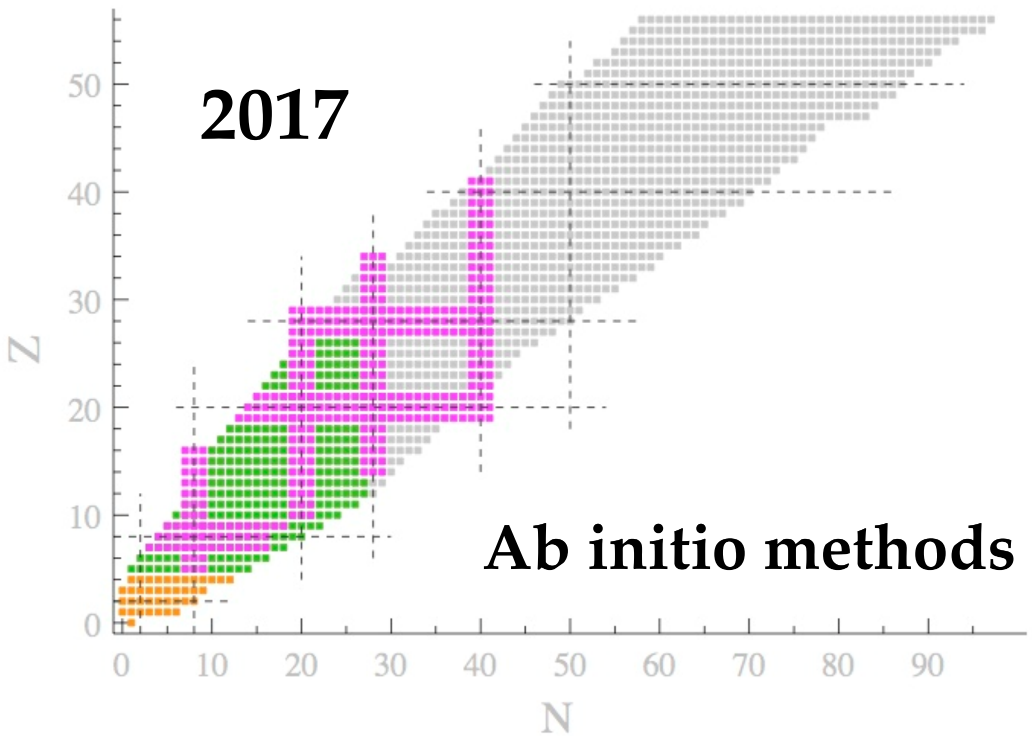
Ab initio calculation of the potential bubble nucleus ^{34}Si



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T. Duguet, V. Somà, S. Lecluse, C. Barbieri, P. Navrátil, Phys. Rev. C95 (2017) 034319

Département de Physique Nucléaire, CEA/Saclay, 17 Novembre 2017

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Ab initio many-body problem

Ab initio (= "from scratch") many-body scheme

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

A-body Hamiltonian

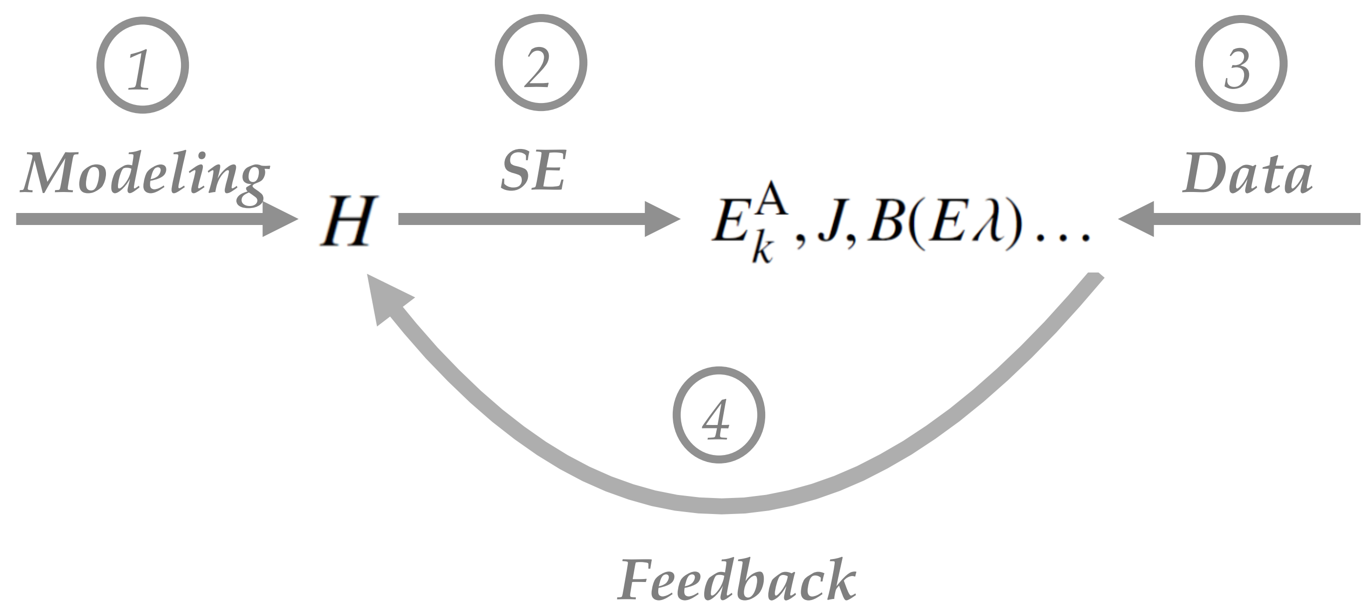
$$H = T + V^{2N} + V^{3N} + V^{4N} + \ldots + V^{AN}$$

A-body wave-function

5 variables x A nucleons

Definition

- *A* structure-less nucleons
- All nucleons active in complete Hilbert space
- Elementary interactions between them
- Solve A-body Schroedinger equation (SE)
- Thorough estimate of error



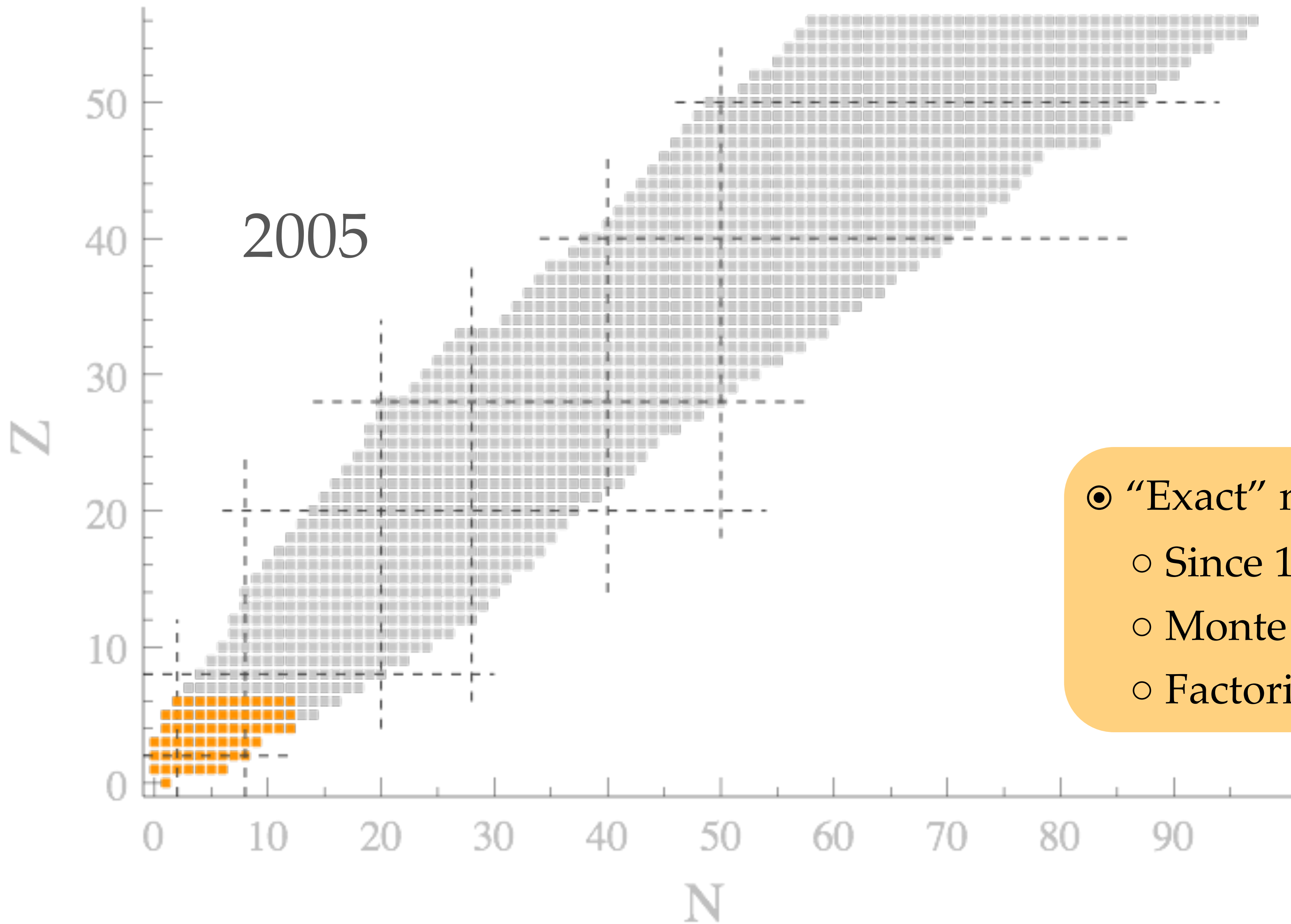
Hamiltonian

Do we know the form of V^{2N}, V^{3N} etc
Do we know how to derive them from QCD?
Why would there be forces beyond pairwise?
Do we need all the terms up to AN forces?

Schroedinger equation

Can we solve the SE with relevant accuracy?
Can we do it for any A=N+Z?
Is it even reasonable for A=200 to proceed this way?
More effective approaches needed?

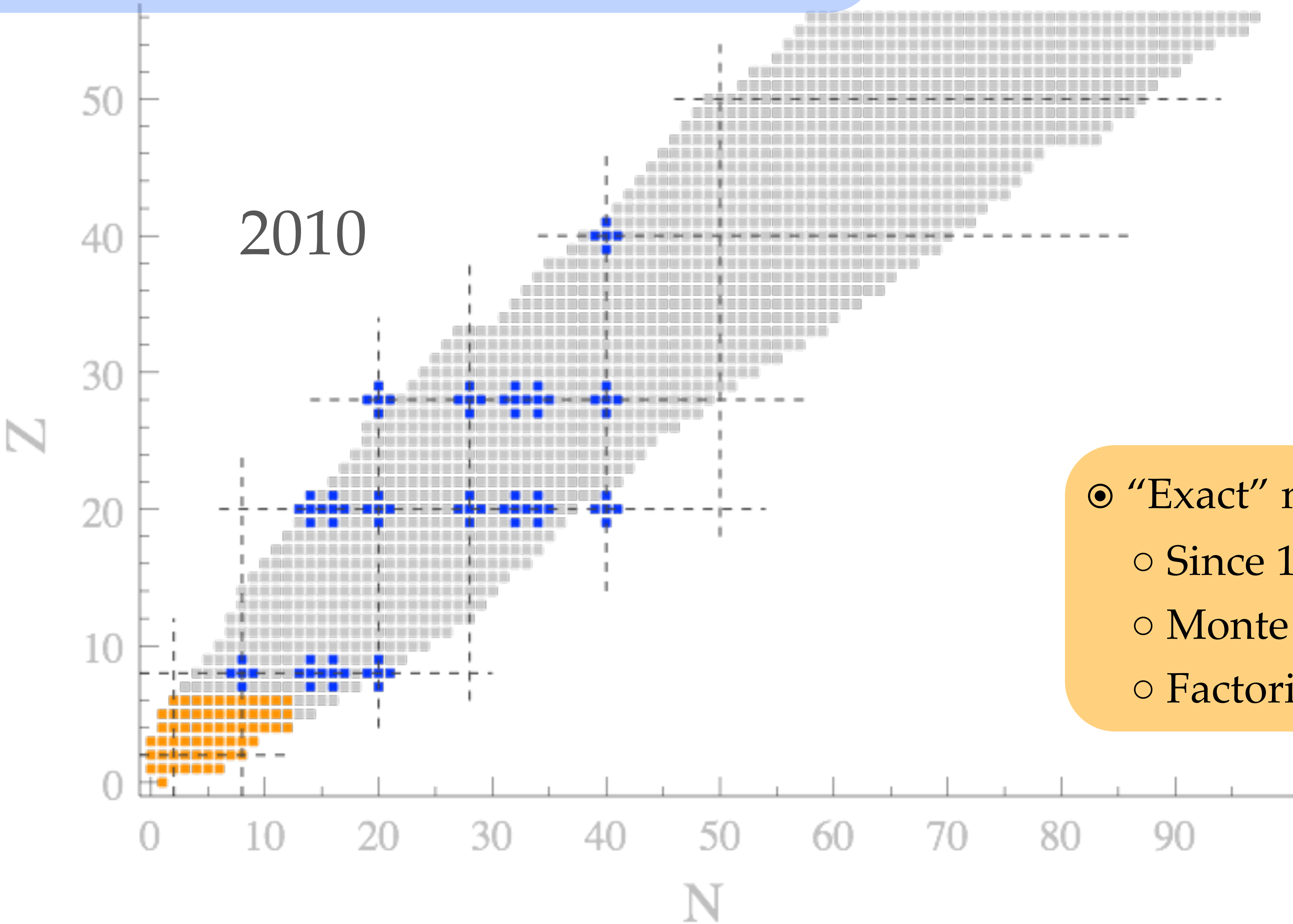
Evolution of *ab initio* nuclear chart



- “Exact” methods
  - Since 1980’s
  - Monte Carlo, CI, …
  - Factorial scaling

Evolution of *ab initio* nuclear chart

- Approximate methods for closed-shells
  - Since 2000's
  - MBPT, SCGF, CC, IMSRG
  - Polynomial scaling



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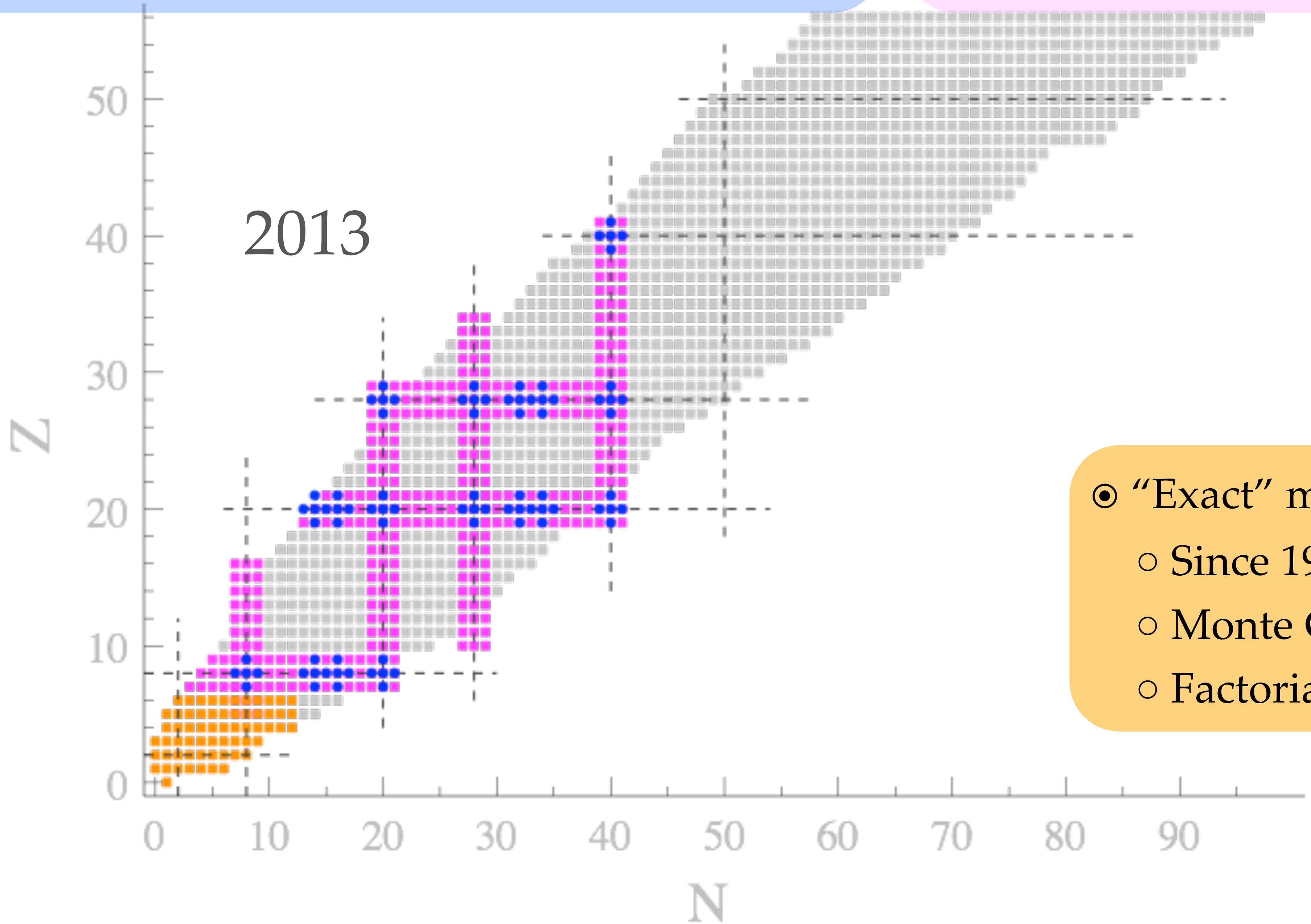
  - Since 2010's
  - BMBPT, GGF, BCC, MR-IMSRG, MCPT
  - Polynomial scaling



- "Exact" methods
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Evolution of *ab initio* nuclear chart

- Approximate methods for closed-shells
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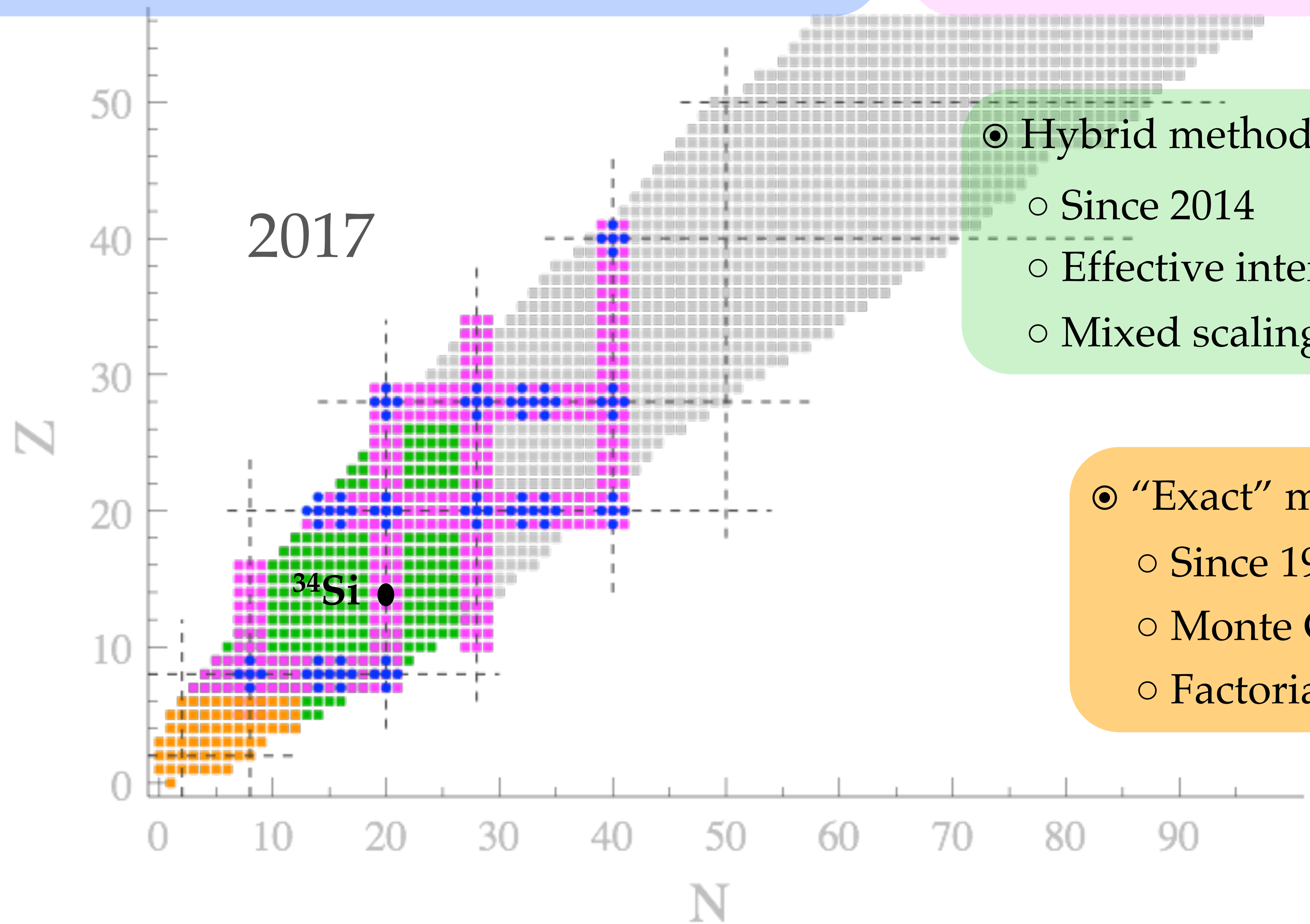


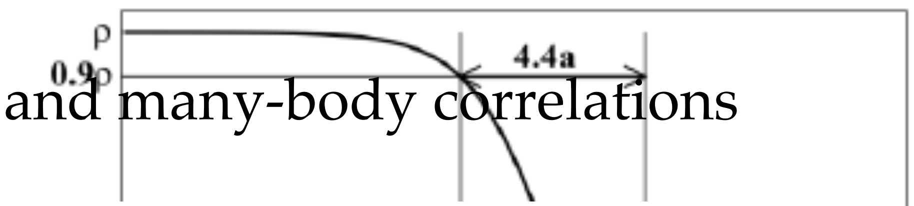
- Hybrid methods (ab initio shell model)
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

- "Exact" methods
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial scaling

Charge density $\rho_{ch}(r)$

- **Tool to probe several basic features of nuclear structure**
  - Nuclear saturation, extension, binding and surface tension
  - Oscillations reflect consistent combinations of shell structure and many-body correlations

$$\rho_C = \rho/(1 + e^{(r-R)/a})$$

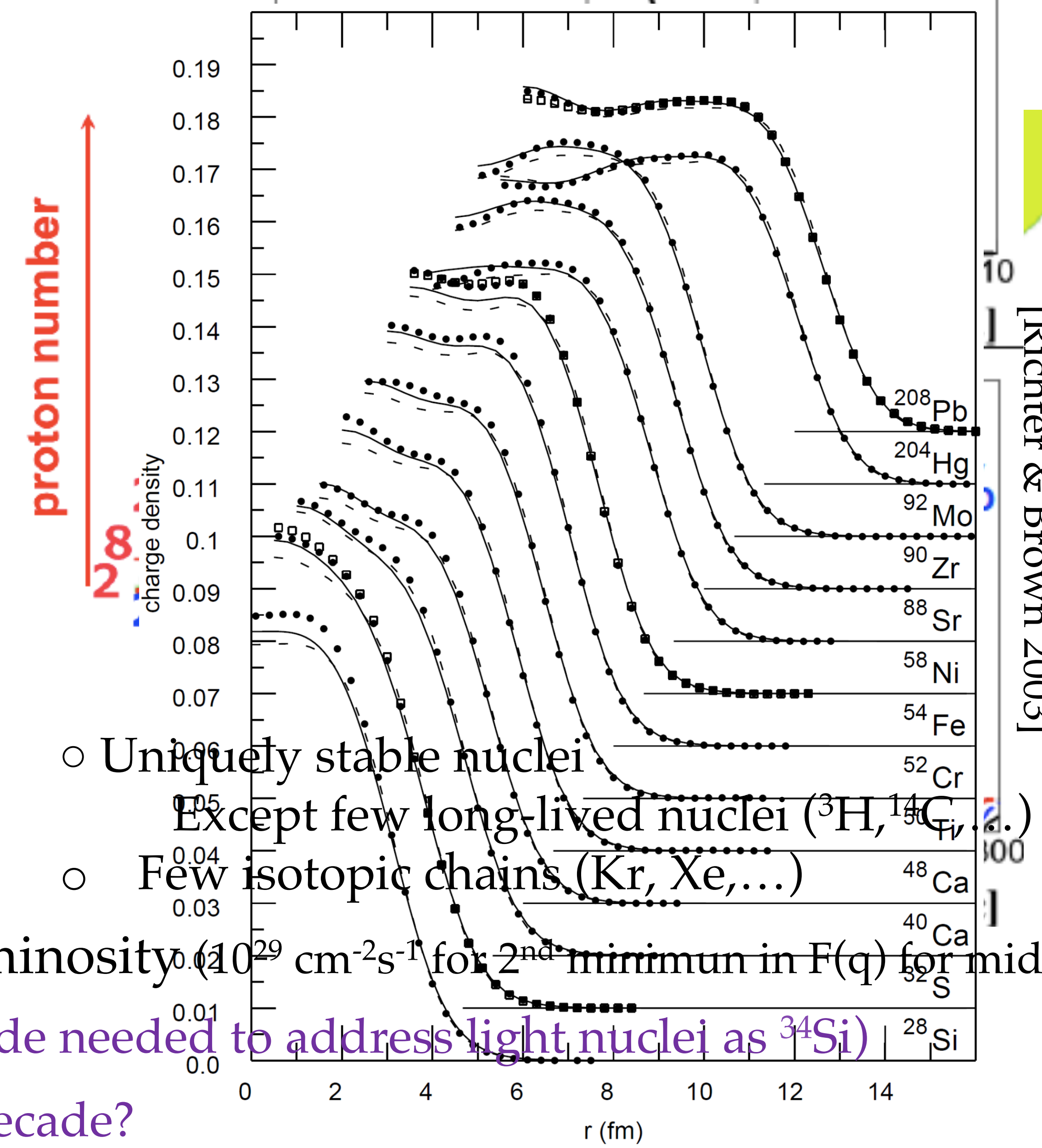


- Experimental probe via electron scattering
  - Sensitive to charge and spin: EM structure
  - Weak coupling: perturbation theory ok

    Ex: elastic scattering between 300 and 700 MeV/c

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{Mott}} \times |F_{\mathrm{Ch}}(q)|^2 \quad \text{with} \quad F_{\mathrm{ch}}(q) = \int d\vec{r}\rho_{\mathrm{ch}}(r)e^{-i\vec{q}\cdot\vec{r}}$$

Mott scattering Nucleus form factor PWBA



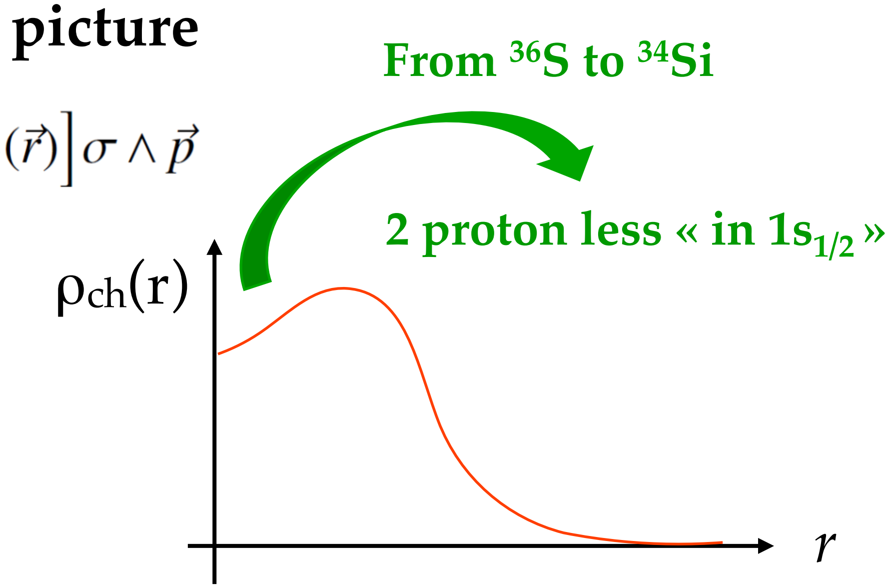
- Nuclei studied in this way so far
  - Uniquely stable nuclei
    Except few long-lived nuclei (^{3}H, ^{14}C, ...)
  - Few isotopic chains (Kr, Xe, ...)
- Challenge is to study unstable nuclei with enough luminosity (10^{29} cm^{-2}s^{-1} for 2nd minimun in F(q) for mid A

  SCRIT@RIKEN with 10^{27} cm^{-2}s^{-1} luminosity (upgrade needed to address light nuclei as ^{34}Si)

  ELISE@FAIR with 10^{28} cm^{-2}s^{-1} luminosity in next decade?

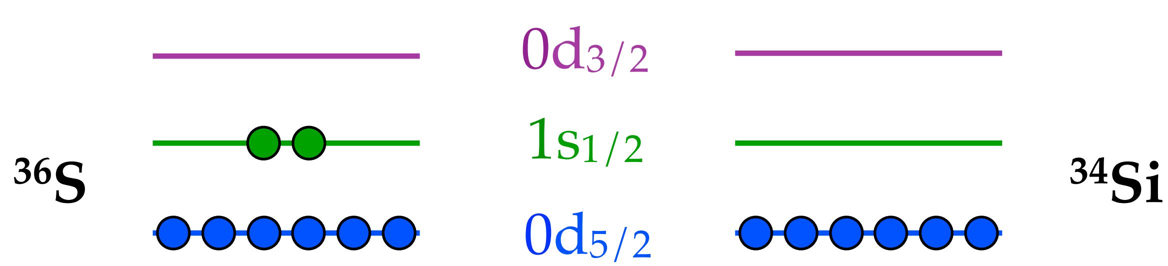
Motivations to study potential (semi-)bubble nuclei

- **Unconventional depletion** ("semi-bubble") in the centre of $\rho_{ch}(r)$ conjectured for certain nuclei
- **Quantum mechanical effect finding intuitive explanation in simple mean-field picture**
  - $\ell = 0$ orbitals display radial distribution peaked at $r = 0$
  - $\ell \neq 0$ orbitals are instead suppressed at small r
  - Vacancy of s states ($\ell = 0$) embedded in larger-ℓ orbitals might cause central depletion
- **Conjectured effect on spin-orbit splitting in simple mean-field picture**
  - Non-zero derivative in the interior $V_q^{so}(\vec{r},\vec{p}) = \frac{1}{2}\left[W_1 \nabla\rho_q(\vec{r}) + W_2 \nabla\rho_{\bar{q}}(\vec{r})\right]\sigma \wedge \vec{p}$
  - One-body spin-orbit potential of "non-natural" sign
  - Reduction of (energy) splitting of low-ℓ spin-orbit partners



- Marked bubbles predicted for hyper-heavy nuclei [Dechargé *et al.* 2003, Bender & Heenen 2013]
- In light/medium-mass nuclei most **promising candidate is ^{34}Si** [Todd-Rutel *et al.* 2004, Khan *et al.* 2008, …]

Naive proton filling



E_{2^+} (^{34}Si)= 3.3MeV
[Ibbotson *et al.* 1998]

Contents

- **Introduction**
- **Theoretical set up**
- **Results**
- **Conclusions**

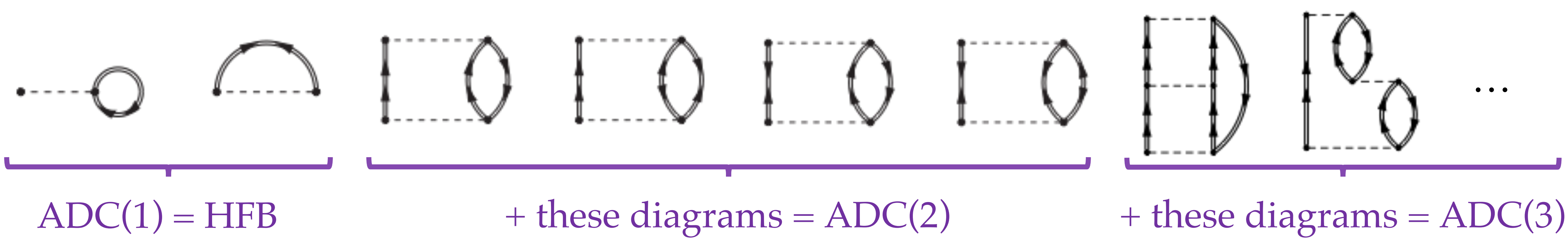
Ab initio self-consistent Green's function approach

⦿ **Solve *A*-body Schrödinger equation** $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$ [Dickhoff, Barbieri 2004]

1) Rewriting it in terms of **1-, 2-, …. *A*-body objects** $G_1 = G$, $G_2, \ldots G_A$ (**Green's functions**)

2) Expanding these objects in perturbation, e.g. $\mathbf{G = G_1}$

➟ **Self-consistent** schemes resum (infinite) subsets of perturbation-theory contributions



⦿ **We employ the Algebraic Diagrammatic Construction (ADC) method** [Schirmer *et al*. 1983]

○ Systematic, improvable scheme for the one-body Green's function, truncated at order n = **ADC(n)**

○ ADC(1) = Hartree-Fock(-Bogolyubov); ADC(∞) = exact solution

○ At present **ADC(1)**, **ADC(2)** and **ADC(3)** are implemented and used

⦿ **Extension to open-shell nuclei: (symmetry-breaking) Gorkov scheme** [Somà, Duguet, Barbieri 2011]

Observables of interest (here)

- Observables: **A-body ground-state binding energy, radii, density distributions**

- Bonus: one-body Green's function accesses ***A*±1 energy spectra**

- **Spectral representation**

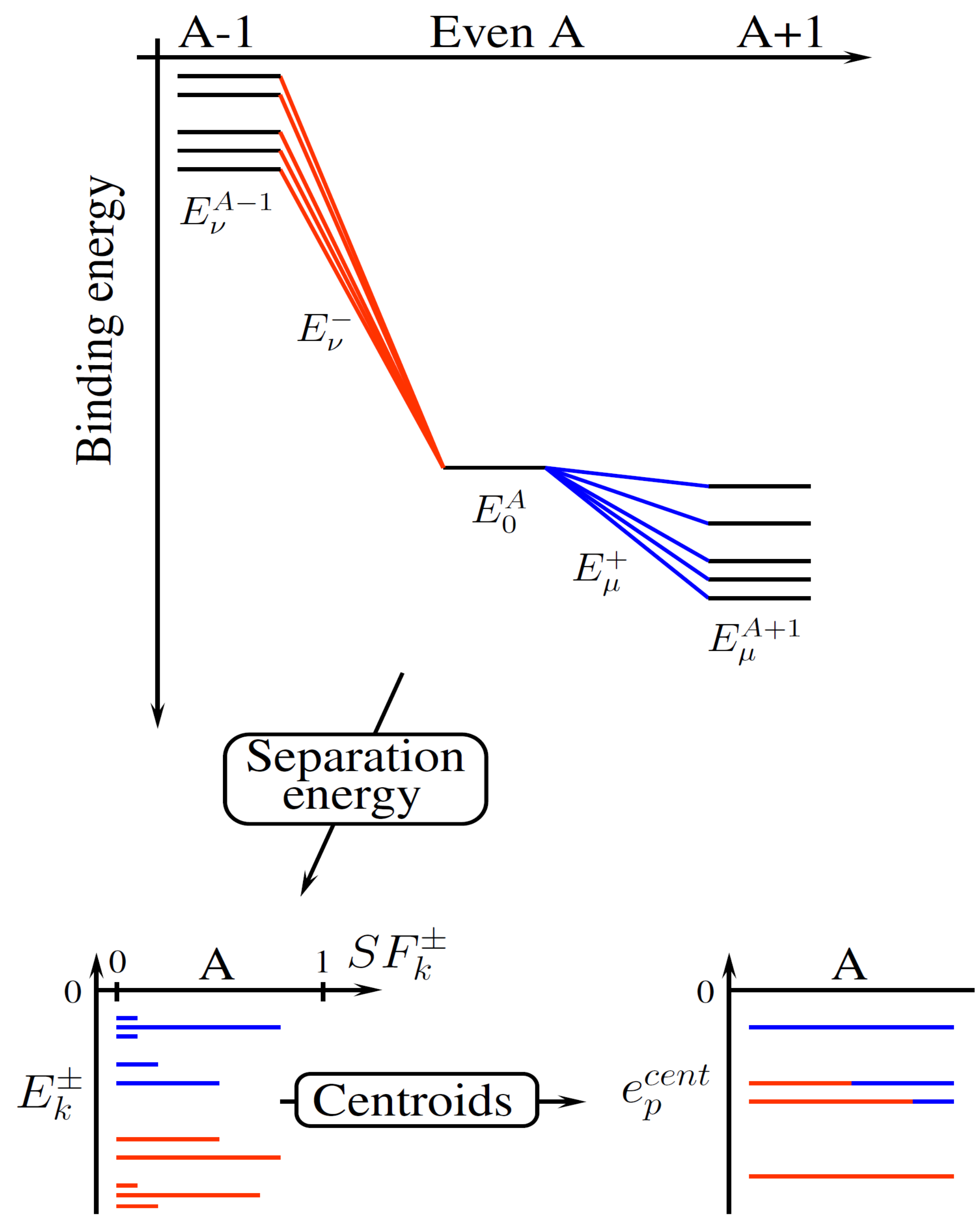
$$G_{pq}(\omega) = \sum_k \left\{ \frac{S_k^{+pq}}{\omega - \omega_k + i\eta} + \frac{S_k^{-pq}}{\omega + \omega_k - i\eta} \right\}$$

where
$$\begin{cases} S_k^{+pq} \equiv \langle \Psi_0^A | a_a | \Psi_k^{A+1} \rangle \langle \Psi_k^{A+1} | a_b^\dagger | \Psi_0^A \rangle \\ S_k^{-pq} \equiv \langle \Psi_0^A | a_a^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | a_b | \Psi_0^A \rangle \end{cases}$$

and
$$\begin{cases} E_k^{+\,(A)} \equiv E_k^{A+1} - E_0^A \equiv \mu + \omega_k \\ E_k^{-\,(A)} \equiv E_0^A - E_k^{A-1} \equiv \mu - \omega_k \end{cases}$$

- **Spectroscopic factors**

$$SF_k^{\pm} \equiv \sum_p S_k^{\pm pp}$$



Calculations set-up

⦿ **Two sets of 2N+3N chiral interactions**

By default in the following calculations

➟ N^2LO 2N+3N (450 MeV) [**$NNLO_{sat}$**]

[Ekström *et al*. 2015]

✓ bare

➟ N^3LO 2N (500 MeV) + N^2LO 3N (400 MeV) [**EM**]

✓ SRG-evolved to 1.88-2.0 fm^{-1}

[Entem & Machleidt 2003; Navrátil 2007; Roth *et al*. 2012]

⦿ **Many-body approaches**

➟ Self-consistent Green's functions

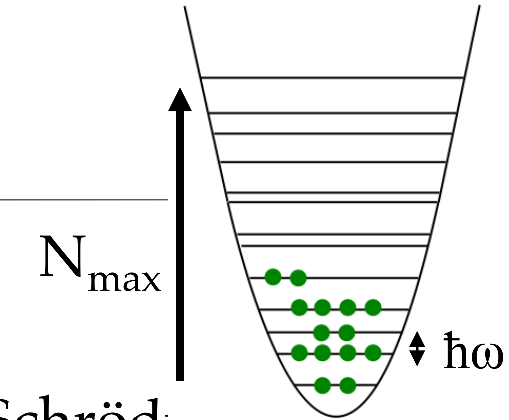
By default in the following calculations

○ Closed-shell Dyson scheme [**DGF**]

○ Open-shell Gorkov scheme [**GGF**]

Contents

Method & convergence

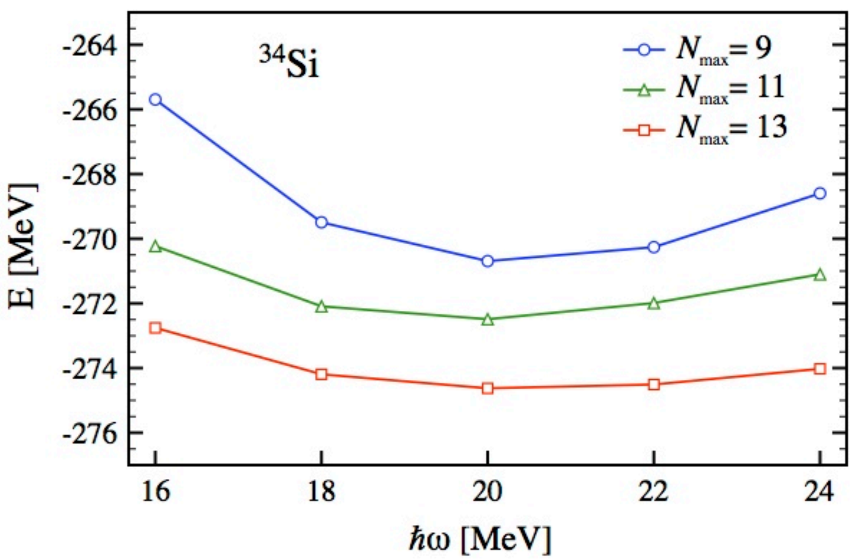


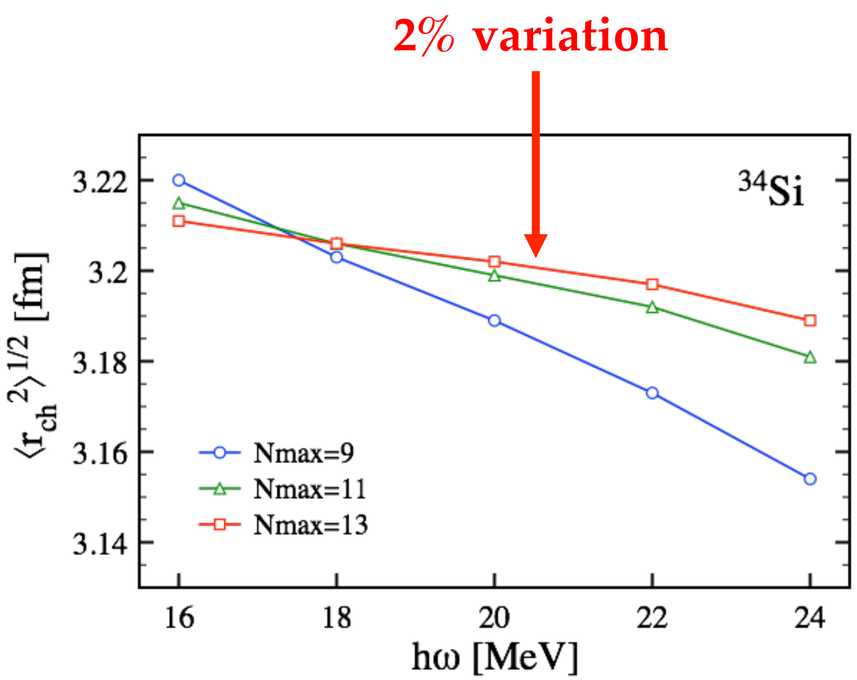
⊙ Many-body calculation implementation

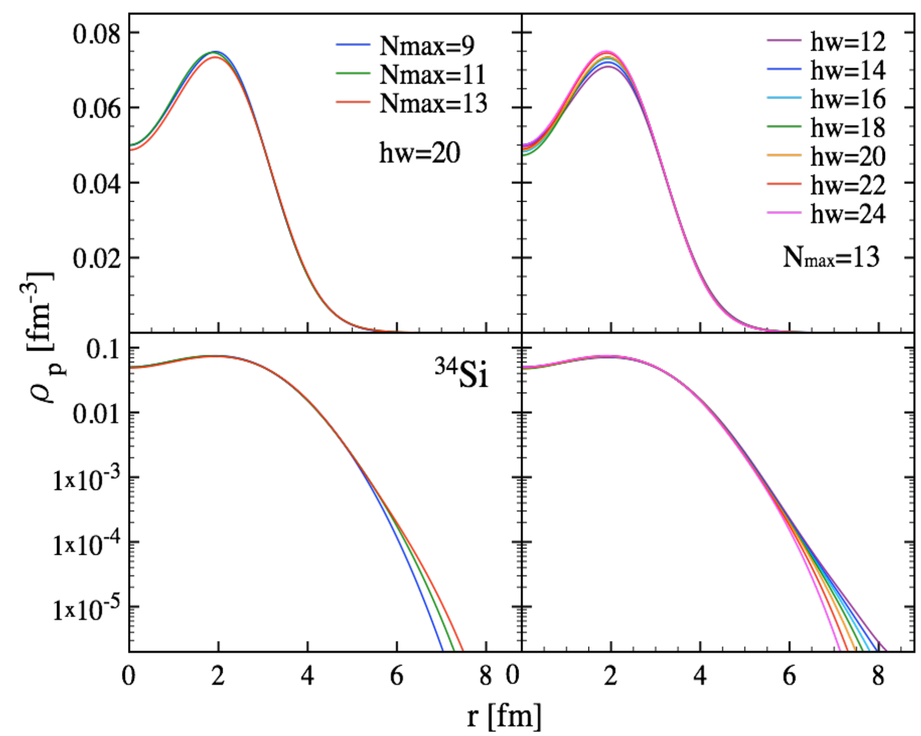
○ Different sizes (N_{max}, ħω) of harmonic oscillator basis to expand AN interactions

○ Different many-body truncations [ADC(1) = HF(B), ADC(2), ADC(3)] to solve Schrödinger equation

⊙ Model space convergence







⊙ Many-body convergence with NNLO$_{sat}$ (densities later on)

Binding energies

E	ADC(1)	ADC(2)	ADC(3)	Experiment
^{34}Si	-84.481	-274.626	-282.938	-283.427
^{36}S	-90.007	-296.060	-305.767	-308.714

1%

ADC(3) brings ~5% additional binding
Missing ADC(4) < 1% binding

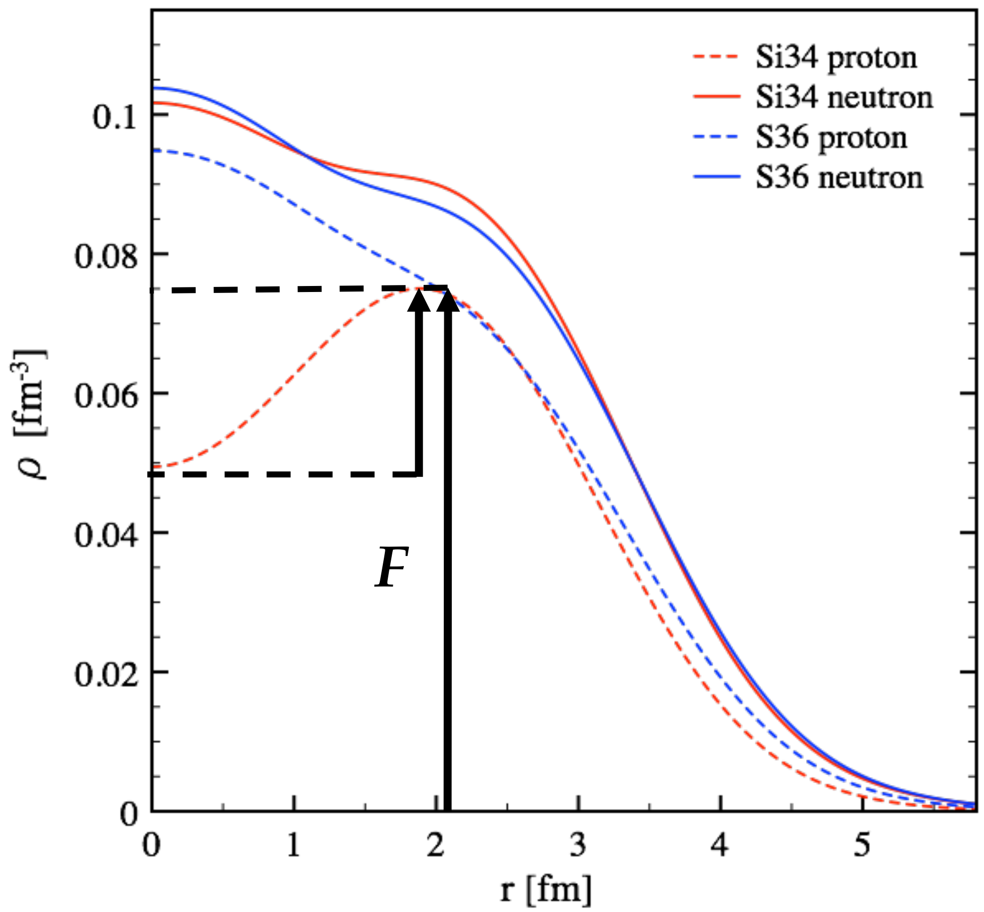
Charge radii

$\langle r_{ch}^2\rangle^{1/2}$	ADC(1)	ADC(2)	ADC(3)	Experiment
^{34}Si	3.270	3.189	3.187	-
^{36}S	3.395	3.291	3.285	3.2985 ± 0.0024

Radii essentially converged at ADC(2) level
Correlations reduce the charge radii

Point-nucleon densities in ^{34}Si and ^{36}S

- **Point-nucleon** density operator $\rho_{p/n}(\vec{r}) \equiv \sum_{i=1}^{N/Z} \delta(\vec{r} - \vec{r}_i)$
- Bubble structure can be quantified by the **depletion factor** $F \equiv \frac{\rho_{\max} - \rho_c}{\rho_{\max}}$



- **Point-proton** density of ^{34}Si displays a **marked depletion in the center**
- **Point-neutron** distributions little affected by removal/addition of two protons

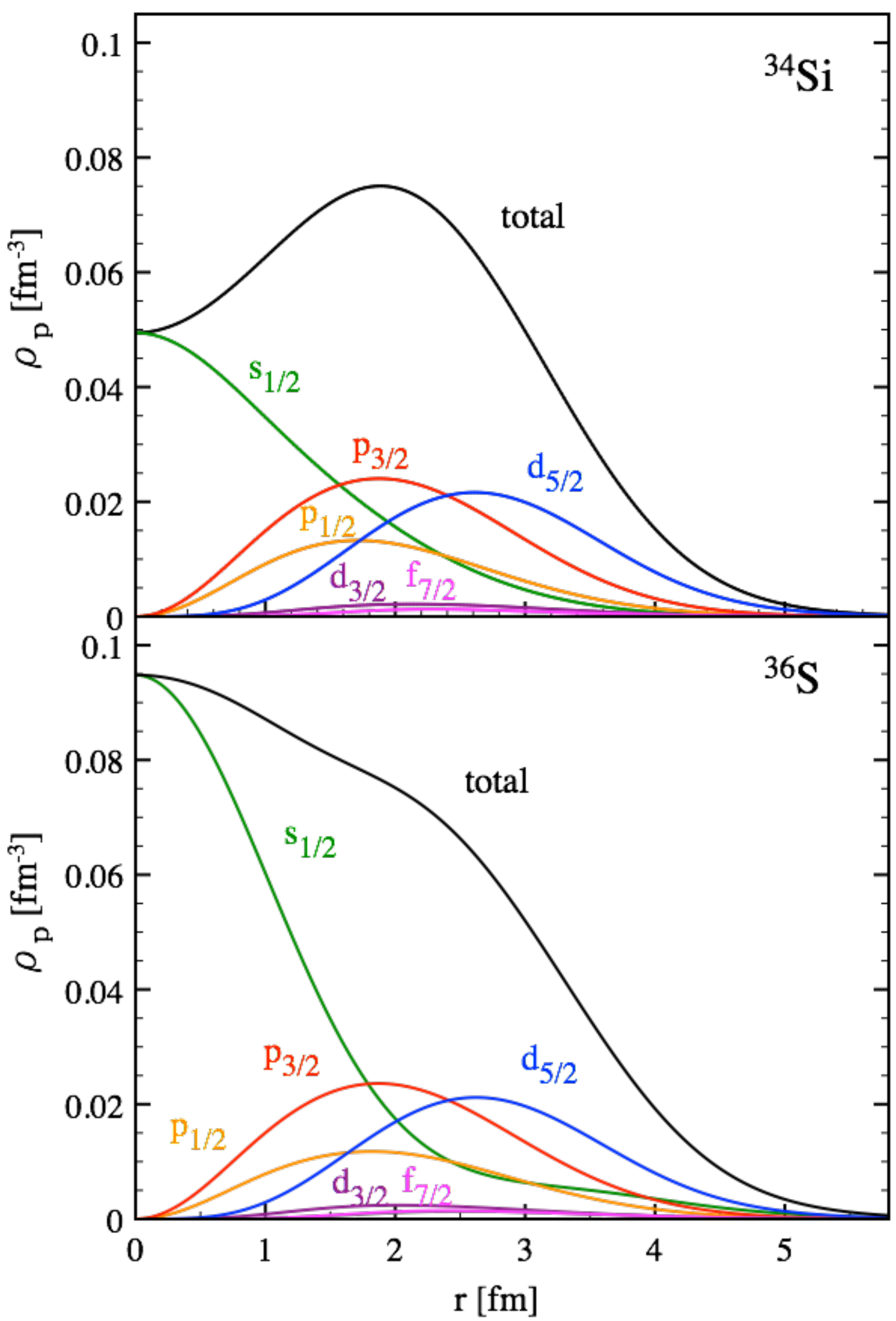
$$\begin{cases} F_p(^{36}\text{S}) = 0 \\ F_p(^{34}\text{Si}) = 0.34 \end{cases}$$

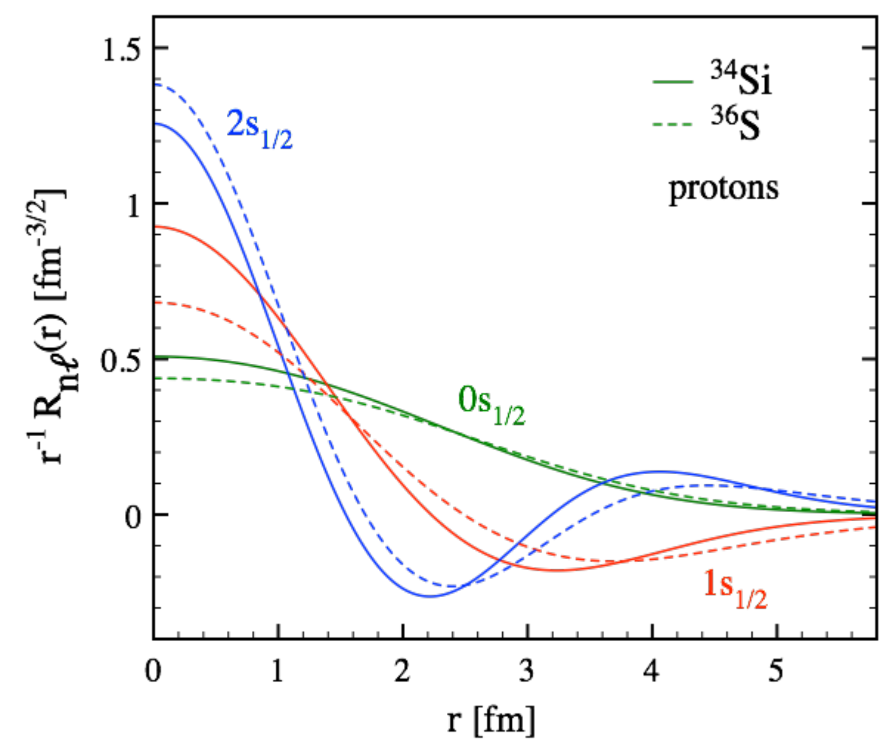
➟ Going from proton density to **observable charge density** will smear out the depletion

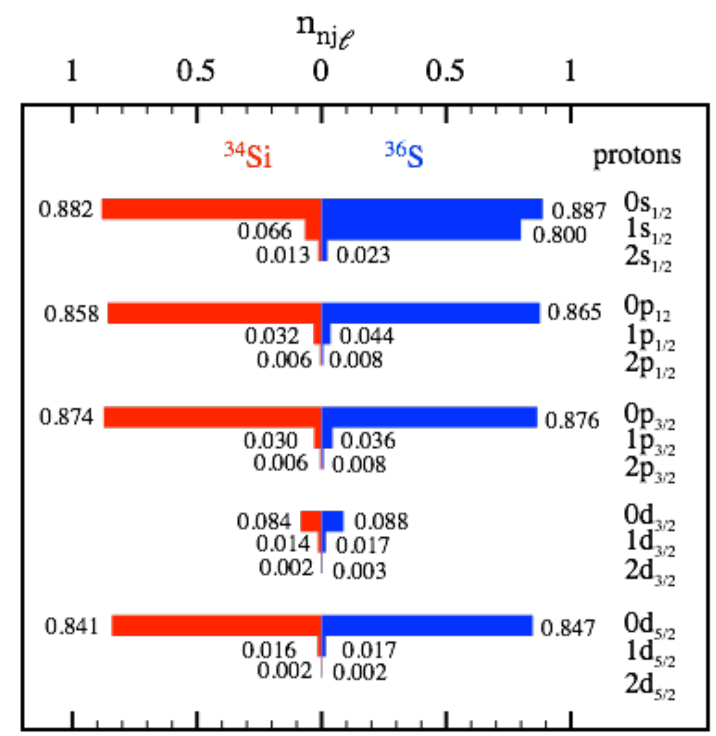
Partial-wave decomposition

⦿ Point-proton distributions can be analysed (internally to the theory) in the **natural basis**

⦿ Consider different partial-wave (l,j) contributions $\rho_{\rm p}(\vec{r}) = \sum_{n\ell j} \frac{2j+1}{4\pi} n_{n\ell j} R^2_{n\ell j}(r) \equiv \sum_{\ell j} \rho_{\rm p}^{\ell j}(r)$







○ Independent-particle filling mechanism **qualitatively OK**

-20% +8%

○ **Quantitatively**

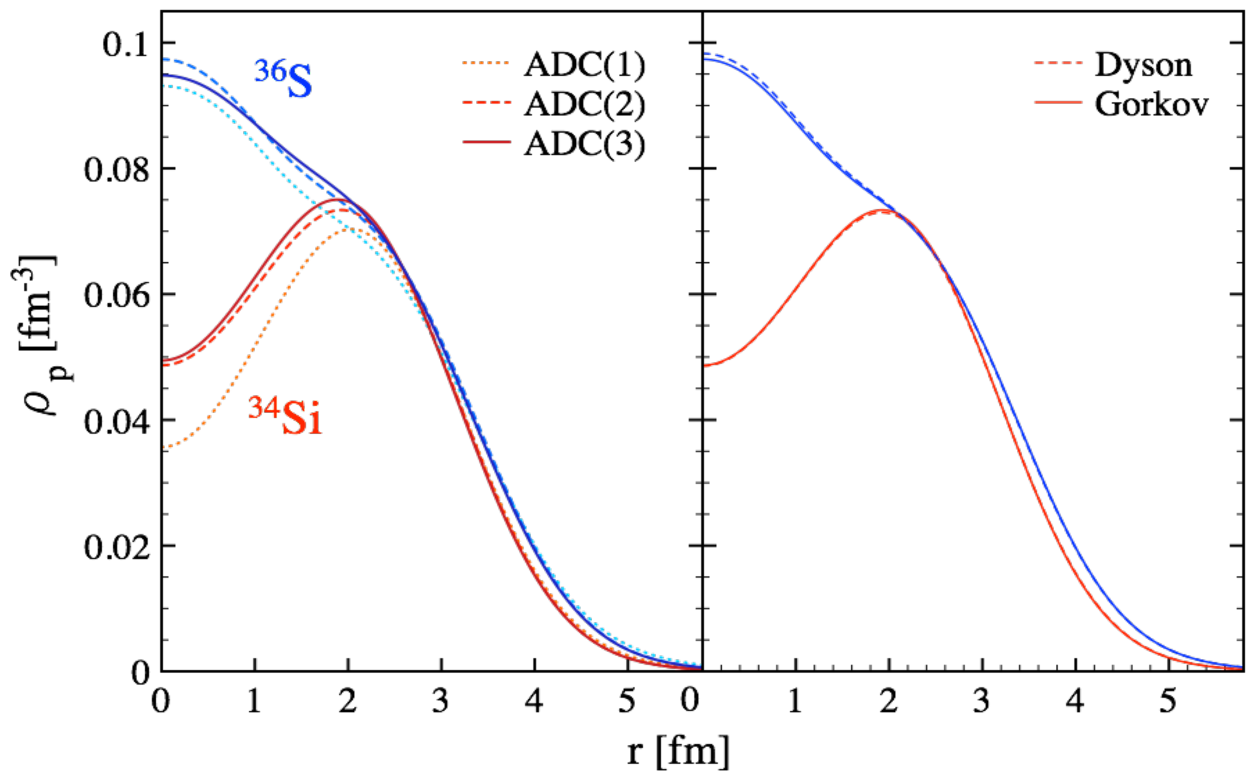
Net effect from **balance between n=0, 1, 2**

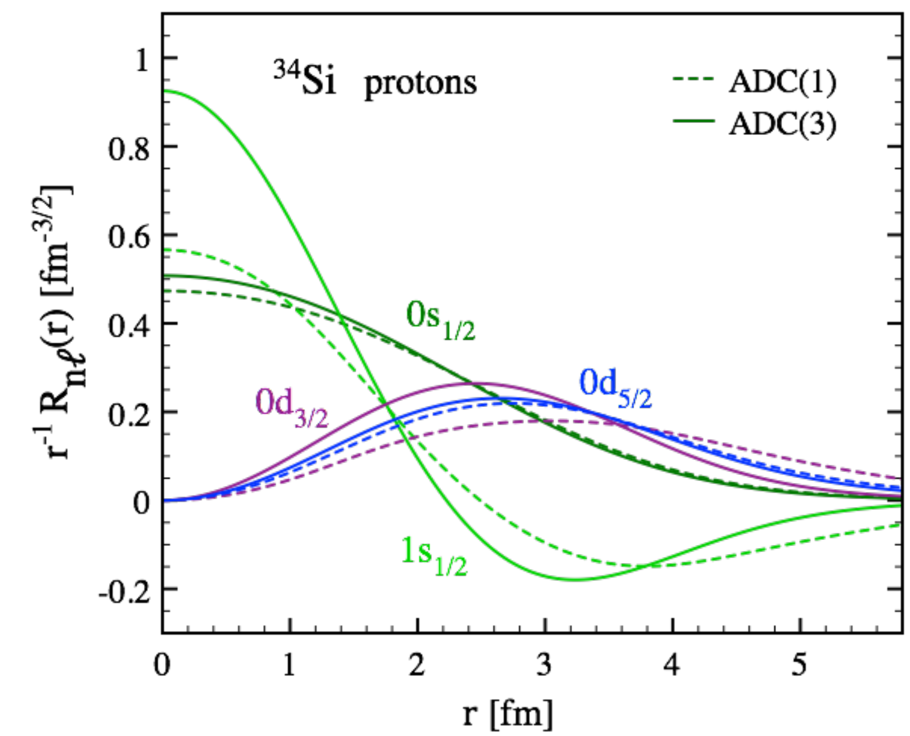
Net effect of **w.f. polarization** and change of occupations

○ Point-neutron contributions & occupations unaffected

Impact of correlations

⦿ Impact of correlations analysed by comparing **different ADC(n) many-body truncation schemes**





○ Dynamical correlations cause an **erosion** of the bubble in ^{34}Si

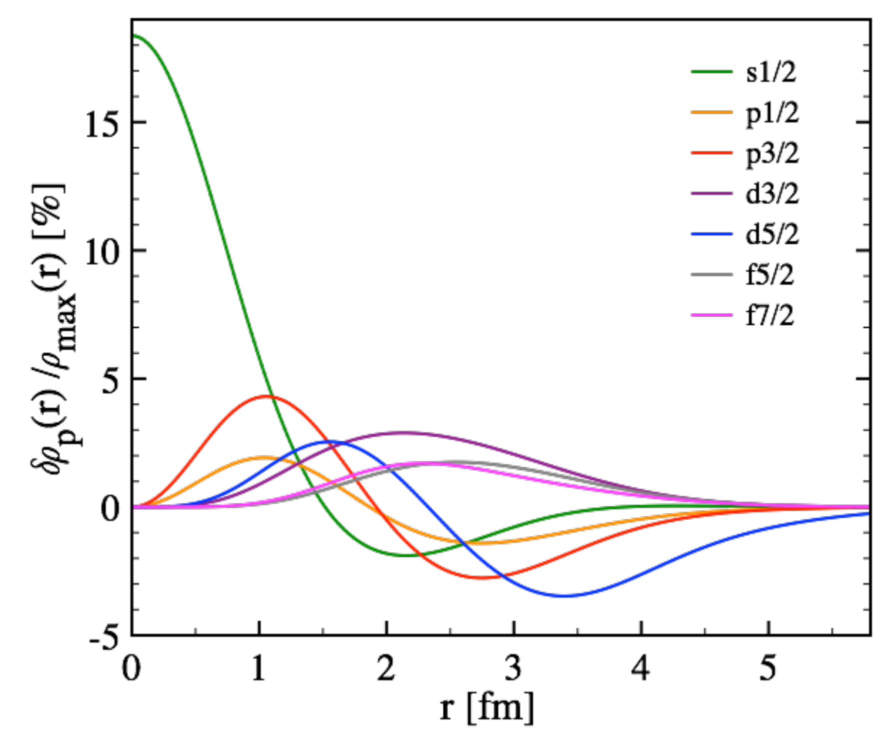
^{34}Si	ADC(1)	ADC(2)	ADC(3)
F_p	0.49	0.34	0.34

○ Traces back to two combining effects of correlations

1) $1s_{1/2}$ orbitals becoming slightly occupied

2) Wave functions get contracted ➟ $1s_{1/2}$ more peaked at $r = 0$

○ Including **pairing** explicitly does not change anything

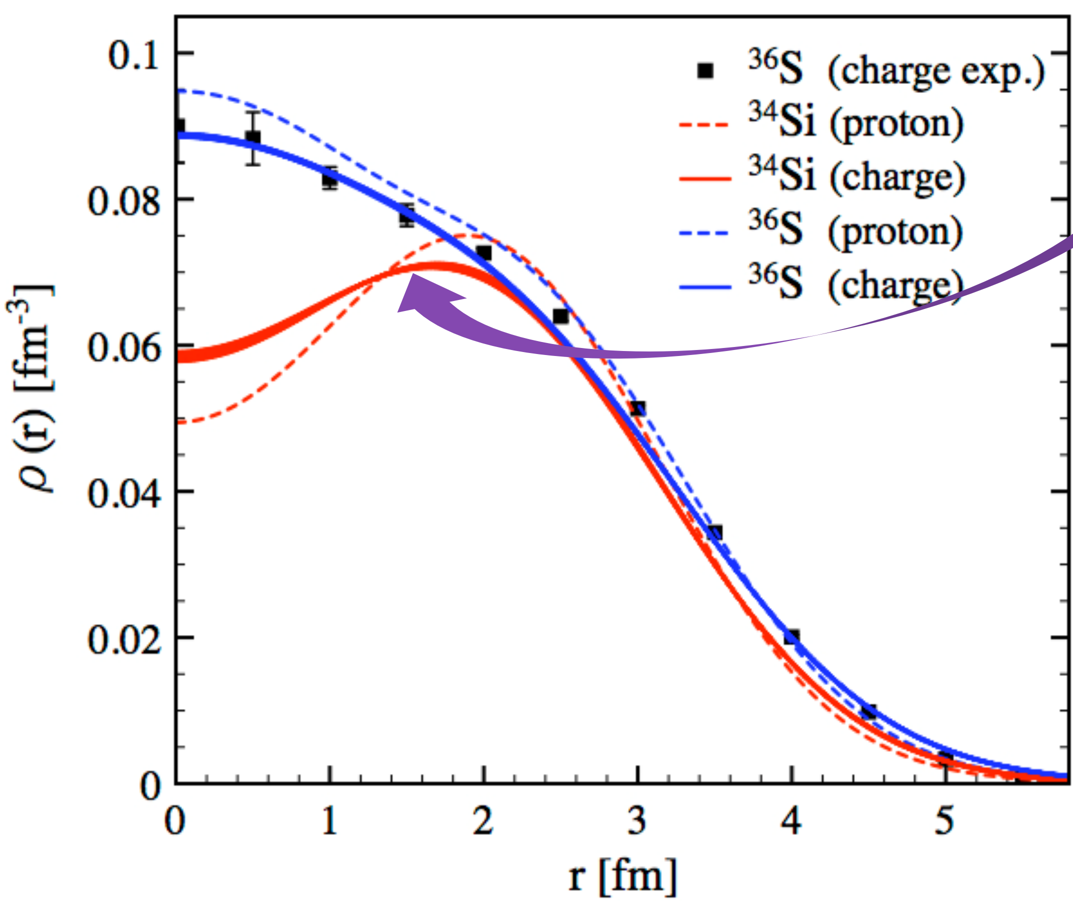


Charge density distribution

- Charge density computed through folding with the finite charge of the proton

$$\rho_{ch}(r) = \frac{1}{a\sqrt{\pi}} \int_0^{+\infty} dr' \, r' \rho_p(r') \left[\frac{e^{-3(r-r')^2/2r_{eff}^2}}{r} - \frac{e^{-3(r+r')^2/2r_{eff}^2}}{r} \right]$$

(no meson-exchange currents here)



$$r_{eff} = \sqrt{\langle R_p^2 \rangle} = 0.8775 \, \text{fm}$$ [Mohr *et al.* 2012]

$$= \sqrt{\langle R_p^2 \rangle + \frac{1}{2}\left(\frac{\hbar}{mc}\right)^2 - \frac{b^2}{A}} \approx 0.82 \, \text{fm}$$ [Brown *et al.* 1979]

Darwin-Foldy correction — **Center-of-mass correction**

r_{eff} = 0.82 fm (SCGF) — **r_{eff} = 0.8 fm** (SCGF*, MREDF [7], MREDF [8], SM [6])

^{34}Si	SCGF	SCGF*	MREDF [7]	MREDF [8]	SM [6]
F_p	0.34	0.34*	0.21	0.22	0.41
F_{ch}	0.15	0.19*	0.09	0.11	0.28

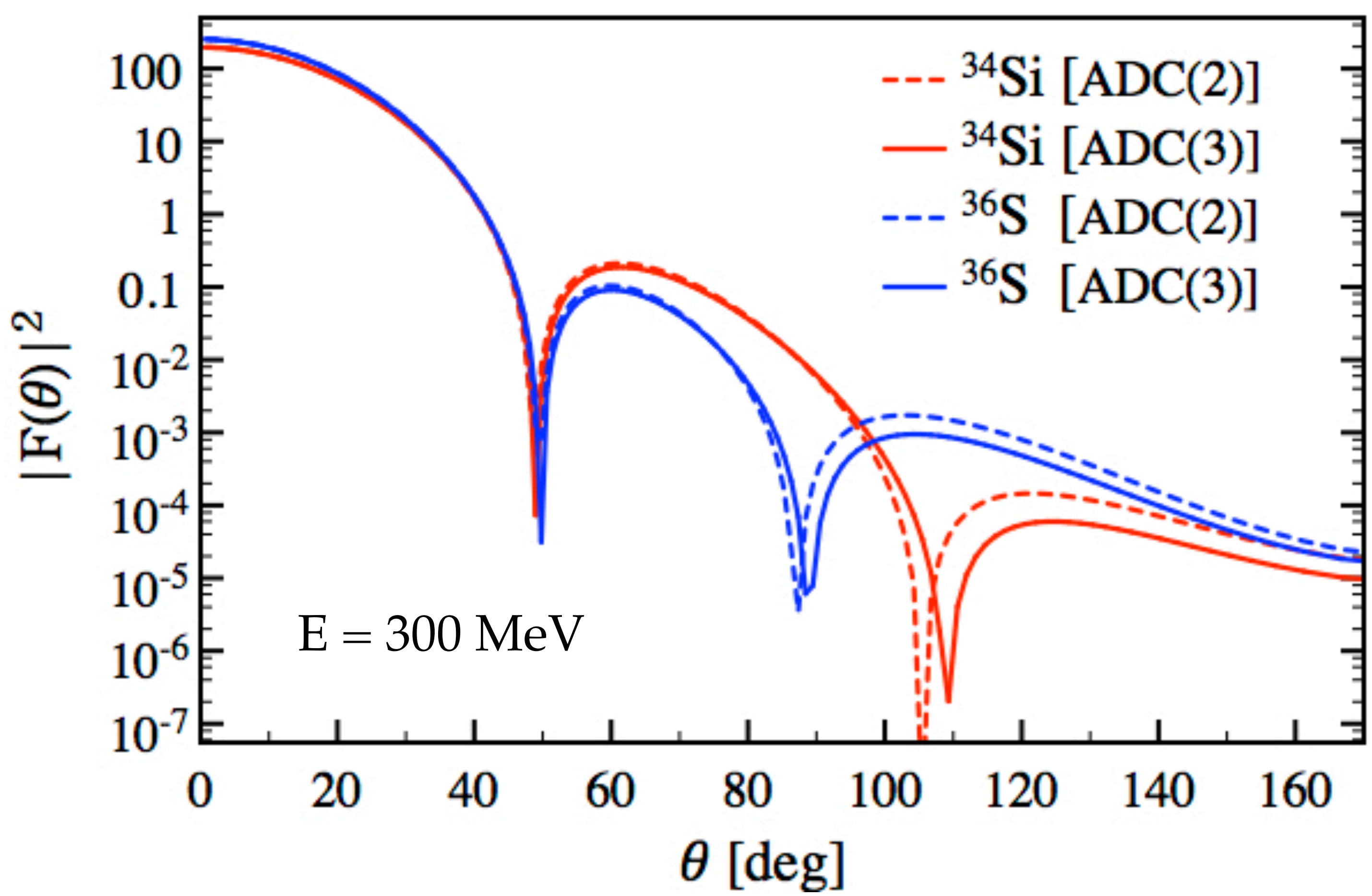
[6] [Grasso *et al.* 2009] [7] [Yao *et al.* 2012] [8] [Yao *et al.* 2013]

- Excellent agreement with experimental charge distribution of ^{36}S [Rychel *et al.* 1983]
- Folding smears out central depletion ➟ **depletion factor decreases from 0.34 to 0.15**
- **Depletion predicted more pronounced than with MR-EDF** (same impact of correlations)

Charge form factor

- Charge form factor measured in (e,e) experiments sensitive to bubble structure?

$$F(q) \overset{\text{PWBA}}{=} \int d\vec{r}\rho_{\text{ch}}(r)e^{-i\vec{q}\cdot\vec{r}} \quad \text{with momentum transfer } q = 2p\sin\theta/2$$



- Central depletion reflects in larger $|F(\theta)|^2$ for **angles 60°<θ<90° and shifted 2$^{\text{nd}}$ minimum by 20°**
- Future **electron scattering** experiments might see its **fingerprints if enough luminosity**

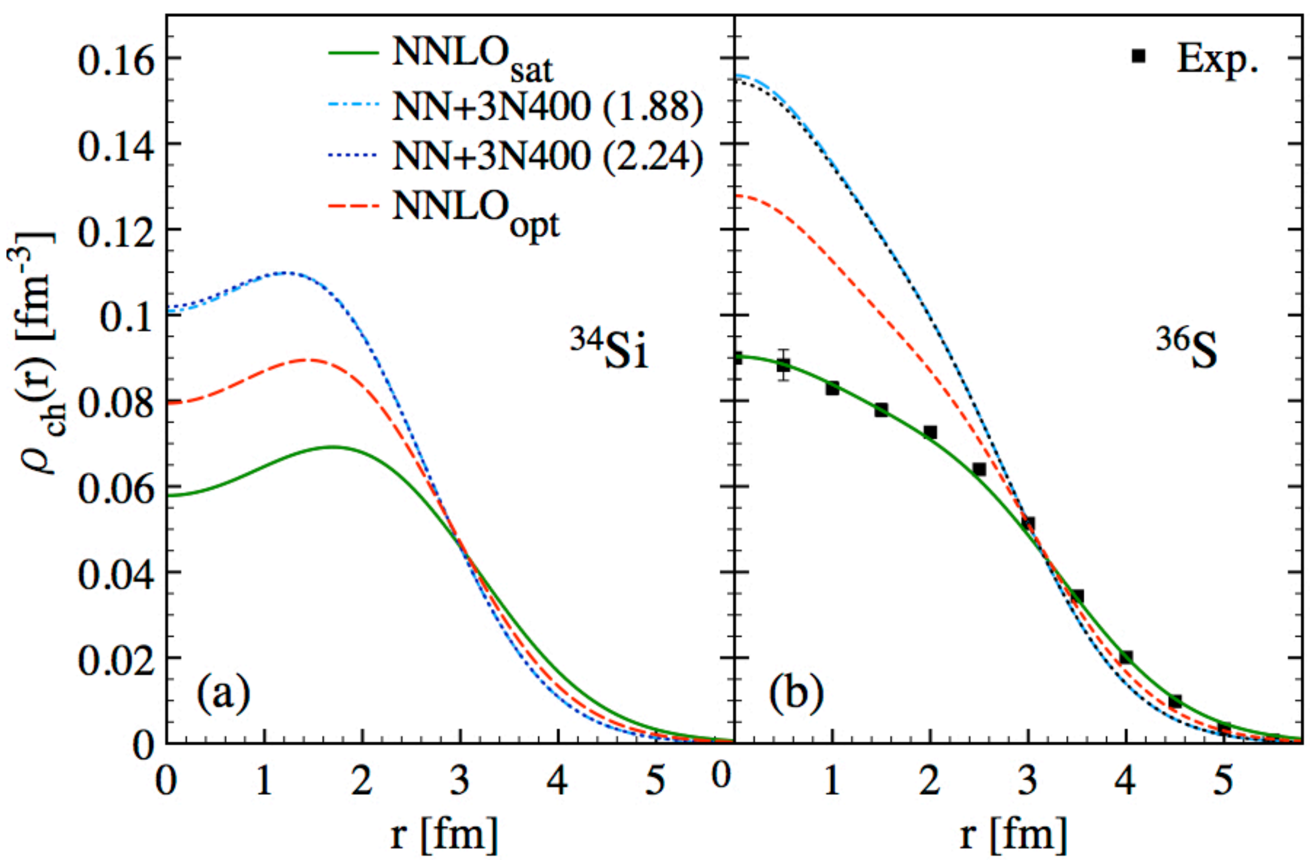
Impact of Hamiltonian (poor man's way…)

- Rms charge radius

^{36}S	NN+3N400(1.88)	NNLO$_{opt}$	NNLO$_{sat}$	Experiment
$\langle r^2_{ch}\rangle^{1/2}$	2.864	3.033	3.291	3.2985 ± 0.0024

Superior (true for BE as well)

- Charge density distribution



Consistent with charge density in ^{36}S

Empirically = NNLO$_{sat}$ is to be better trusted
Fundamentally = several question marks

Most pronounced bubble

- Consequence on the central depletion in ^{34}Si

^{34}Si	NN+3N400(1.88)	NNLO$_{opt}$	NNLO$_{sat}$
F_{ch}	0.08	0.11	0.15

- 3N interaction has severe/modest impact for NNLO$_{sat}$/NN+3N400 = leaves some question marks

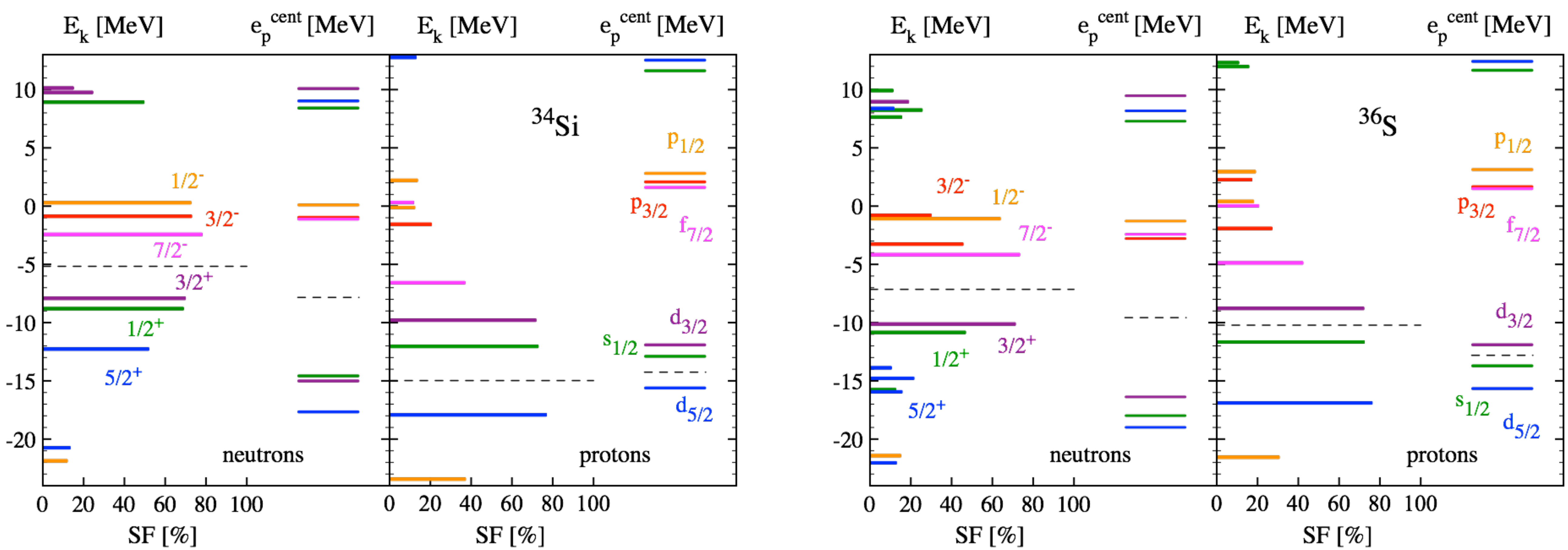
Spectroscopy in A+/-1 nuclei

- Green's function calculations access **one-nucleon addition & removal spectra**

One-nucleon separation energies vs. *Spectroscopic factors*

$$E_k^{\pm} \equiv \pm(E_k^{\mathrm{A}\pm 1} - E_0^{\mathrm{A}})$$

$$SF_k^{\pm} \equiv \sum_p S_k^{\pm pp}$$



- **Effective single-particle energies** can be reconstructed **for interpretation**

[Duguet, Hagen 2012]

[Duguet *et al.* 2015]

$$e_p^{\mathrm{cent}} = \sum_{k\in\mathcal{H}_{A-1}} E_k^{-} S_k^{-pp} + \sum_{k\in\mathcal{H}_{A+1}} E_k^{+} S_k^{+pp}$$

Comparison to data

- Addition and removal spectra can be compared to **transfer** and **knock-out reactions**

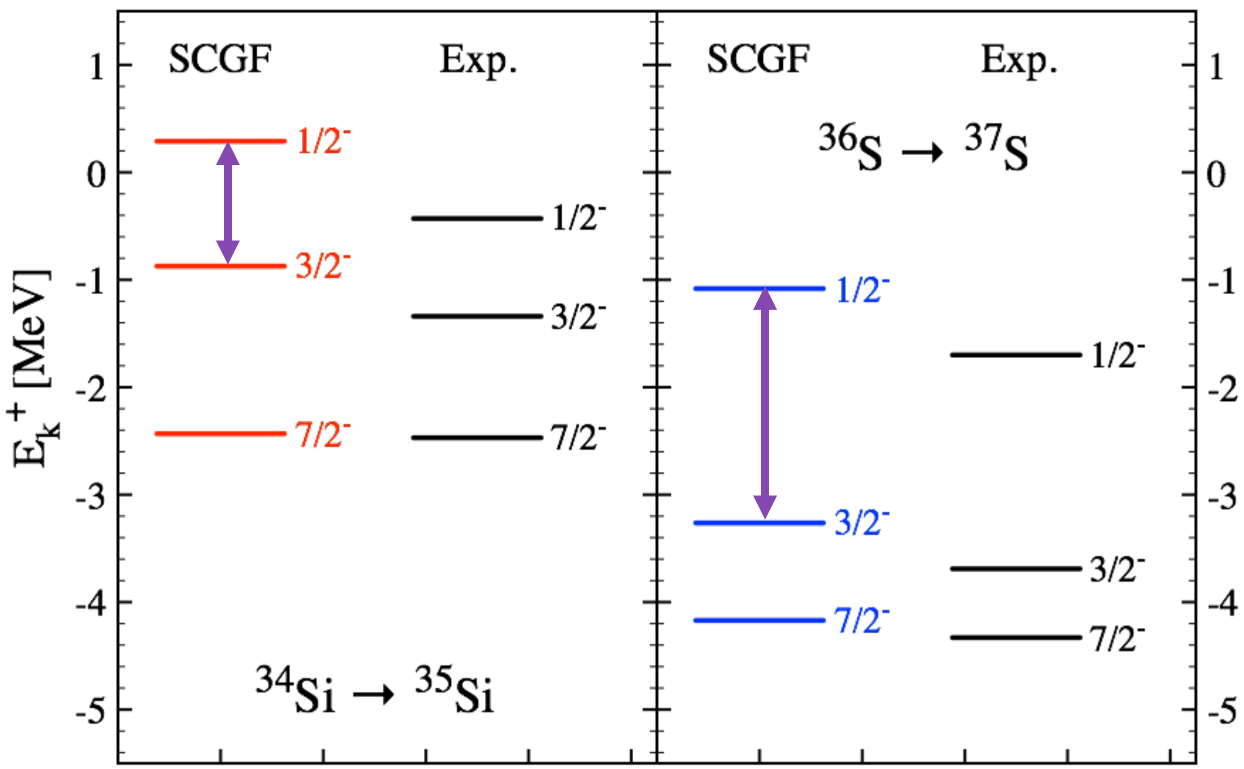
One-neutron addition

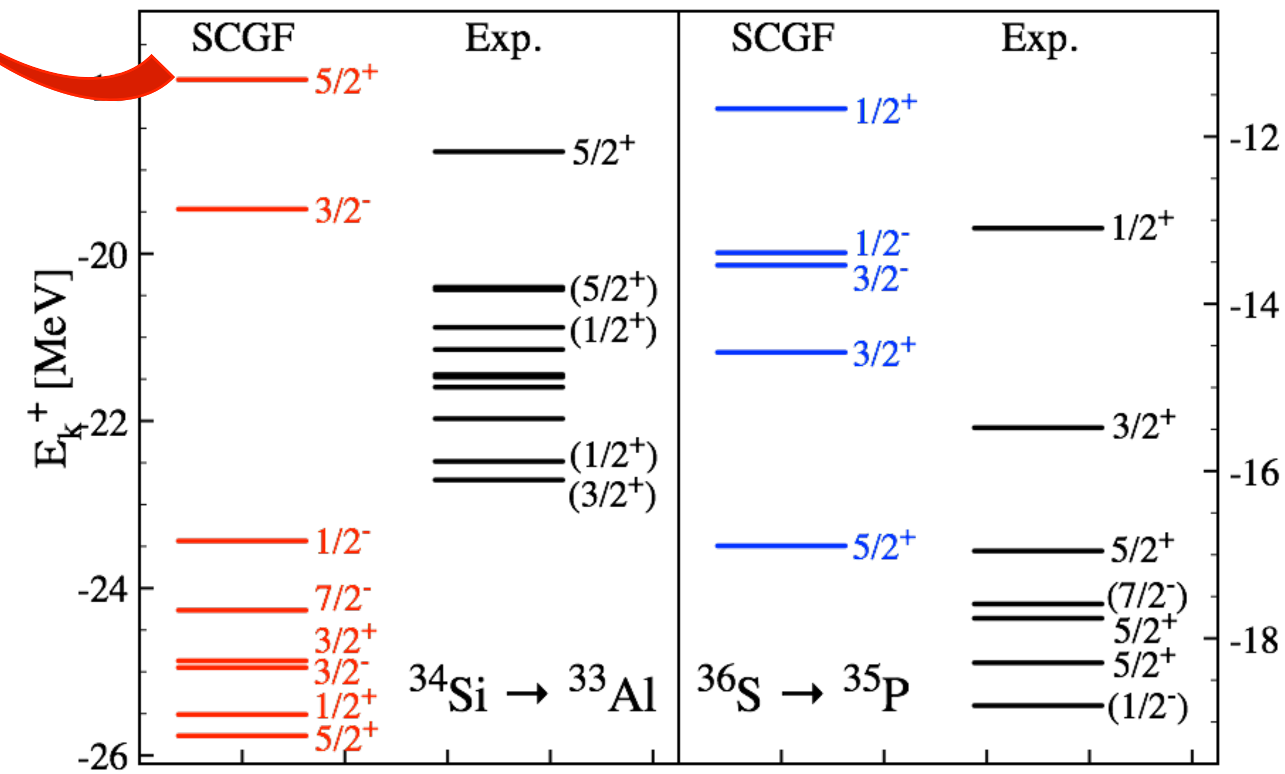
Exp. data: [Thorn *et al.* 1984] [Eckle *et al.* 1989] [Burgunder *et al.* 2014]

Quadrupole moment [Heylen *et al.* 2016]

One-proton knock-out

Exp. data: [Khan *et al.* 1985] [Mutschler *et al.* 2016] [Mutschler *et al.* 2017]





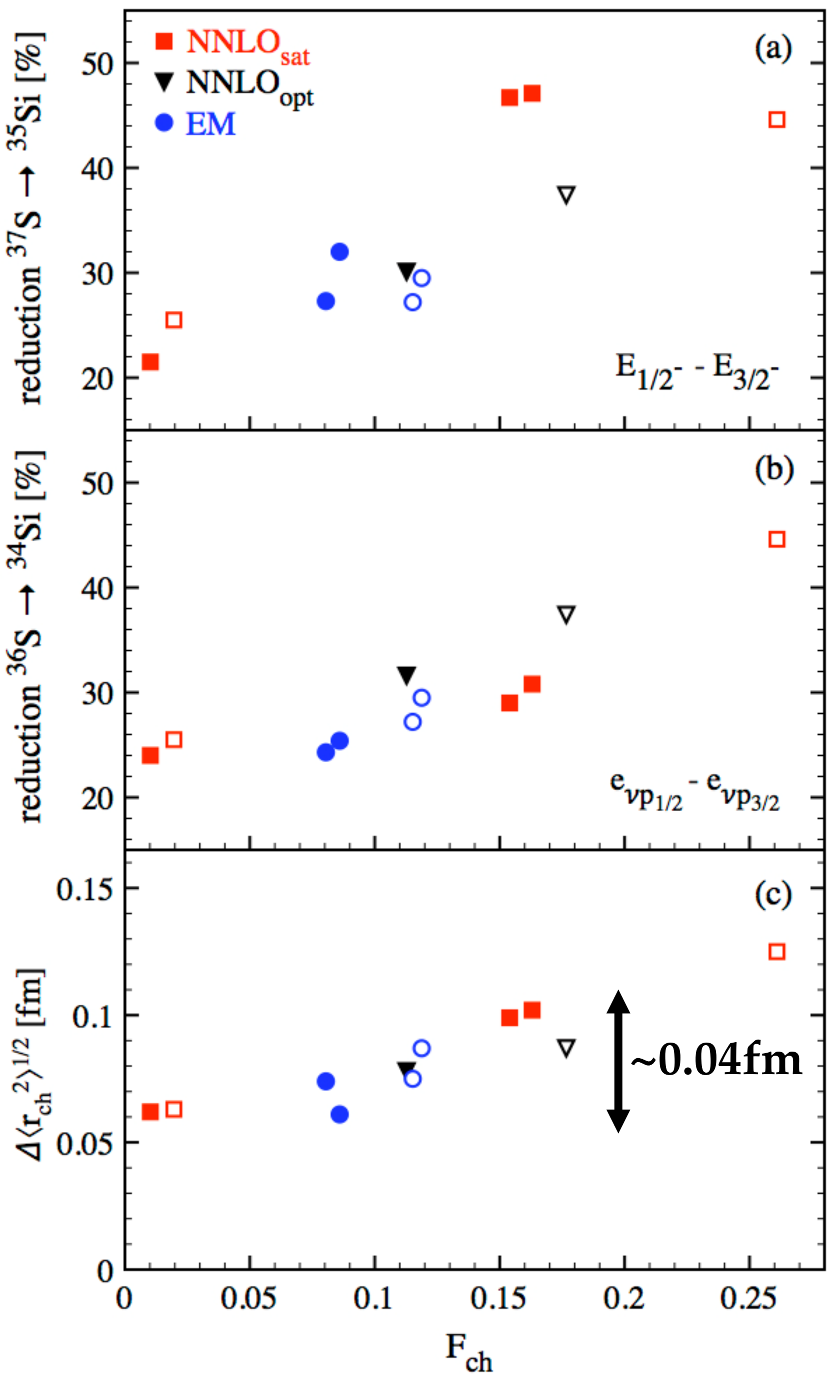
- **Good agreement** for one-neutron addition to ^{35}Si and ^{37}Si (1/2$^-$ state in ^{35}Si needs continuum)
- Much less good for one-proton removal; ^{33}Al on the edge of island of inversion: challenging!
- **Correct reduction of splitting $E_{1/2^-}$ - $E_{3/2^-}$ from ^{37}S to ^{35}Si**

Such a sudden reduction of 50% is unique
Any correlation with the bubble?!

$E_{1/2^-} - E_{3/2^-}$	^{37}S	^{35}Si	^{37}S→^{35}Si
SCGF	2.18	1.16	-1.02 (-47%)
(d,p)	1.99	0.91	-1.08 (-54%)

Bubble and spin-orbit splitting

- **Correlation** between bubble and reduction of spin-orbit splitting?
- **Gather set of calculations (various Hamiltonians, various ADC(n) orders)**



Many-body separation energies *(observable)*

○ Calculations support existence of a correlation

Effective single-particle energies *(within fixed theoretical scheme)*

○ Linear correlation holds for ESPEs in present scheme
○ Account for 50% of $E_{1/2^-}$ - $E_{3/2^-}$ reduction (+fragmentation of 3/2$^-$ strength)

Charge radius difference between ^{36}S and ^{34}Si

○ Also correlates with F_{ch}

❖ Great motivation to measure $\rho_{ch}(r)$ in ^{34}Si
❖ Very valuable to measure $\Delta\langle r^2\rangle_{ch}^{1/2}$ in the meantime

Contents

Conclusions

- Ab initio Self-consistent Green's function calculation predicts
  - Existence of a **significant depletion in $\rho_{ch}(r)$ of ^{34}Si**
  - **Correlation** between **bubble** and **weakening of many-body spin-orbit splitting**
  - **Correlation** between **bubble** and **$\Delta\langle r^2\rangle_{ch}^{1/2}$**

- Next
  - Measurement of $\delta\langle r^2\rangle_{ch}^{1/2}$ **from high-resolution laser spectroscopy@NSCL (R. Garcia-Ruiz)**
  - **Revise with**
    - **Future χ-EFT Hamiltonians**
    - **Meson-exchange currents**
  - Study other bubble candidates, e.g. in excited states
  - **Measure $\rho_{ch}(r)$ in ^{34}Si from e^- scattering?**

Nuclei	$T_{1/2}$	I^{π}	μ[nm]	Q[b]	$\langle r^2\rangle^{1/2}$ [fm]
^{24}Si	140 ms	0^+			
^{25}Si	220 ms	$5/2^+$			
^{26}Si	2.2 s	0^+			
^{27}Si	4.1 s	$5/2^+$	(-)0.8554(4)	(+)0.060(13)	
^{28}Si	stable	0^+			3.106(30)
^{29}Si	stable	$1/2^+$	-0.55529(3)		3.079(21)
^{30}Si	stable	0^+			3.193(13)
^{31}Si	157.3 m	$3/2^+$			
^{32}Si	153 y	0^+			
^{33}Si	6.1 s	$(3/2)^+$	(+)1.21(3)		
^{34}Si	2.8 s	0^+			
^{35}Si	0.8 s	$(7/2)^-$	(-)1.638(4)		

Collaborators on ab initio many-body calculations

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