Update 28/02

Michael Heines

Theory progress

- QED from Paul: Only ^{41}K left
- Konstantin is working on k and α → I will do a mudirac test after this
- Misha finished his nucleon polarization → Uncertainty treatment agreed upon
- Igor is wrapping up his nuclear polarization → Uncertainty treatment agreed upon
- Natalia is checking 1s and 2s electron screening
- Wouter and Pepijn are giving me charge distributions for V_2

QED from Paul

QED contributions

Rms radius

Z	A	RMS	J total	Nb. Conf.	Eigenv. #	E(Coul+VP11)	E(Magnetic)_	E(Retardat.)	E(Ret._>w2)_	E(Self.En.)_	E(S.E_FNS)__	E(Welt._Scr)	not used	not used	E(VP_had11)_	E(El.Den.VP)	E(Vac._P_13)	E ...
19	39	3.4006	1	1	1	-255429.3718	0.0000	0.0000	0.0000	-1.0737	0.2583	0.0000	0.0000	0.0000	-0.0069	0.0000	1.0518	
19	39	3.4006	1	1	1	-968222.4933	0.0000	0.0000	0.0000	300.8085	-106.4934	0.0000	0.0000	0.0000	-9.2211	0.0000	5.0209	
19	39	3.4023	1	1	1	-255429.3044	0.0000	0.0000	0.0000	-1.0737	0.2585	0.0000	0.0000	0.0000	-0.0069	0.0000	1.0518	
19	39	3.4023	1	1	1	-968178.6914	0.0000	0.0000	0.0000	300.8085	-106.5477	0.0000	0.0000	0.0000	-9.2182	0.0000	5.0206	
19	39	3.4040	1	1	1	-255429.2369	0.0000	0.0000	0.0000	-1.0737	0.2588	0.0000	0.0000	0.0000	-0.0069	0.0000	1.0518	
19	39	3.4040	1	1	1	-968134.8843	0.0000	0.0000	0.0000	300.8085	-106.6019	0.0000	0.0000	0.0000	-9.2153	0.0000	5.0202	
19	39	3.4057	1	1	1	-255429.1694	0.0000	0.0000	0.0000	-1.0737	0.2590	0.0000	0.0000	0.0000	-0.0069	0.0000	1.0518	
19	39	3.4057	1	1	1	-968091.0718	0.0000	0.0000	0.0000	300.8085	-106.6561	0.0000	0.0000	0.0000	-9.2124	0.0000	5.0199	
19	39	3.4074	1	1	1	-255429.1018	0.0000	0.0000	0.0000	-1.0737	0.2592	0.0000	0.0000	0.0000	-0.0069	0.0000	1.0518	
19	39	3.4074	1	1	1	-968047.2543	0.0000	0.0000	0.0000	300.8085	-106.7102	0.0000	0.0000	0.0000	-9.2096	0.0000	5.0196	
19	39	3.4091	1	1	1	-255429.0342	0.0000	0.0000	0.0000	-1.0737	0.2595	0.0000	0.0000	0.0000	-0.0069	0.0000	1.0518	
19	39	3.4091	1	1	1	-968003.4316	0.0000	0.0000	0.0000	300.8085	-106.7644	0.0000	0.0000	0.0000	-9.2067	0.0000	5.0192	
19	39	3.4109	1	1	1	-255428.9625	0.0000	0.0000	0.0000	-1.0737	0.2597	0.0000	0.0000	0.0000	-0.0069	0.0000	1.0518	
19	39	3.4109	1	1	1	-967957.0215	0.0000	0.0000	0.0000	300.8085	-106.8217	0.0000	0.0000	0.0000	-9.2037	0.0000	5.0189	
19	39	3.4126	1	1	1	-255428.8947	0.0000	0.0000	0.0000	-1.0737	0.2600	0.0000	0.0000	0.0000	-0.0069	0.0000	1.0518	
19	39	3.4126	1	1	1	-967913.1870	0.0000	0.0000	0.0000	300.8085	-106.8758	0.0000	0.0000	0.0000	-9.2008	0.0000	5.0185	
19	39	3.4143	1	1	1	-255428.8269	0.0000	0.0000	0.0000	-1.0737	0.2602	0.0000	0.0000	0.0000	-0.0069	0.0000	1.0518	
19	39	3.4143	1	1	1	-967869.3430	0.0000	0.0000	0.0000	300.8085	-106.9300	0.0000	0.0000	0.0000	-9.1979	0.0000	5.0182	

Only term with significant radius sensitivity

Spread with radius ~ 1eV

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What to do

- QED from Paul: Transition energy as function of c

$$\rho(r) = \frac{\rho_0}{1 + \exp\left[4 \ln 3 \left(\frac{r - c}{2.3\ fm}\right)\right]}$$

- Add NP (constant on top) and recoil correction (almost constant)

- Calculate Barrett radius for all c:
  - Cutoff radius for integral?
  - Step size in r for Riemann sum?

- What order polynomial to fit with?

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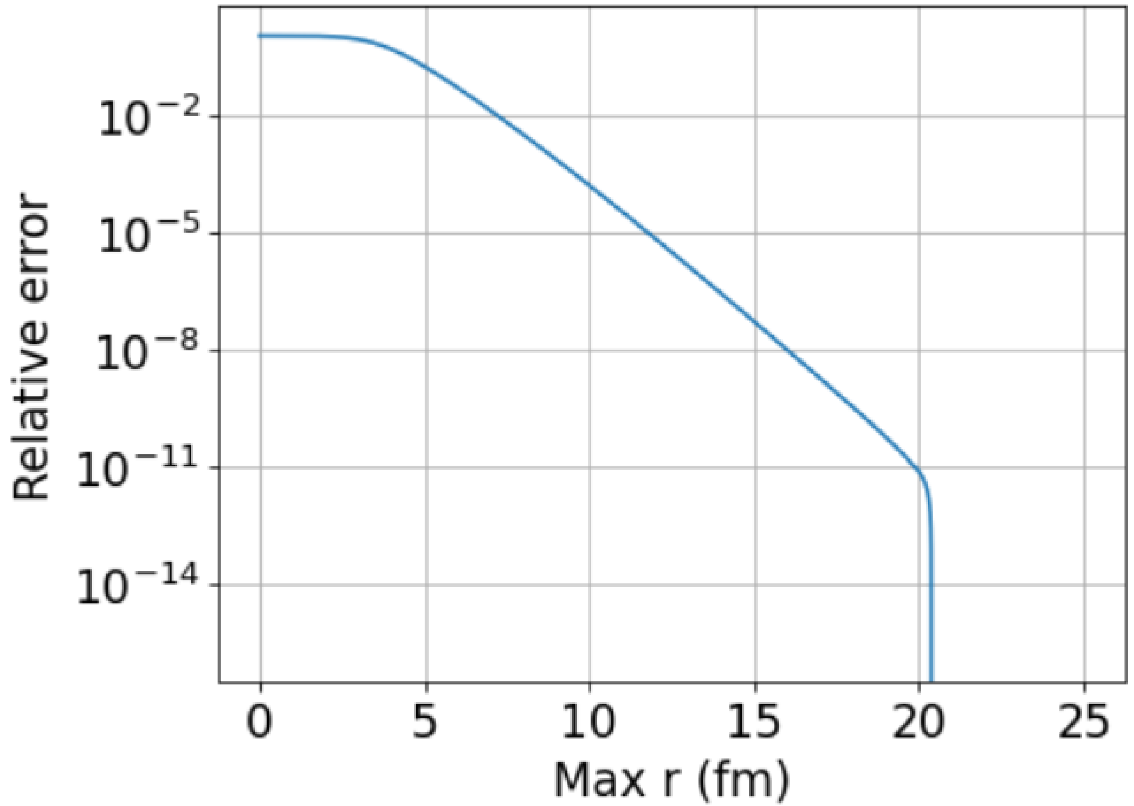
Cutoff radius

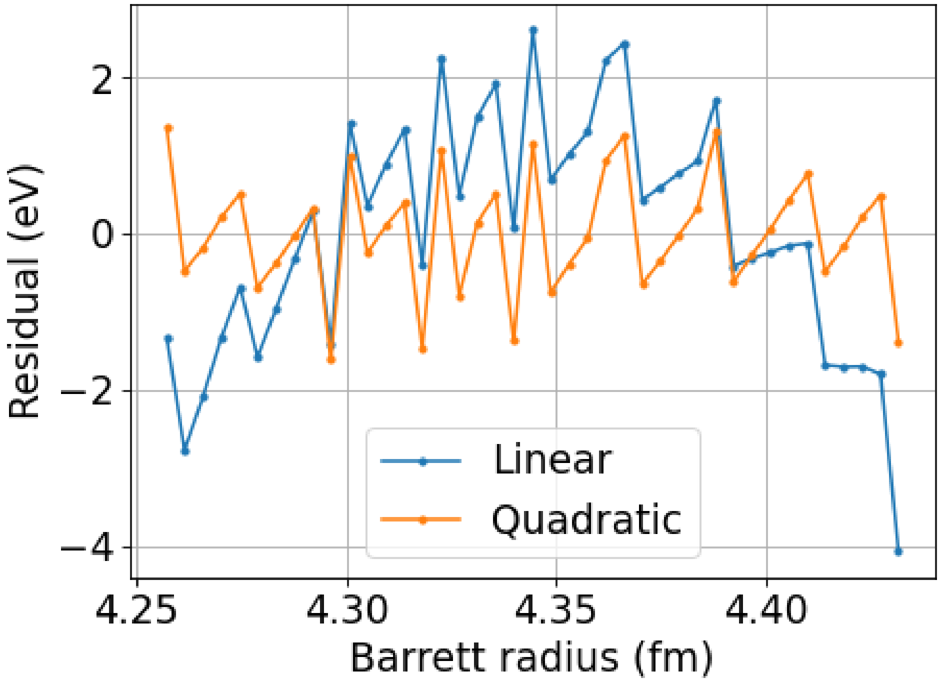
- Charge distribution drops of fast, but:
  - r^2 in Jacobian
  - r^2 for rms / $r^{k\approx 2.1}$ for Barrett
- How far is far enough?
  - 1e-7 precision at Max = 15 fm
  - Complete crash around 20 fm
  - Proceeded with 25 fm



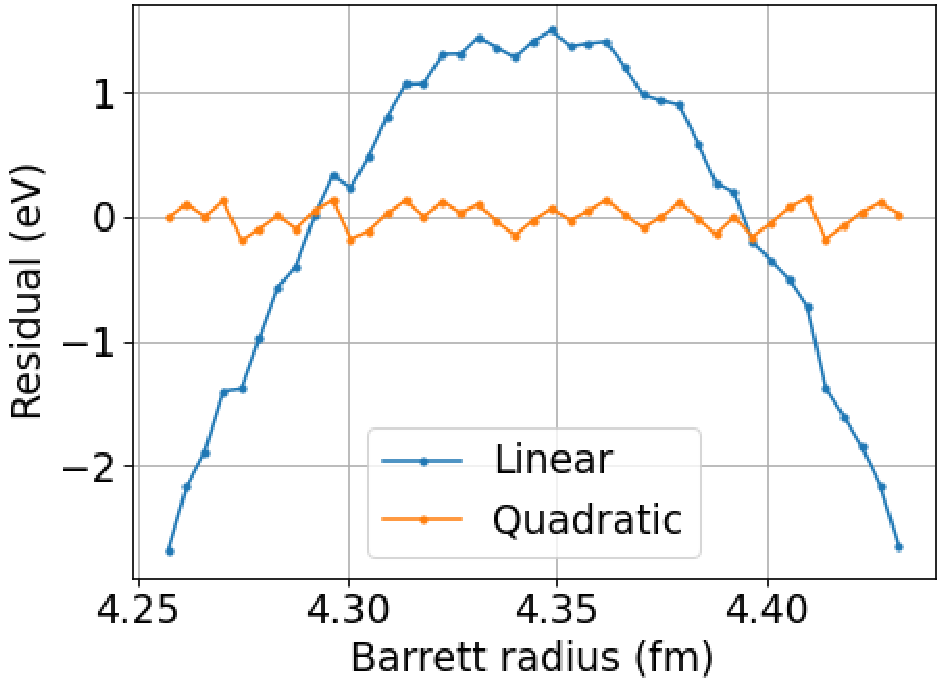
Coarseness in r

Riemann sums → How small is small enough?

- 0 → 25 fm with 1e-4 fm spacing (~10-20 seconds)



- 0 → 25 fm with 1e-5 fm spacing (~2 minutes)



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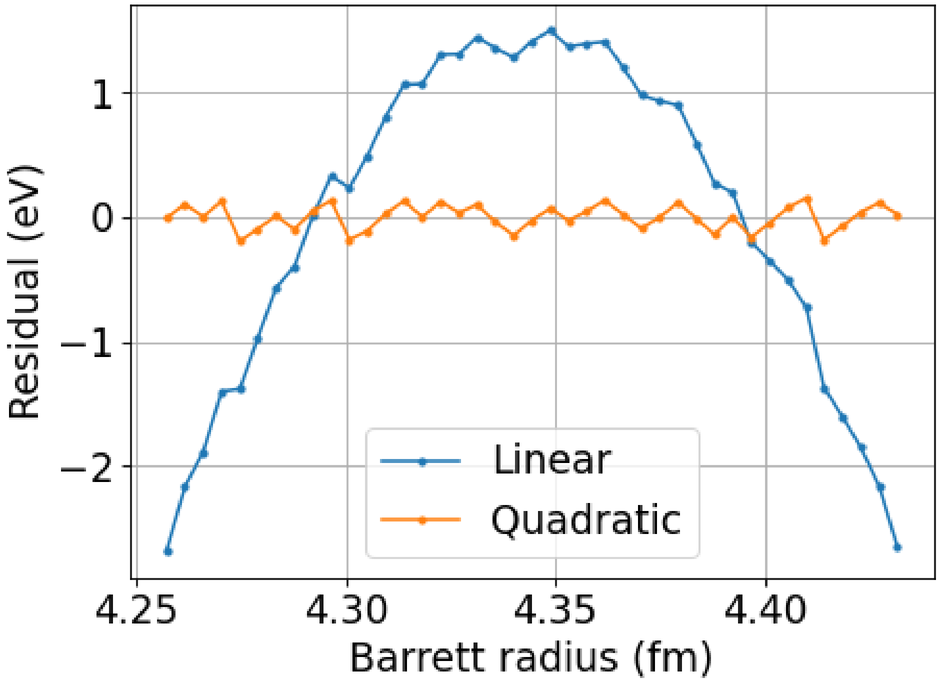
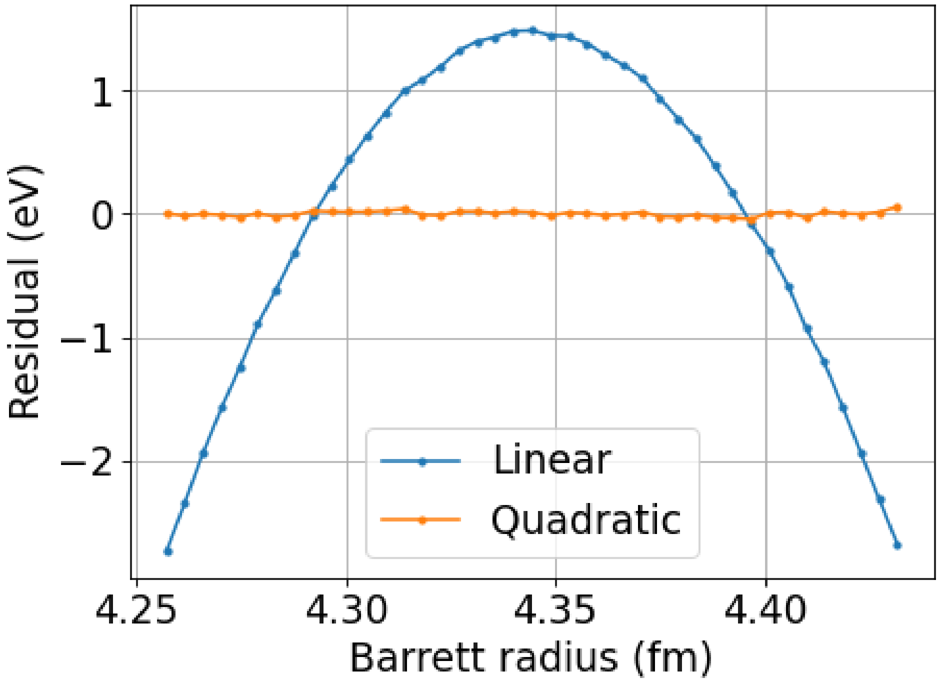
Coarseness in r

Riemann sums → How small is small enough?

- 0 → 25 fm with 1e-5 fm spacing (few minutes)



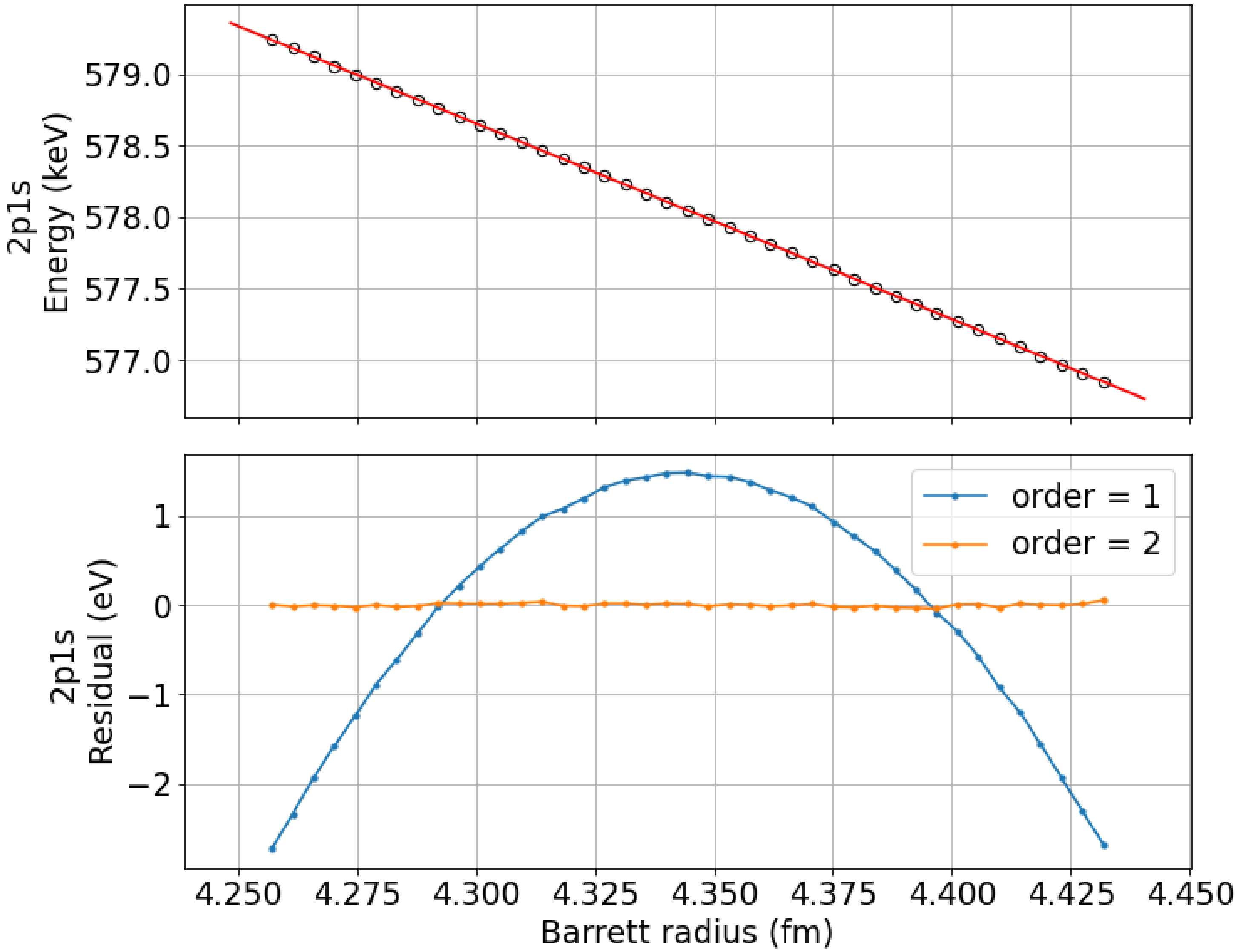
- 0 → 25 fm with 1e-6 fm spacing (~20-30 mins)



Decision

- Using 1e-6 fm steps
- < 0.05 eV deviation in CI

- Precision:
  - Exp = ~15 eV
  - NP = ~40 eV



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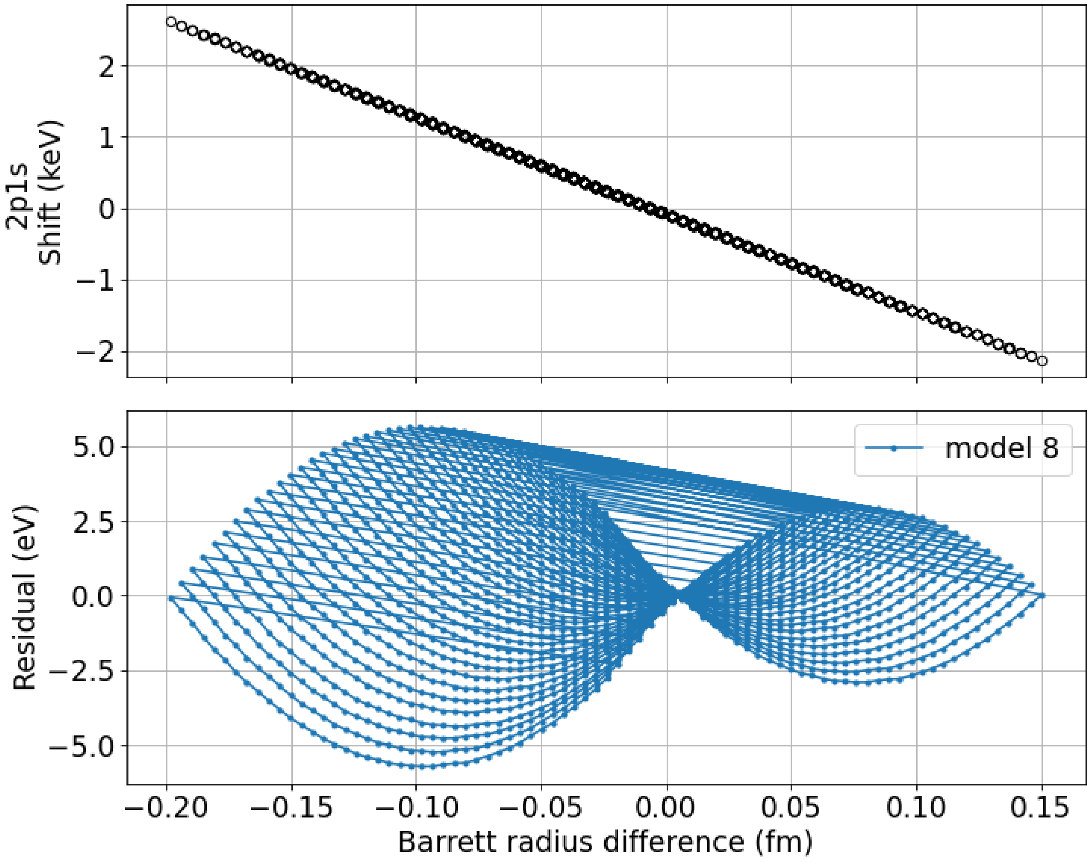
What about differences?

- Isotope shifts better than absolute energies
- NP on difference better than absolute values
- Calculate the isotope shift as function of Barrett radius difference
- Mostly linear, some weird additional trends



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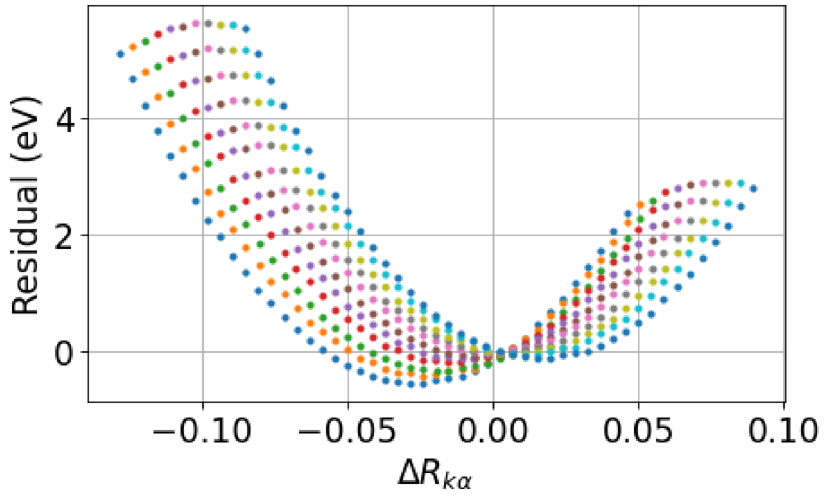
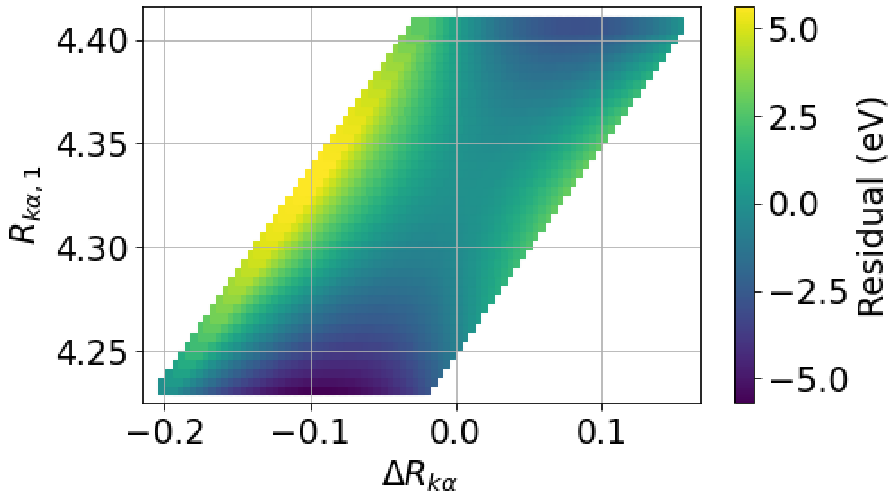
What is it? Do we care?

- $R_{k\alpha,1}$ not completely decoupled from $\Delta R_{k\alpha}$
- Minor shift in fit for different $R_{k\alpha,1}$
- Options:
  - 2D fit constraining $R_{k\alpha,1}$ to previous extraction
  - Ignore → $\sigma_{exp} > 5\ eV; \sigma_{NP} \approx 10\ eV$





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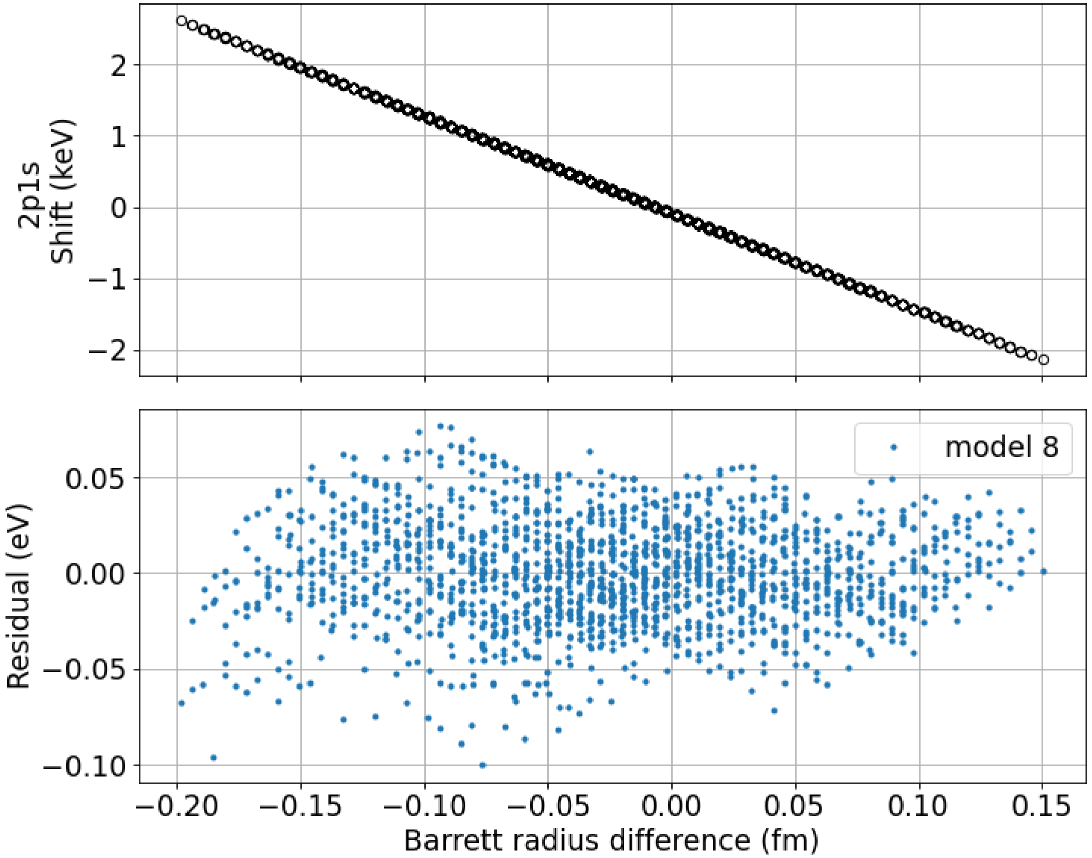
Accounting for $R_{k\alpha}$

- Checked different models. Best model is

$$\Delta E = b_0 + b_1 \Delta R_{k\alpha} + b_2 \Delta R_{k\alpha} + b_3\, R_{k\alpha,1} \Delta R_{k\alpha} + b_4 R_{k\alpha,1}$$

- Residual reduced to ~50 meV!



Drumroll...

^{39}K $R_{k\alpha}$:

Literature: 4.4077(16)[18] fm

Literature E + our theory: 4.4075(16)[?] fm

Our 2p1s: 4.4091(7)[?] fm

Our 3p1s: 4.4083(8)[?] fm

Our 4p1s: 4.4102(8)[?] fm

Our average: 4.4092(6)[?] fm $\chi_\nu^2 = 1.61\ (p \approx 0.2)$

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Radii of Cl

Radius	Value	σ_E	σ_{NP}	σ_{V_2}	σ_{Tot}
R (^{35}Cl)	3.3358	0.0005	0.0020	0.0041	0.0065
R (^{37}Cl)	3.3463	0.0008	0.0020	0.0041	0.0068
R (^{37}Cl) - R (^{35}Cl)	0.0113	0.0006	0.0007	0.0013	0.0026
$\delta\langle r^2\rangle$	0.0755	0.0039	0.0049	0.0086	0.0175

Assuming 95% V2 correlation

Literature:

- R (^{35}Cl) = 3.388(15) → ~3.5σ too high (2.3x larger error)
- R (^{37}Cl) = 3.384(15) → ~2.5 σ too high (2.2x larger error)

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Assuming 95% V2 correlation

X10 improvement on literature

Literature:

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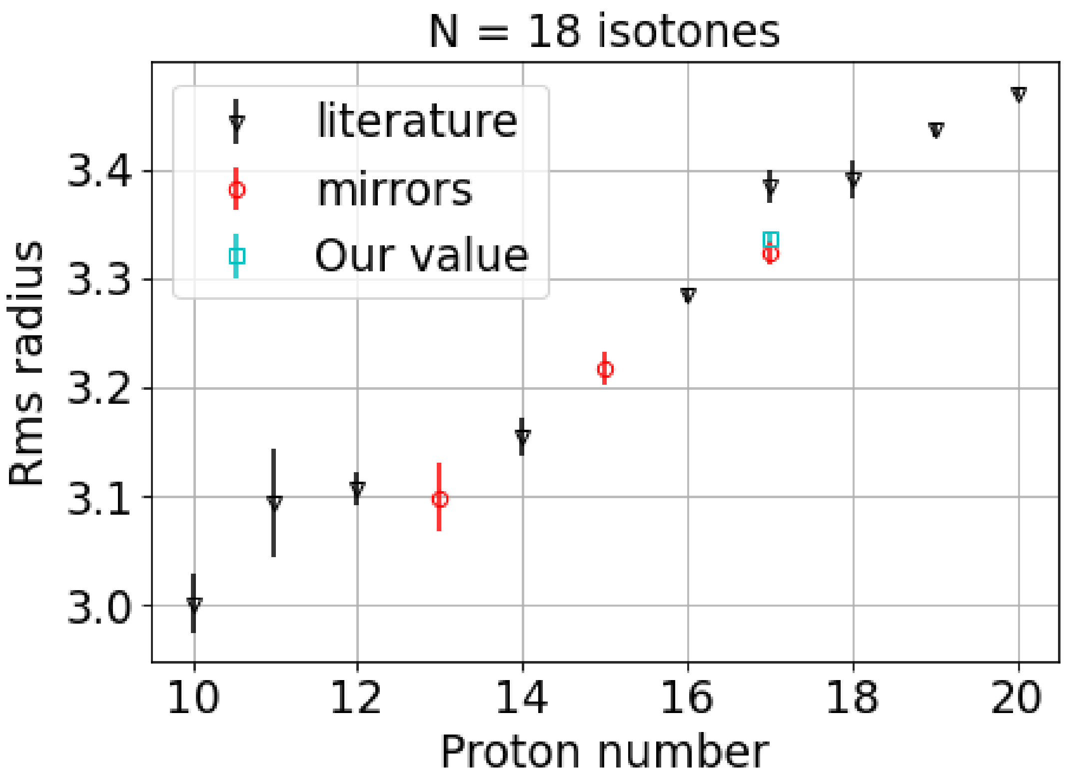
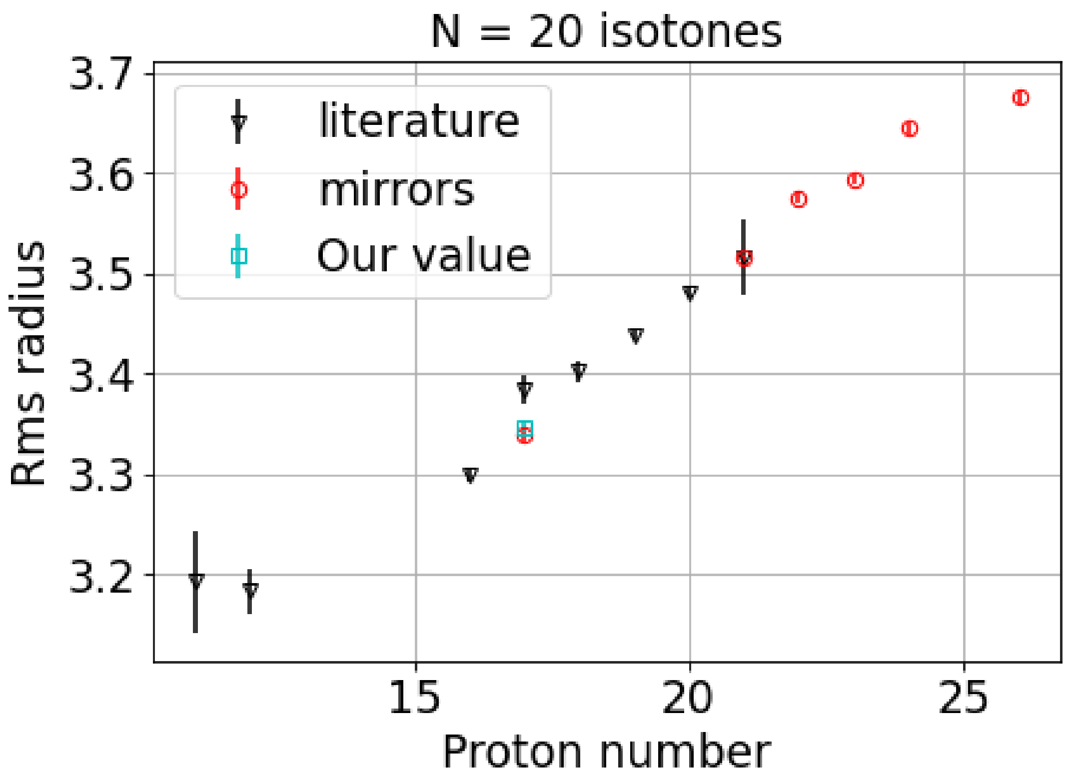
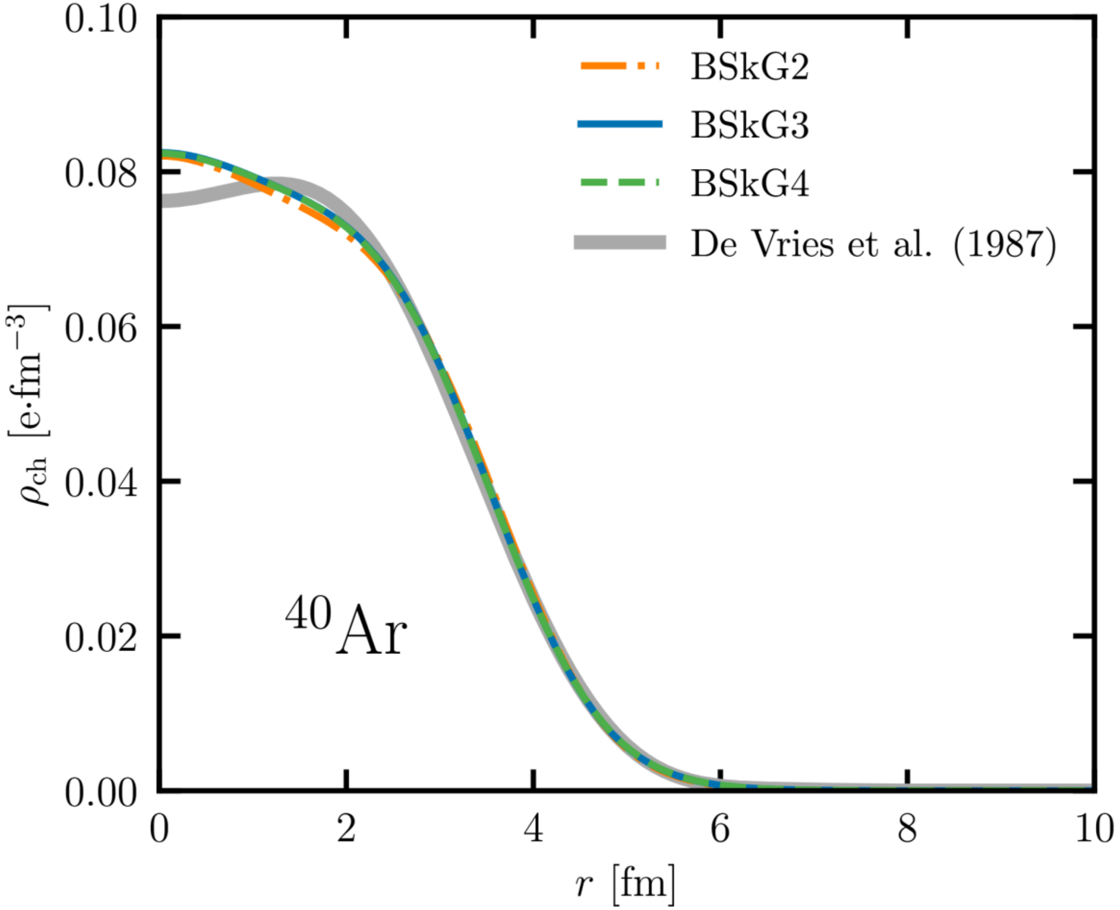
Do those preliminary radii make sense



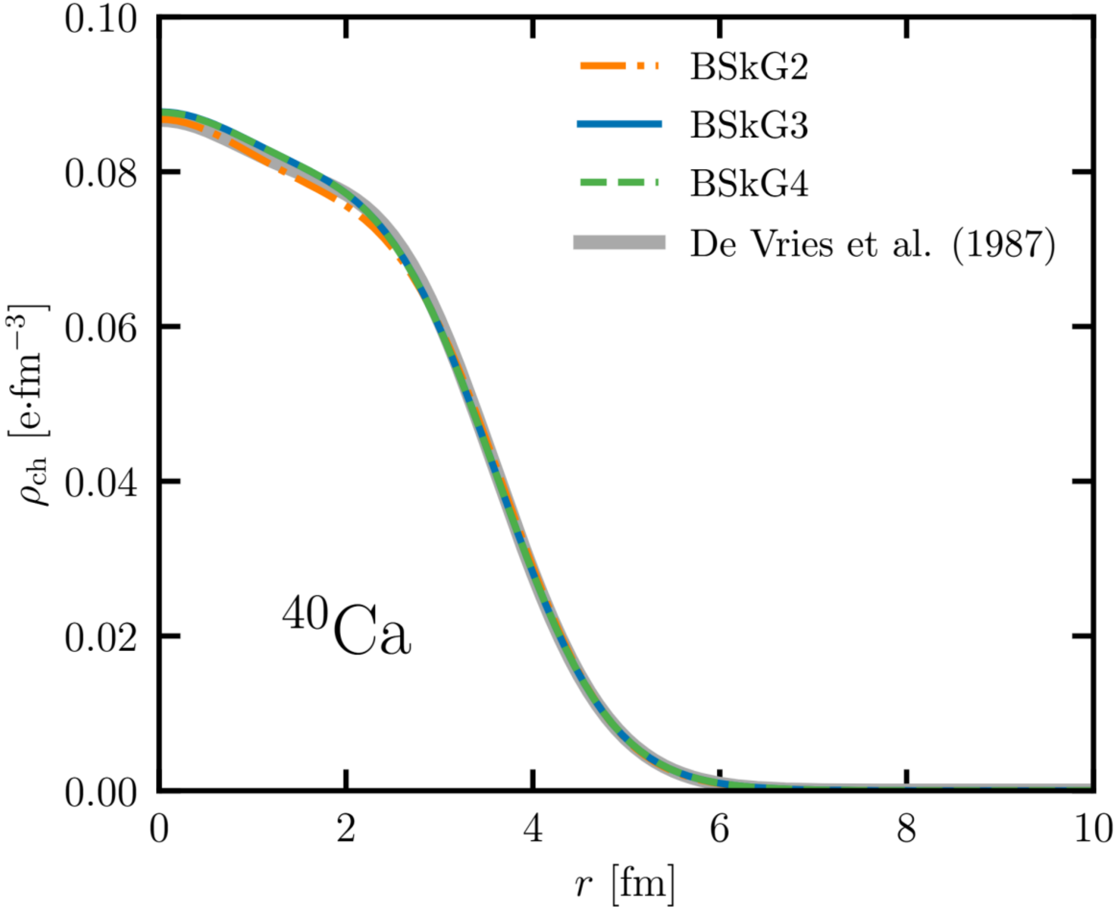


V_2 from DFT nuclear theory

$q_{max} = 1.8$



$q_{max} = 3.7$



V_2 from DFT nuclear theory

- For now: some test cases

$$\Delta V_2 = V_2(Exp) - V_2(DFT)$$

Very good agreement! Equivalent to high q scattering experiment?

Isotope (measurement)	**ΔV_2(BSkG2) (1e-4)**	**ΔV_2(BSkG3) (1e-4)**	**ΔV_2(BSkG4) (1e-4)**	**$\delta V_2(Exp)$ (1e-4)**
^{40}Ar	-7.7	-3.4	-2.5	15
^{40}Ca (Si73)	-12.6	-7.9	-7.8	8.2
^{40}Ca (Em83b)	4.4	9.1	9.1	8.2
^{48}Ca (Em83b)	4.0	9.9	9.4	8.7
^{30}Si (Mi82+)	-8.9	-3.5	-3.1	16

Differences better than absolutes

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