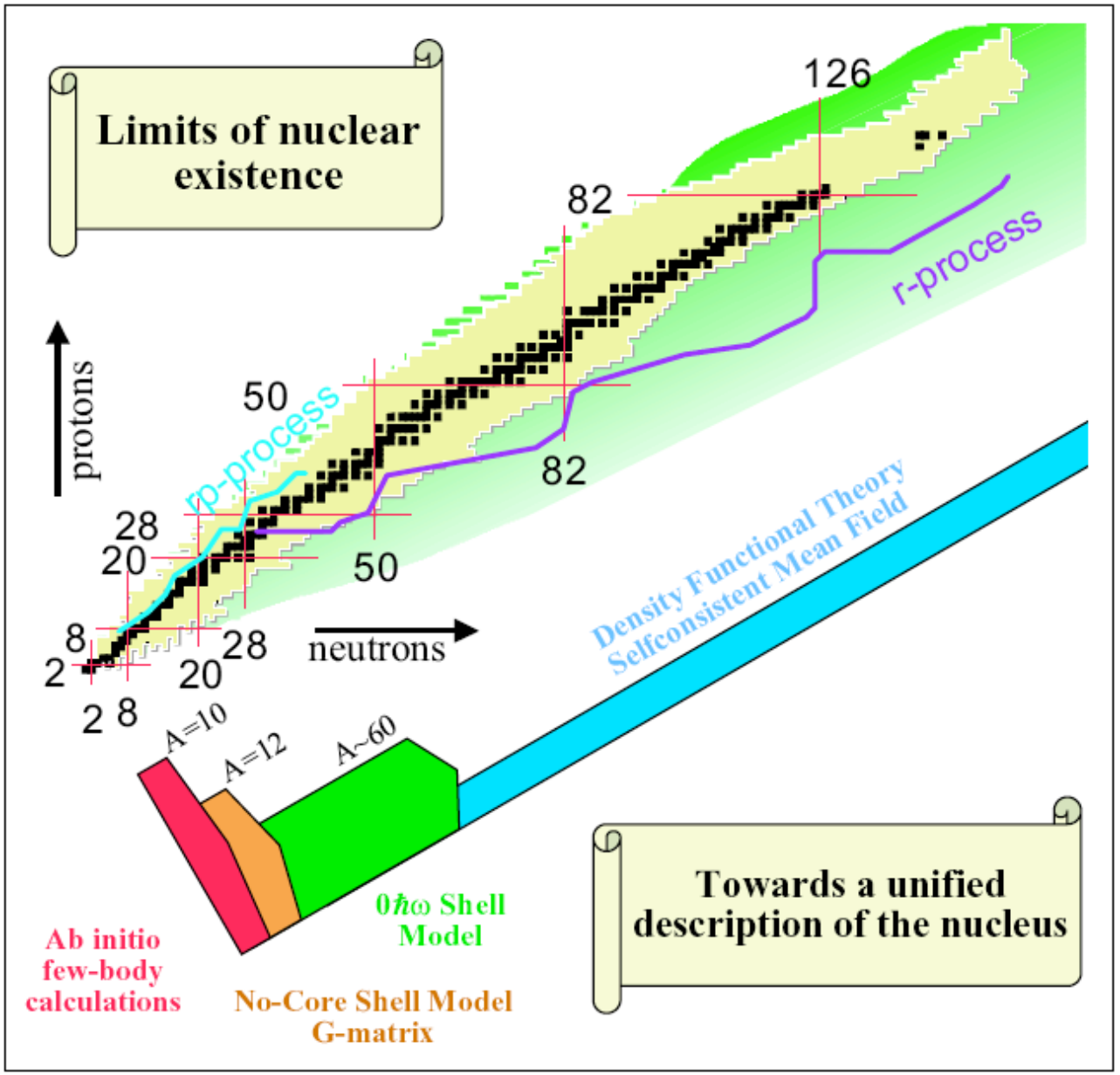
While ground-state energies are closer to exp in DFT than in HF

"Single-particle energies" from mean-field/DFT calculations of nuclei



M.Bender slide JUSTIPEN workshop Oak Ridge, March 2007

Chart of nuclides



Interpretation: Nazarewicz

Fourier transform of G (Lehmann representation)

$$G(\alpha,\beta;E) = \left\langle \Psi_0^N \middle| a_\alpha \frac{1}{E-\left(\hat{H}-E_0^N\right)+i\eta} a_\beta^\dagger \middle| \Psi_0^N \right\rangle \quad \Leftarrow \text{Particle part}$$

$$+\left\langle \Psi_0^N \middle| a_\beta^\dagger \frac{1}{E+\left(\hat{H}-E_0^N\right)-i\eta} a_\alpha \middle| \Psi_0^N \right\rangle \quad \Leftarrow \text{Hole part}$$

$$= \sum_n \frac{\left\langle \Psi_0^N \middle| a_\alpha \middle| \Psi_n^{N+1} \right\rangle \left\langle \Psi_n^{N+1} \middle| a_\beta^\dagger \middle| \Psi_0^N \right\rangle}{E-\left(E_n^{N+1}-E_0^N\right)+i\eta} + \sum_n \frac{\left\langle \Psi_0^N \middle| a_\beta^\dagger \middle| \Psi_n^{N-1} \right\rangle \left\langle \Psi_n^{N-1} \middle| a_\alpha \middle| \Psi_0^N \right\rangle}{E+\left(E_n^{N-1}-E_0^N\right)-i\eta}$$

$$= \sum_n \frac{\left(z_n^{(+)}\right)_\alpha \left(z_n^{(+)}\right)_\beta^*}{E-\varepsilon_n^{(+)}+i\eta} + \sum_n \frac{\left(z_n^{(-)}\right)_\alpha \left(z_n^{(-)}\right)_\beta^*}{E-\varepsilon_n^{(-)}-i\eta}$$

Poles $\varepsilon_n^{(+)}$ in addition domain $\left(\varepsilon_0^{(+)},+\infty\right)$

Poles $\varepsilon_n^{(-)}$ in addition domain $\left(-\infty,\varepsilon_0^{(-)}\right)$

Density and Removal Energy Matrices

One-body density matrix

$$N^{(-)}_{\alpha,\beta} = \int \frac{dE}{2\pi i} e^{i\eta E} G(\alpha,\beta;E) = \sum_n \left(z_n^{(-)}\right)_\alpha \left(z_n^{(-)}\right)^*_\beta = \left\langle \Psi_0^N \left| a^\dagger_\beta a_\alpha \right| \Psi_0^N \right\rangle$$

Removal energy matrix

$$M^{(-)}_{\alpha,\beta} = \int \frac{dE}{2\pi i} e^{i\eta E} E\, G(\alpha,\beta;E) = \sum_n \varepsilon_n^{(-)} \left(z_n^{(-)}\right)_\alpha \left(z_n^{(-)}\right)^*_\beta = \left\langle \Psi_0^N \left| a^\dagger_\beta \left[a_\alpha, \hat{H} \right] \right| \Psi_0^N \right\rangle$$

Removal part of propagator yields any one-body observable plus

$$E_0^N = \frac{1}{2} Tr\left([H_0][N^{(-)}] + [M^{(-)}] \right)$$ the total energy (Migdal-Galitskii)

Spectral function

Single-particle spectral function

$$\left[S(E)\right] = \frac{1}{2\pi i} sign(\varepsilon_F - E)\left(\left[G(E)\right] - \left[G(E)\right]^{\dagger}\right)$$

$$= \sum_n \left(z_n^{(+)}\right)\left(z_n^{(+)}\right)^{\dagger} \delta\left(E - \varepsilon_n^{(+)}\right) + \sum_n \left(z_n^{(-)}\right)\left(z_n^{(-)}\right)^{\dagger} \delta\left(E - \varepsilon_n^{(-)}\right)$$

Sum rules

$$N_{\alpha,\beta} = \int_{-\infty}^{+\infty} dE\ S(\alpha,\beta;E) = \left\langle \Psi_0^N \left| \left\{ a_\beta^{\dagger}, a_\alpha \right\} \right| \Psi_0^N \right\rangle$$

$$M_{\alpha,\beta} = \int_{-\infty}^{+\infty} dE\ E\ S(\alpha,\beta;E) = \left\langle \Psi_0^N \left| \left\{ a_\beta^{\dagger}, \left[a_\alpha, \hat{H} \right] \right\} \right| \Psi_0^N \right\rangle$$

Integrations over the entire energy axis

Split integration

$$N_{\alpha,\beta} = \int_{-\infty}^{\varepsilon_F} dE\ S(\alpha,\beta;E) + \int_{\varepsilon_F}^{+\infty} dE\ S(\alpha,\beta;E) = N_{\alpha,\beta}^{(-)} + N_{\alpha,\beta}^{(+)}$$

and similarly for

$$M_{\alpha,\beta} = \int_{-\infty}^{\varepsilon_F} dE\ E\ S(\alpha,\beta;E) + \int_{\varepsilon_F}^{+\infty} dE\ E\ S(\alpha,\beta;E) = M_{\alpha,\beta}^{(-)} + M_{\alpha,\beta}^{(+)}$$

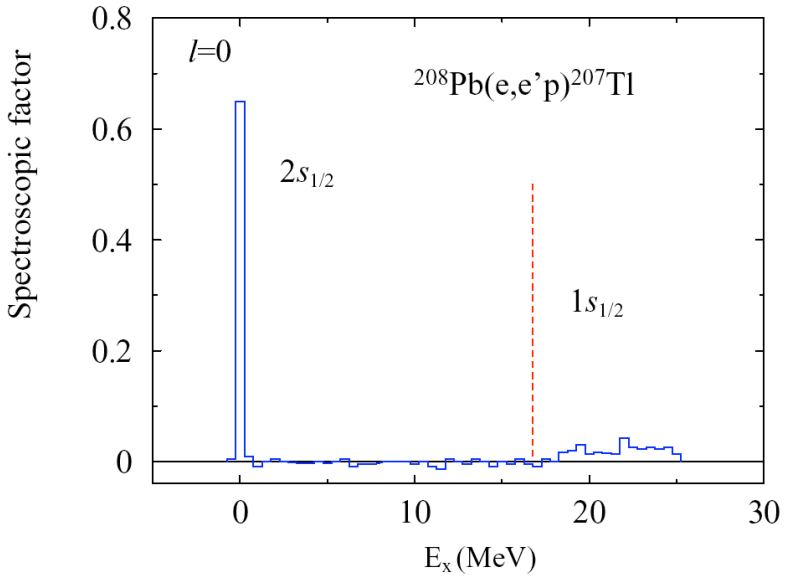
Evaluating (anti)commutators (previous slide) sum rule can be written in closed form

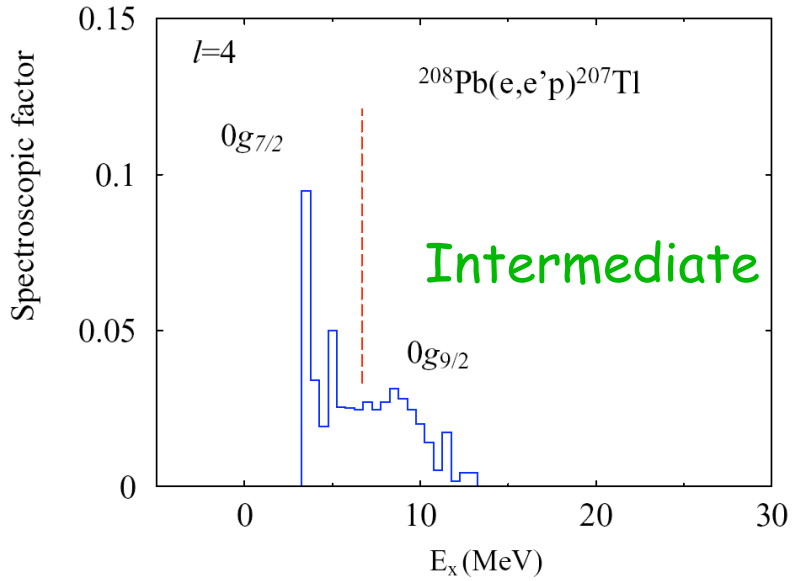
$$N_{\alpha,\beta} = \delta_{\alpha,\beta} \quad \text{or} \quad [N] = [I]$$

and $$M_{\alpha,\beta} = \langle \alpha | H_0 | \beta \rangle + \sum_{\gamma\delta} \langle \alpha\gamma | V | \beta\delta \rangle N_{\delta\gamma}^{(-)} \quad \text{or} \quad [M] = [H_0] + [\tilde{V}_{HF}]$$

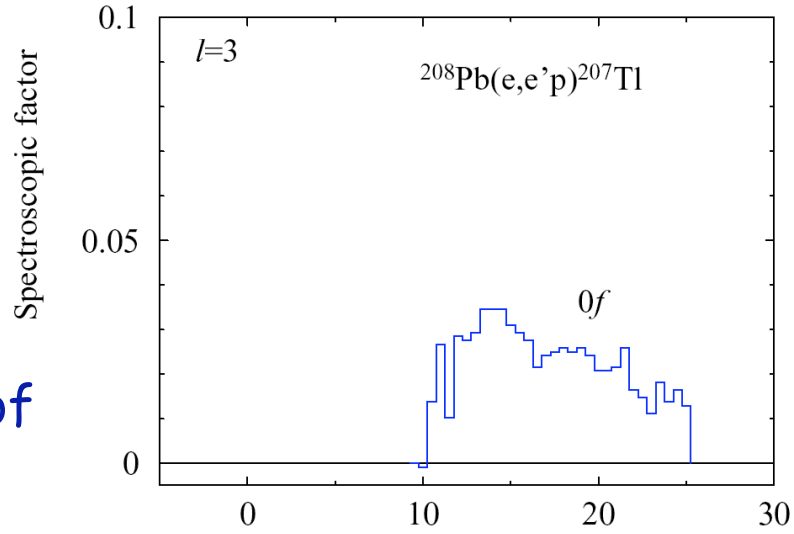
Quasiholes in nuclei

E. Quint, Ph.D.thesis NIKHEF, 1988





Quasihole strength or
spectroscopic factor $Z(2s_{1/2})$=0.65
$n(2s_{1/2})$ = 0.75
from elastic electron scattering



Strong fragmentation of
deeply-bound states

F-RPA, DOM and QP-DFT 20

Main result: QP equations

Require background contributions $\left[M_B^{\pm}\right]$

$\left[N_B^{\pm}\right]$

as functional of the density matrix $\left[N^{(-)}\right]$ to obtain

$$\left(\left[H_0\right]+\left[\tilde{V}_{HF}\left\{N^{(-)}\right\}\right]-\left[M_B\left\{N^{(-)}\right\}\right]\right)u_j=\varepsilon_{Qj}\left(\left[I\right]-\left[N_B\left\{N^{(-)}\right\}\right]\right)u_j$$

Then eigenvalue problem can be solved yielding QP energies ε_{Qj}

and QP orbits $z_{Qj}=\left(\left[I\right]-\left[N_B\left\{N^{(-)}\right\}\right]\right)u_j$

$$\left[N\right]=\left[N_Q\right]+\left[N_B\right]$$

$$\left[M\right]=\left[M_Q\right]+\left[M_B\right]$$

$$\left[N_Q^{(-)}\right]=\sum_{j=1}^{N}z_{Qj}z_{Qj}^{\dagger}\qquad\left[N_Q^{(+)}\right]=\sum_{j=N+1}^{\infty}z_{Qj}z_{Qj}^{\dagger}$$

$$\left[M_Q^{(-)}\right]=\sum_{j=1}^{N}\varepsilon_{Qj}z_{Qj}z_{Qj}^{\dagger}\qquad\left[M_Q^{(+)}\right]=\sum_{j=N+1}^{\infty}\varepsilon_{Qj}z_{Qj}z_{Qj}^{\dagger}$$

Procedure

Initial estimate for $\left[N^{(-)}\right]$ allows construction of $\left[N_B\right]$ and $\left[M_B\right]$ but also $\left[\tilde{V}_{HF}\right]$

N lowest energy solutions belong in *N*-1 and can be used to update the density matrix

$$\left[N_{new}^{(-)}\right] = \sum_{j=1}^{N} z_{Qj} z_{Qj}^{\dagger} + \left[N_B^{(-)}\left\{N^{(-)}\right\}\right]$$

closing the self-consistency loop!

Total energy follows from

$$E_0^N = \frac{1}{2}\sum_{j=1}^{N} z_{Qj}^{\dagger}\left(\left[H_0\right] + \varepsilon_{Qj}\right) z_{Qj} + \frac{1}{2} Tr\left(\left[H_0\right]\left[N_B^{(-)}\left\{N^{(-)}\right\}\right] + \left[M_B^{(-)}\left\{N^{(-)}\right\}\right]\right)$$

Comments

- Formalism generates total energy, density matrix, and individual QP energies and orbits (with correct spectroscopic factors) starting from a representation for the background contributions $[M_B^{(\pm)}]$ and $[N_B^{(\pm)}]$ as a functional of the density matrix.
- M_B plays different role in nuclear systems as compared to electronic systems (responsible for attraction that binds system)
- F-RPA for atoms provides complete electron self-energy
- Recent work on modeling the complete nucleon self-energy $\Rightarrow$ DOM (Charity *et al.*) provides information to generate functionals near and at intermediate energies from the Fermi energy
- Intermediate implementations are possible

  $\Rightarrow$ adapt Skyrme functional approach
- Formalism includes *HF* and *KS-DFT* (see Van Neck paper)

DOM = Dispersive Optical Model

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

Green's function formulation "Mahaux analysis"

goal: extract propagator from data

- Data-driven extrapolations / predictions to the dripline
- Input to QP-DFT for nuclei based on data

FRAMEWORK FOR EXTRAPOLATIONS BASED ON EXPERIMENTAL DATA

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), in press.

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!

Correlations for nuclei with N very different from Z?

⇒ Radioactive beam facilities

Nuclei are TWO-component Fermi liquids

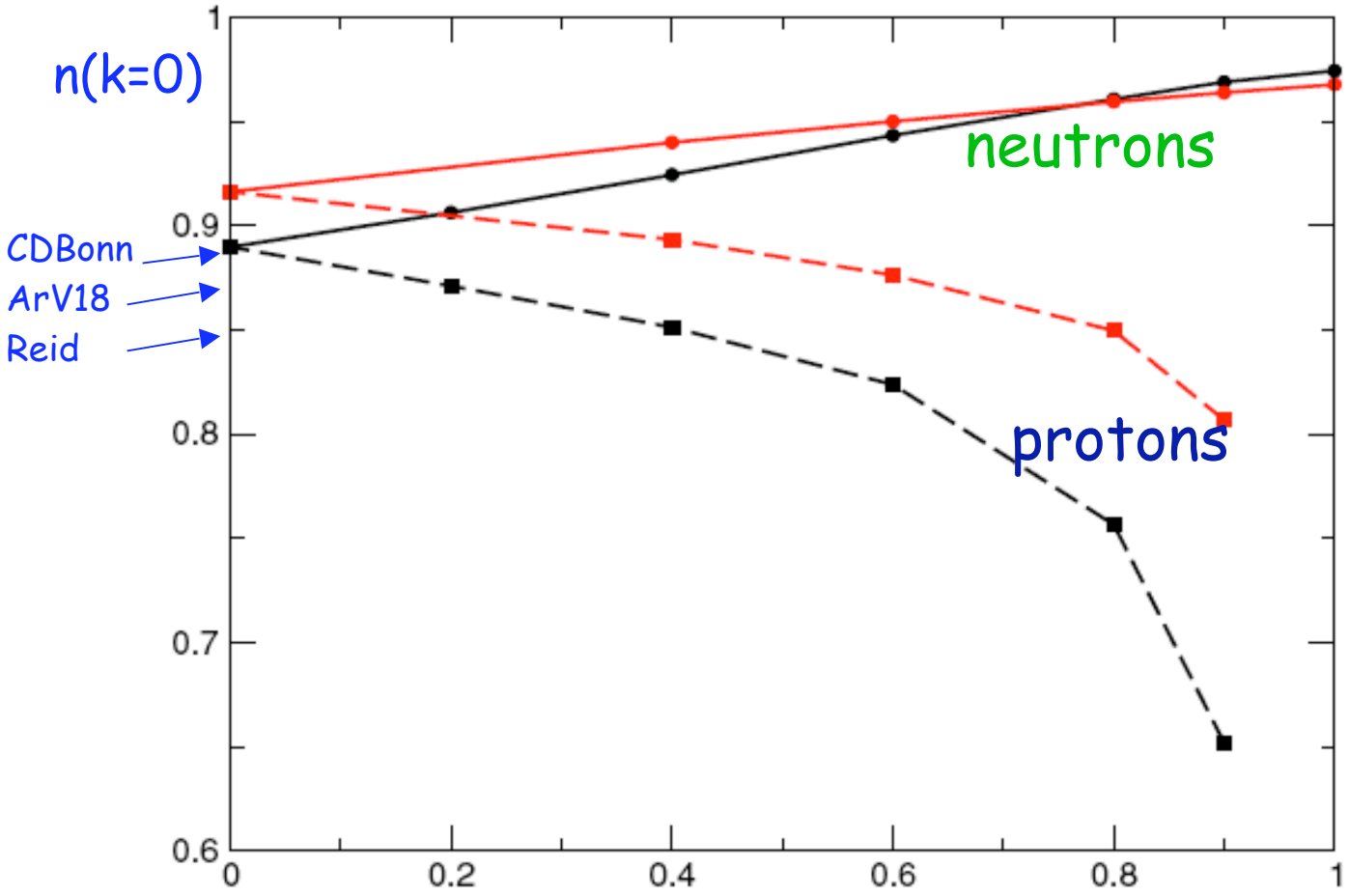
- SRC about the same between pp, np, and nn
- Tensor force disappears for n when N >> Z but …

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

Some pointers: both from theory and experiment

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

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



0.16 fm^{-3}

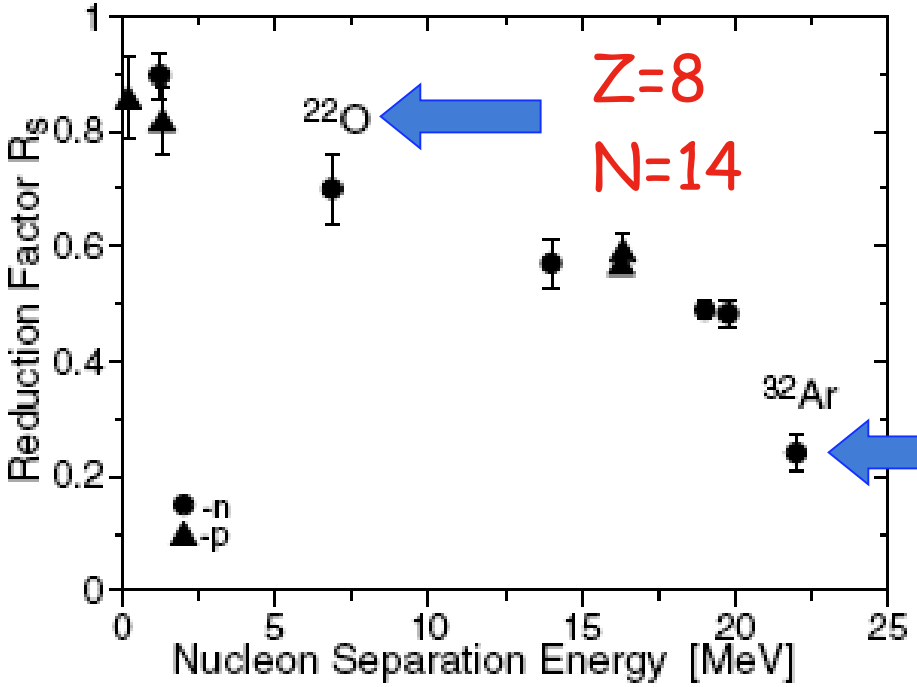
0.32 fm^{-3}

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)



Z=8
N=14

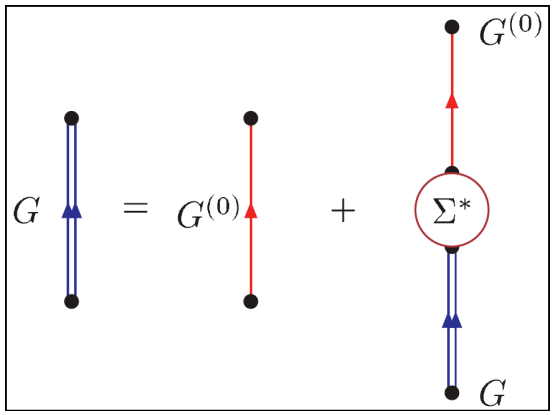
Z=18
N=14

$R_S \neq$ 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

⇒ as observed in (e,e'p)

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

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

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*

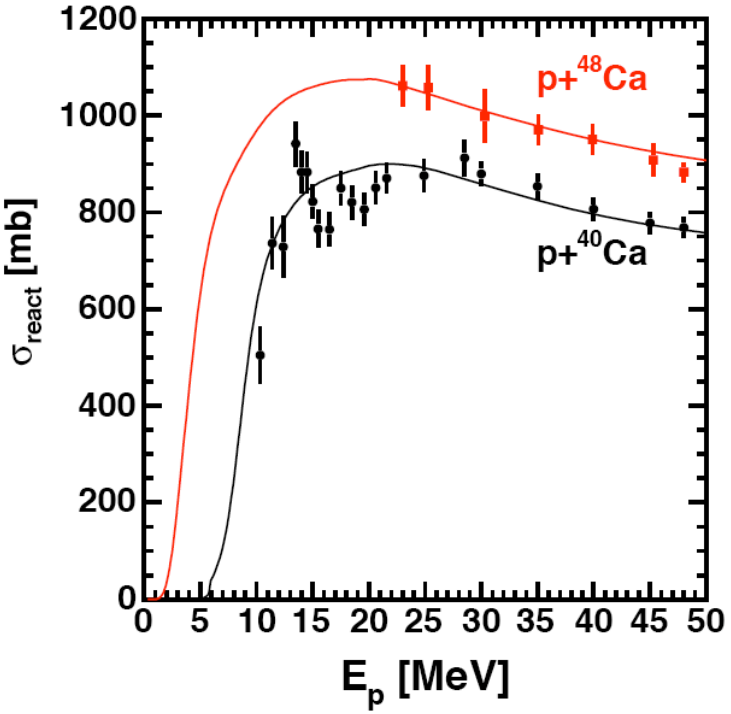
$$\left\langle\Psi_0^{N}\middle|a_{\vec{r}m}\middle|\Psi_k^{N+1}\right\rangle=\psi_k^{N+1}(\vec{r}m)$$ *Bound states in N+1*

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

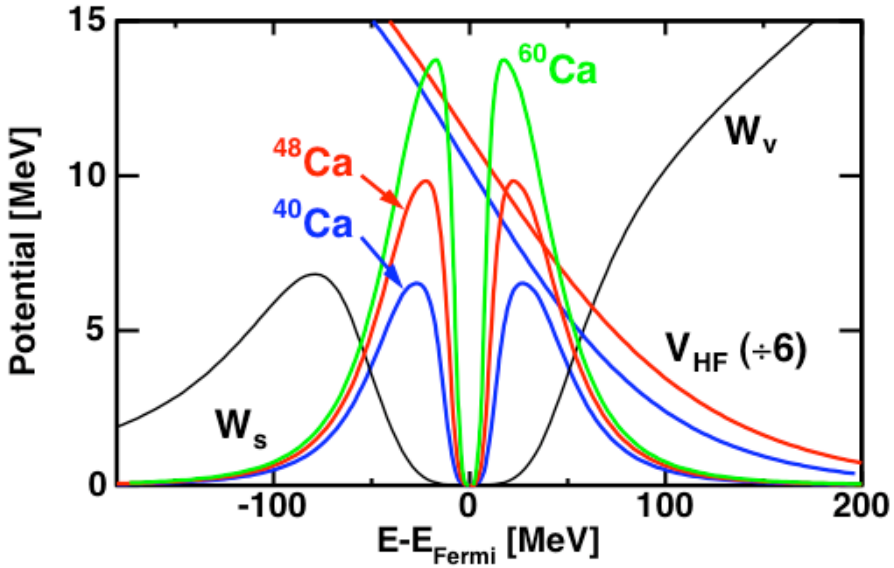
Reaction cross section ^{40}Ca and ^{48}Ca



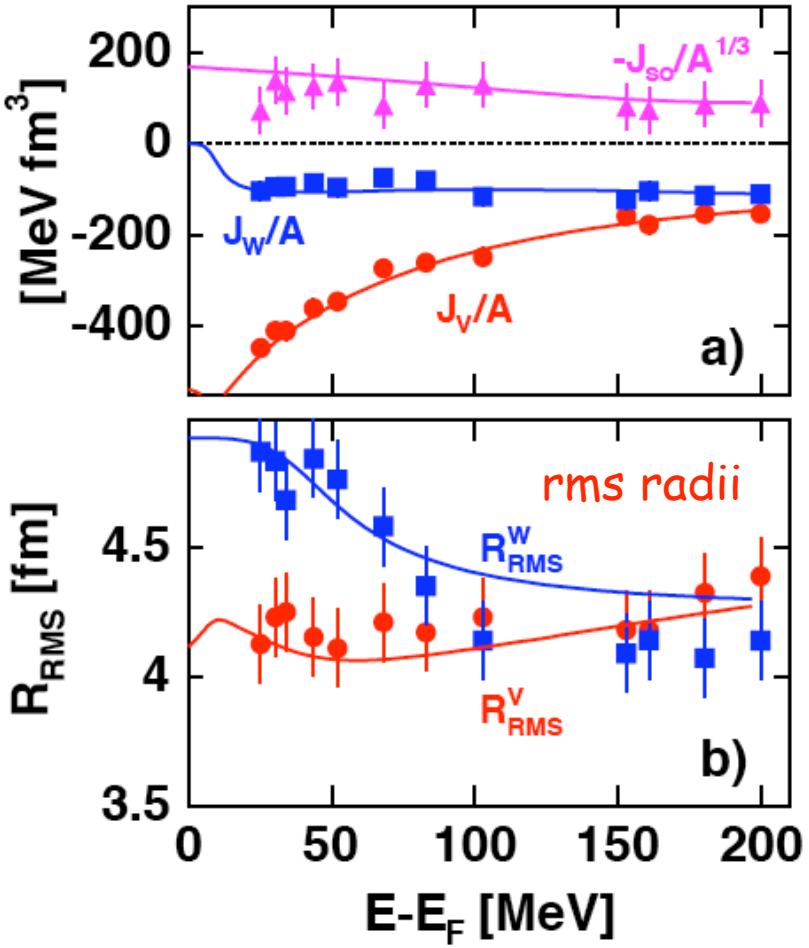
Loss of flux in the elastic channel

Potentials

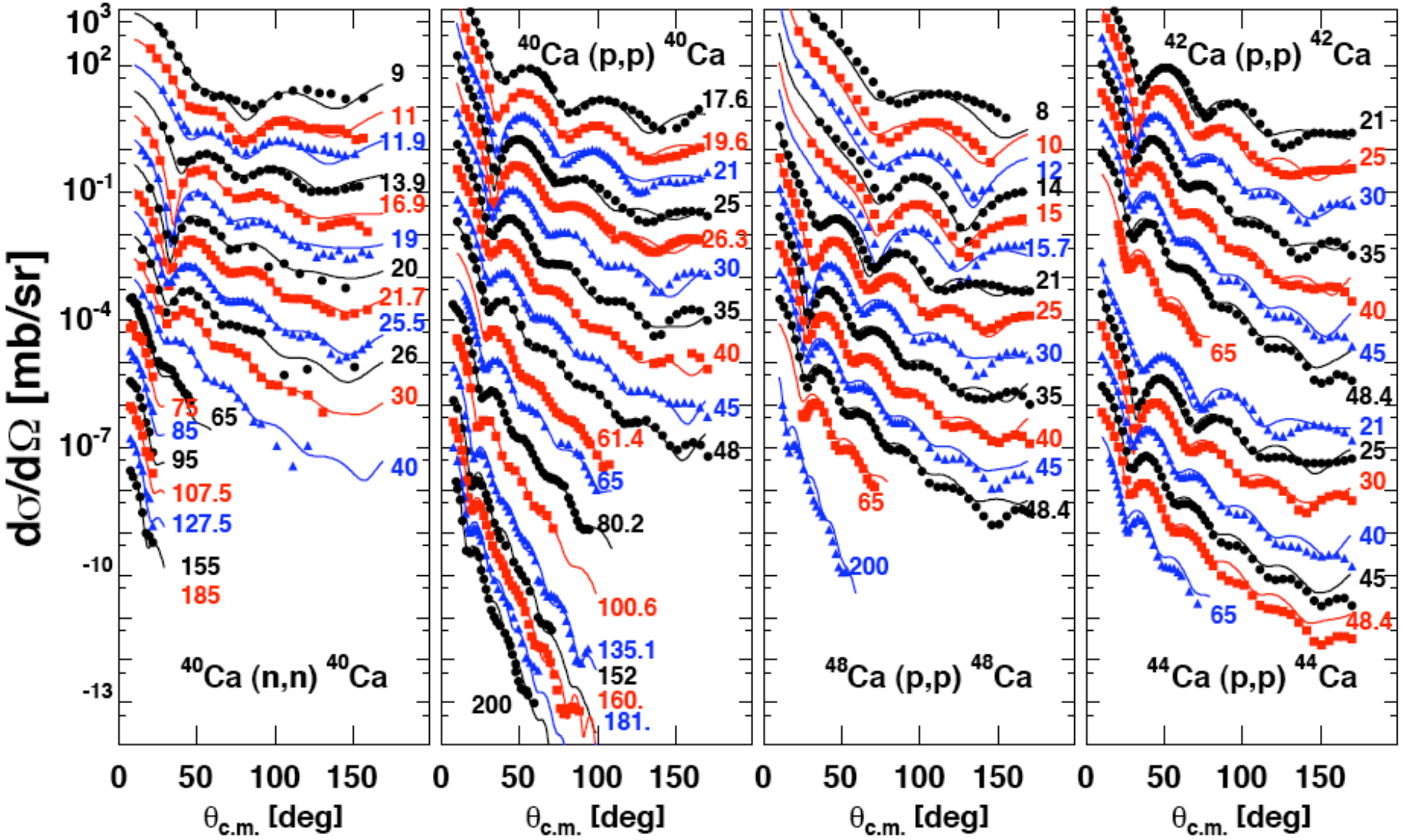
Surface potential strengthens with increasing asymmetry for protons



Volume integrals

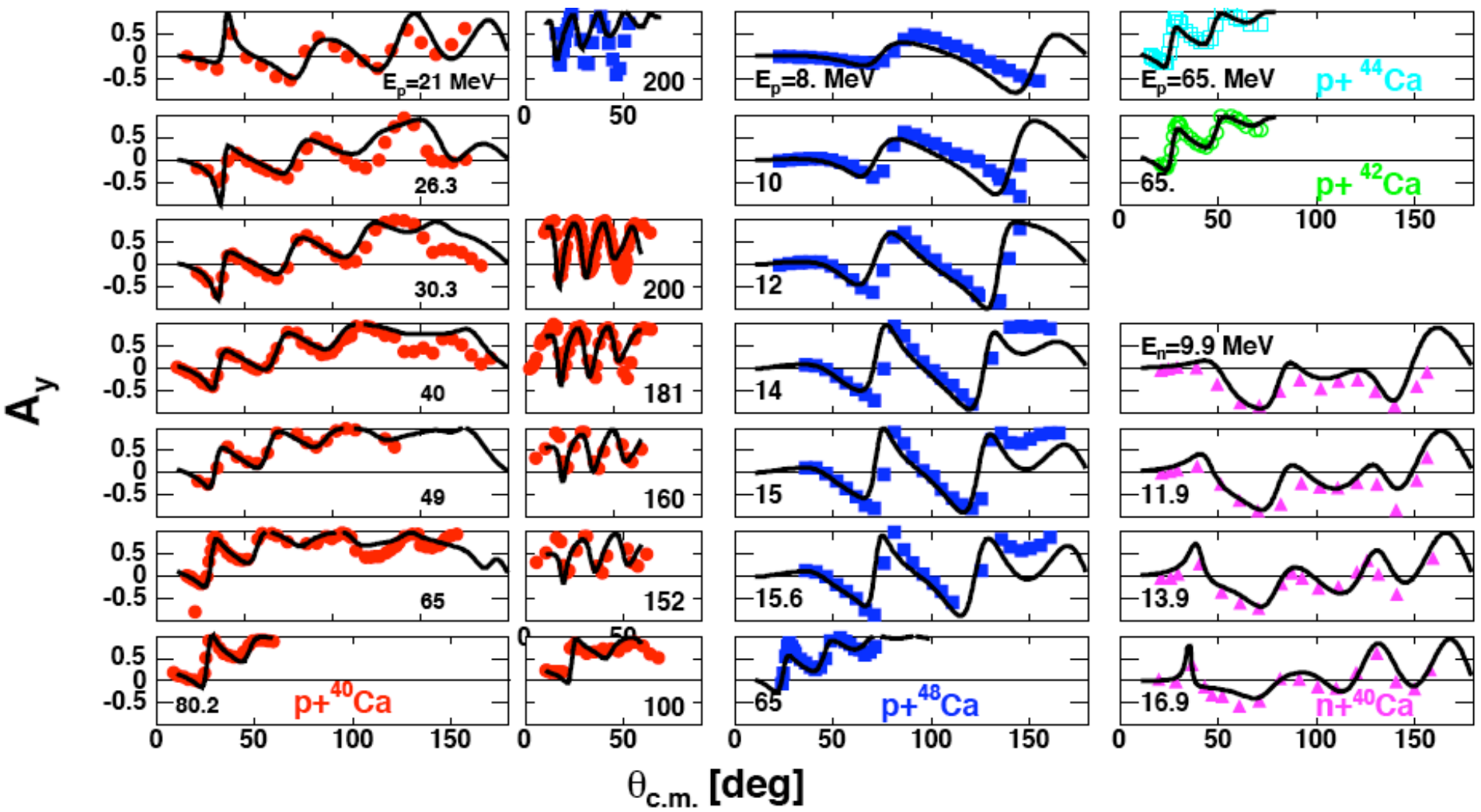


Fit and predictions of n & p elastic scattering cross sections

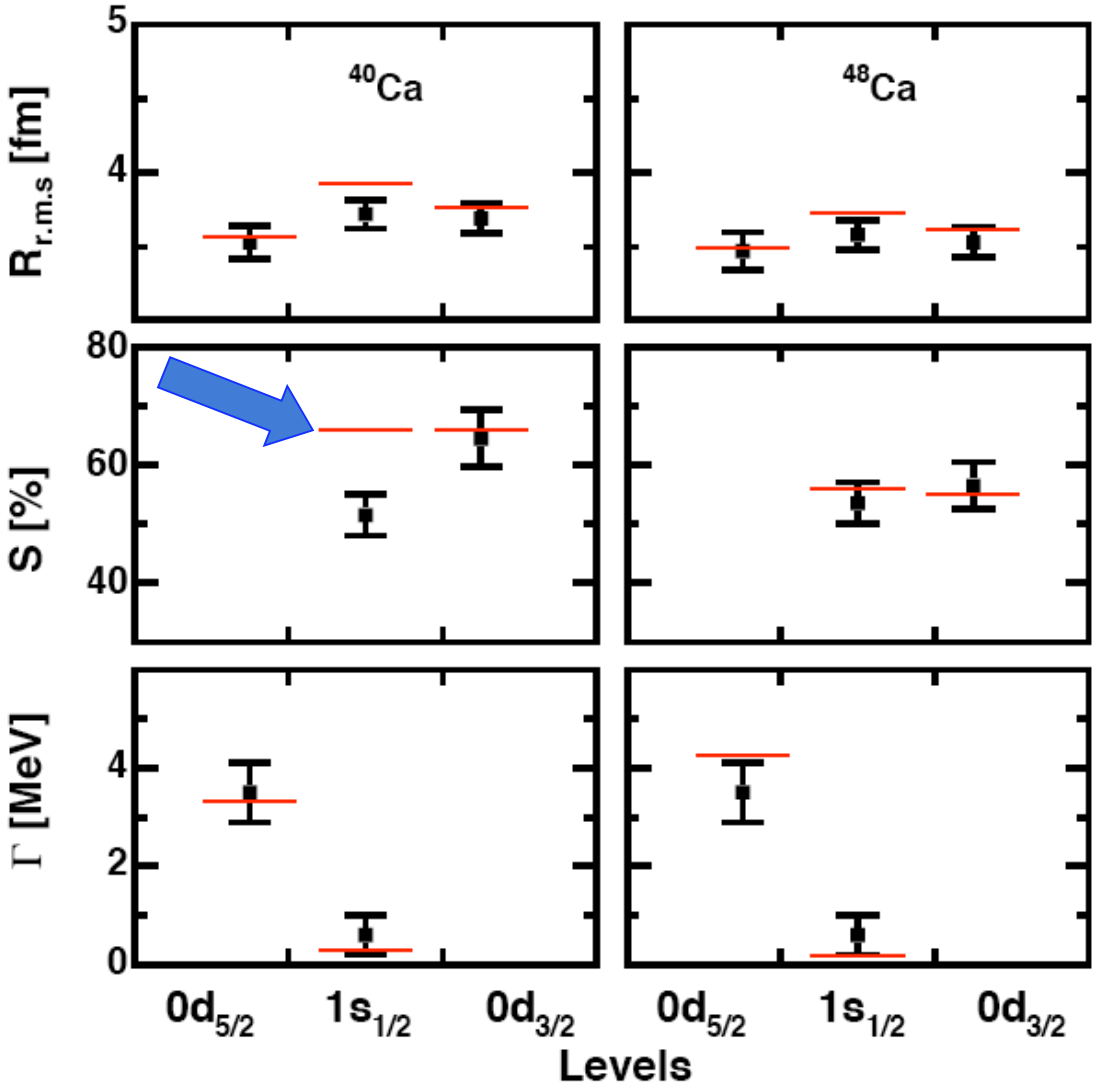


F-RPA, DOM and QP-DFT 32

Present fit and predictions of polarization data



Present fit to (e,e'p) data

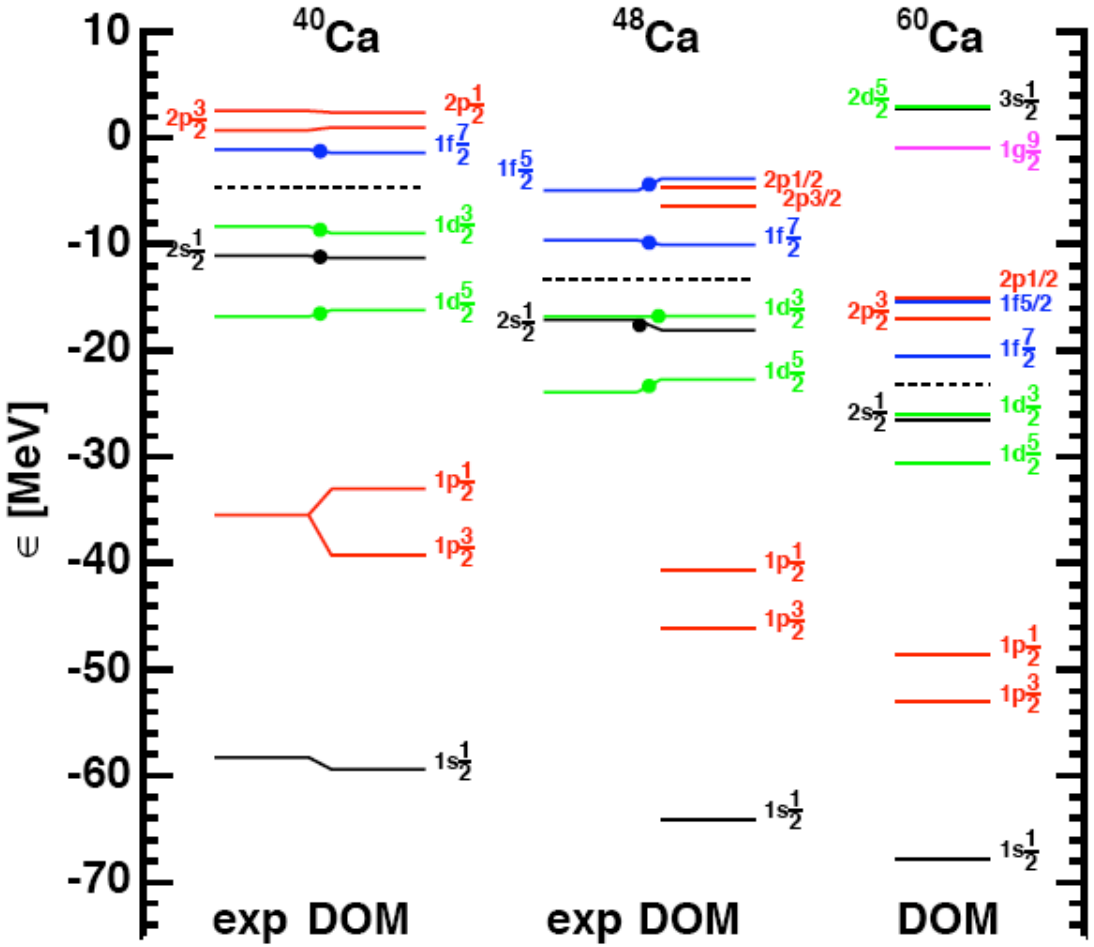


radii of
bound state
wave functions

spectroscopic
factors

widths of strength
distribution

Proton single-particle structure and asymmetry



Pairing of protons due to *pn* correlations?!

Increased correlations with increasing asymmetry!

Extrapolation in δ

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

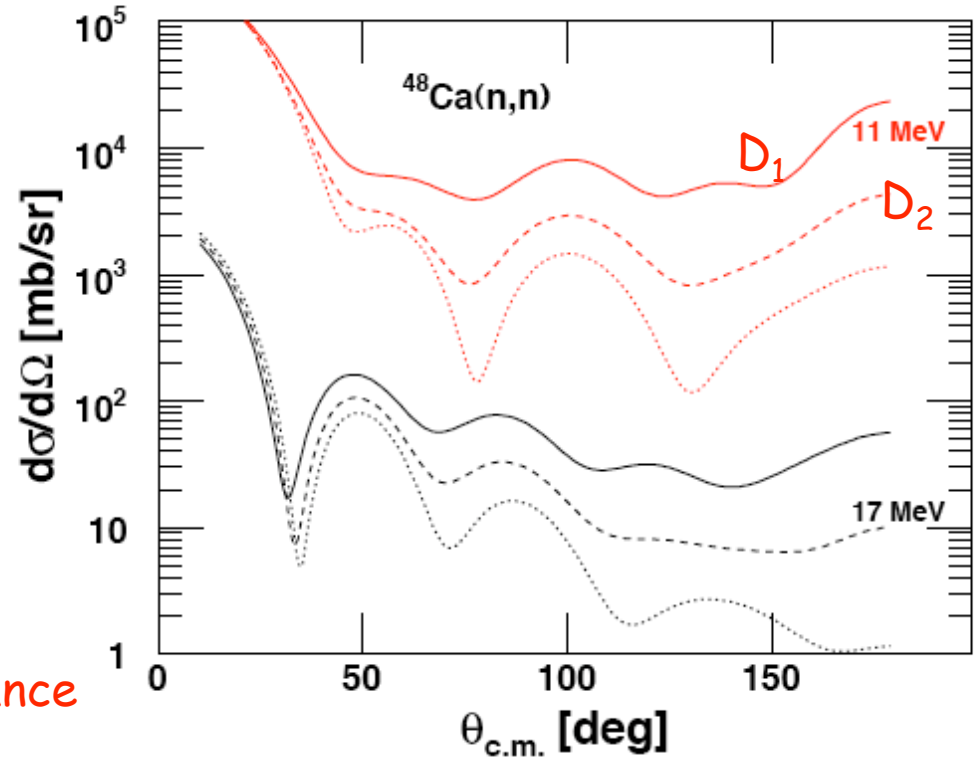
Cannot be extrapolated for n

Less naïve:

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

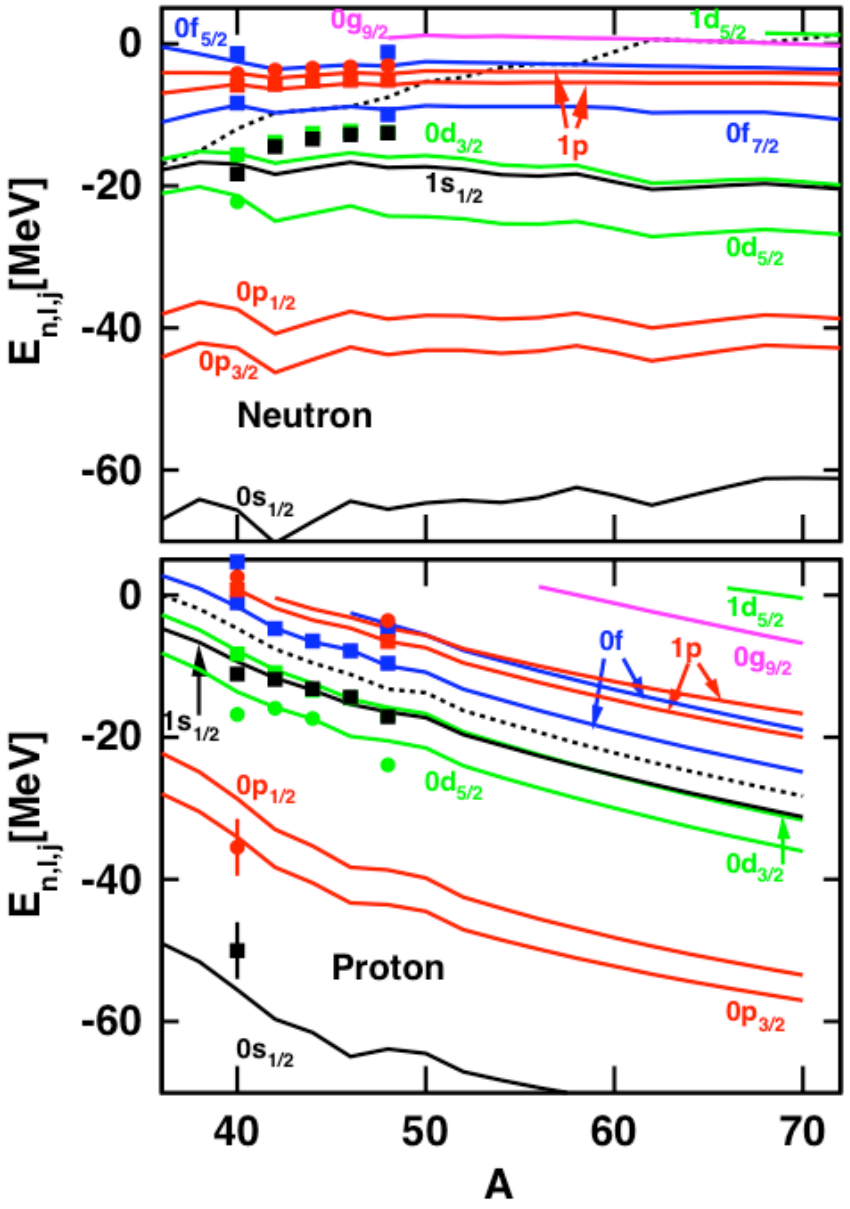
Emphasizes coupling to GT resonance
Consistent with n+^{A}Mo data

Need *n*+^{48}Ca elastic scattering data!!!
In progress at TUNL (Sobotka & Charity)

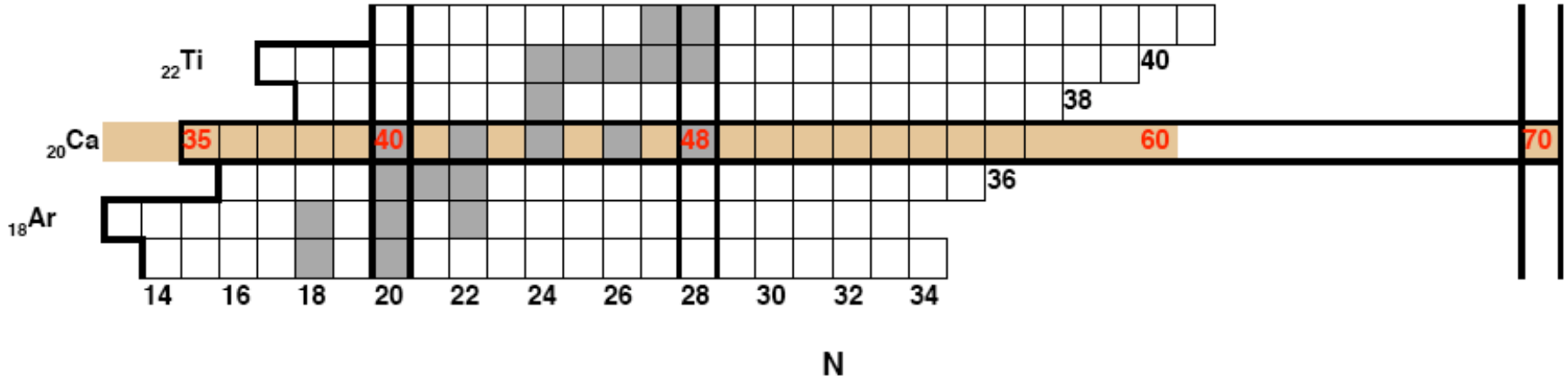


"D2" Extrapolation for large N of sp levels

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



Driplines



Proton dripline wrong by 2

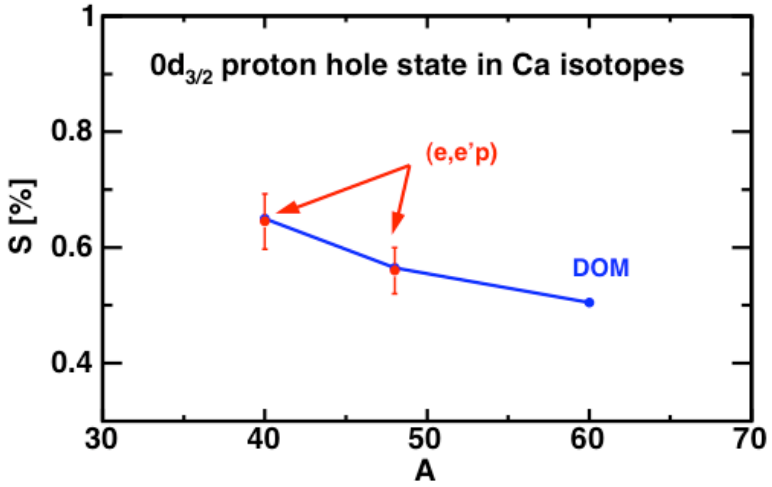
Neutron dripline more complicated:

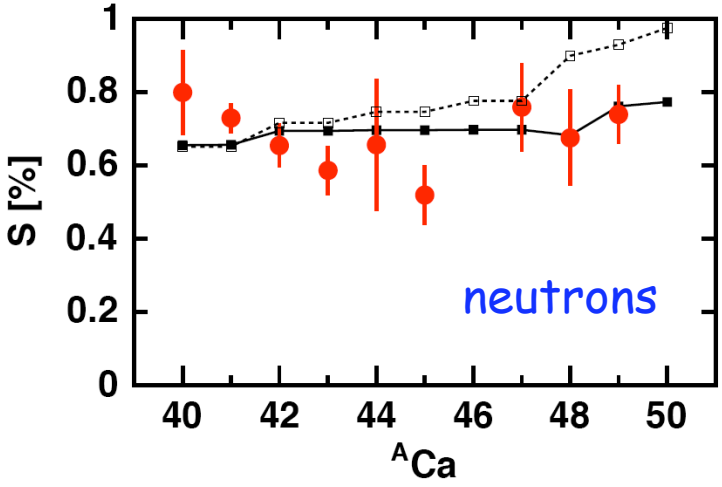
^{60}Ca and ^{70}Ca particle bound

Intermediate isotopes unbound

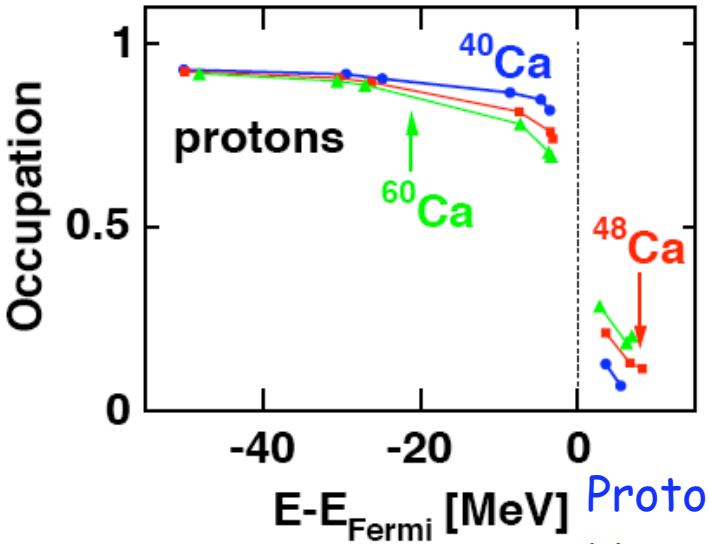
Reef?

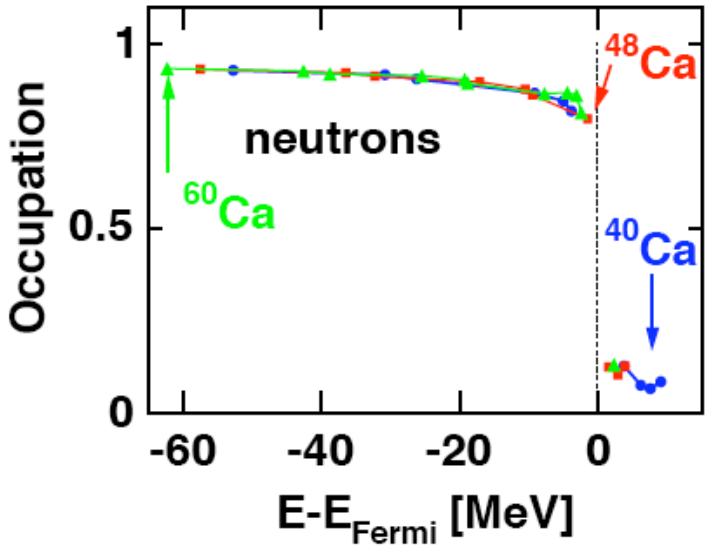
Spectroscopic factors as a function of δ





Occupation numbers





Protons more correlated with δ

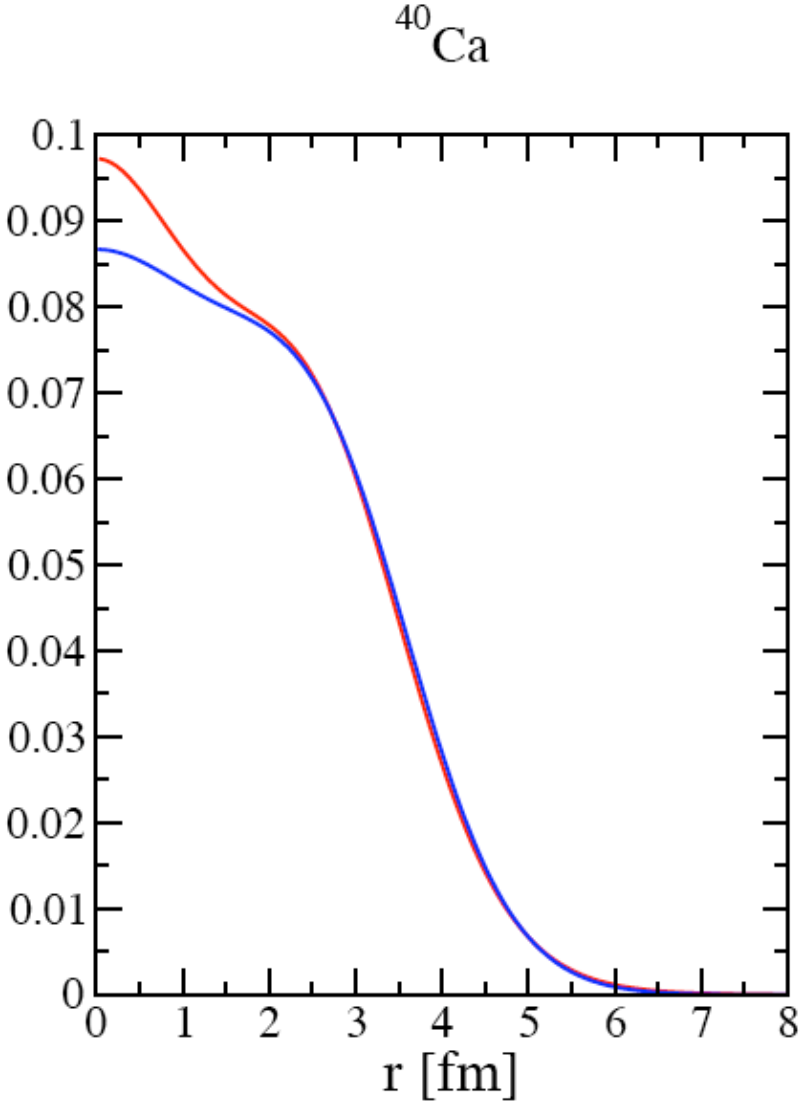
Neutrons not much change

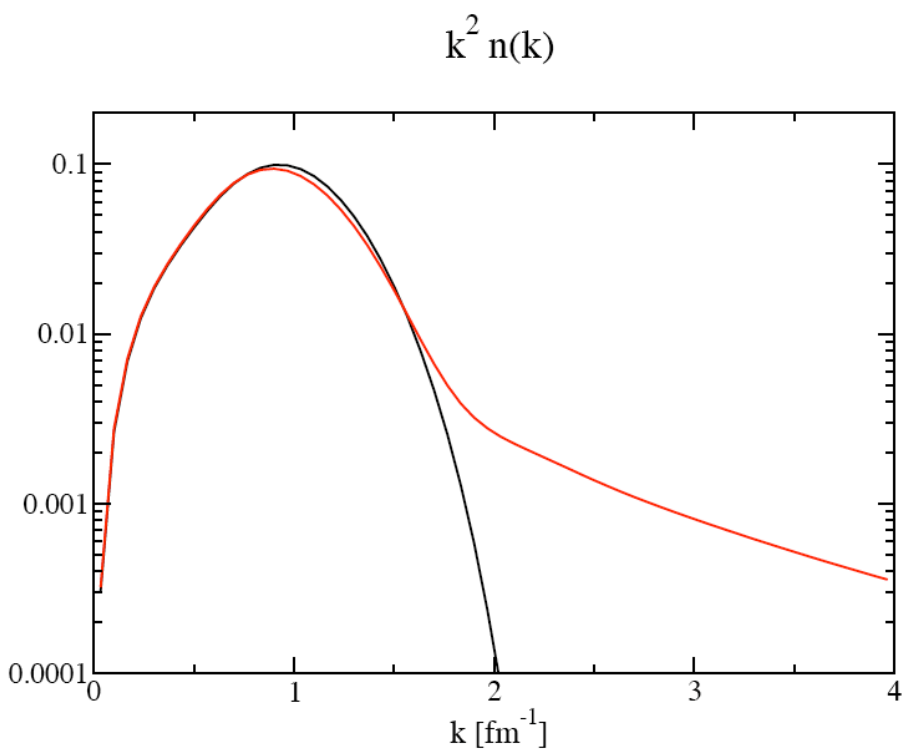
Improvements in progress

Replace treatment of nonlocality in terms of local equivalent
but energy-dependent potential by explicitly nonlocal potential
⇒ 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 ⇒ TNI
- NN Tensor force can be included explicitly
- Generate functionals for QP-DFT

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!

DOM Summary

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

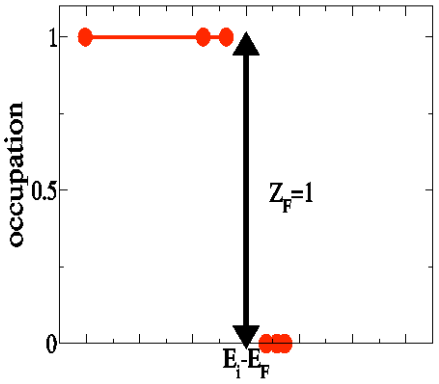
Predictions

- 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)

Correlations in ...

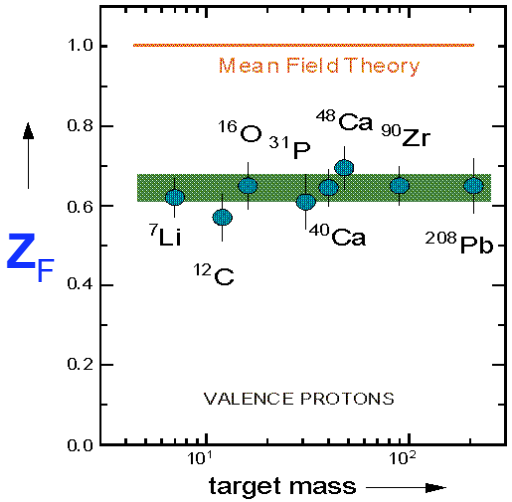
Atoms

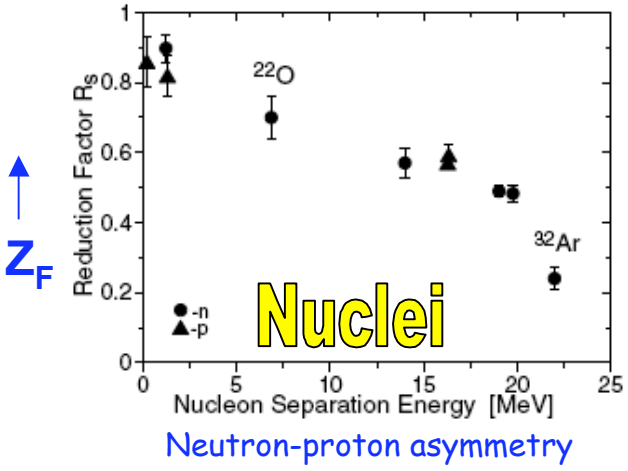
weak correlations



electrons in Ne
Data from (e,2e)

(e,e'p)

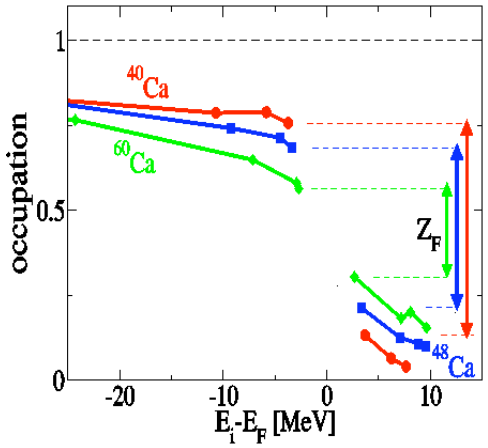




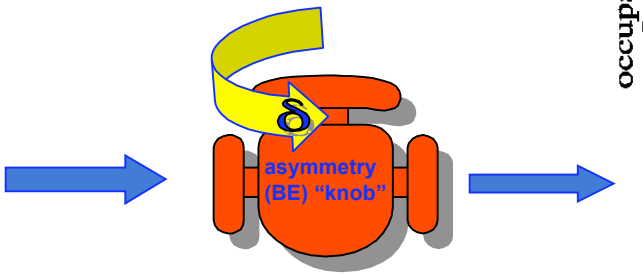
Nuclei

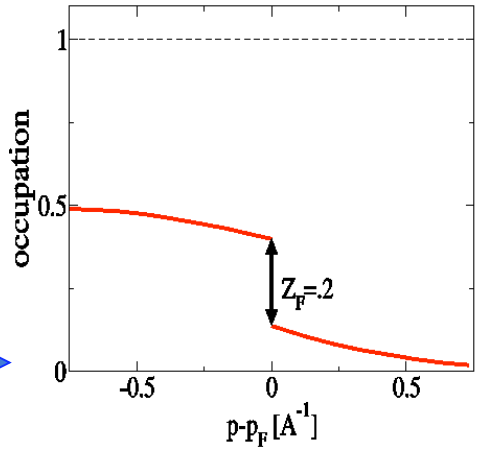
Neutron-proton asymmetry

DOM



protons in stable
closed-shell nuclei





protons in Ca

Liquid 3He

very strong correlations
Data from (n,n')

F-RPA, DOM and QP-DFT 43

Future of Green's function method in nuclear systems

Calculations starting from V_{NN}

- *Faddeev-RPA* method (Barbieri) including $N \neq Z$ systems in order to understand DOM results ($\Rightarrow$ GT connection)
- Pairing & SRC in neutron stars & nuclear matter / EOS (Polls, Rios)

Extensions of DOM

- Include aspects of V_{NN} ($\Rightarrow$ tensor force)
- More data on stable systems (^{48}Ca) and nuclei like ^{36}Ca
- Analyze more systems
- Include (e,e) and (e,e'p) data by treating nonlocality (Van Neck)
- Radioactive beam data including (p,2p)
- Include higher-energy (p,p') data

Construction of QP-DFT functionals (Van Neck)

- starting with extension of Skyrme functionals
- then including aspects of realistic interactions
- or microscopic calculations

Conclusion

F-RPA

- Self-energy of small atoms accurate with F-RPA
- Contains the relevant ingredients for the electron gas including a (possibly) correct self-energy

DOM

- suggests new experiments (some in the pipeline)
- data-driven extrapolation to the dripline

QP-DFT

- F-RPA⇒ study background functionals for QP-DFT
- DOM ⇒ study background functionals for QP-DFT