Ab-Initio Building Blocks for Nuclear DFT

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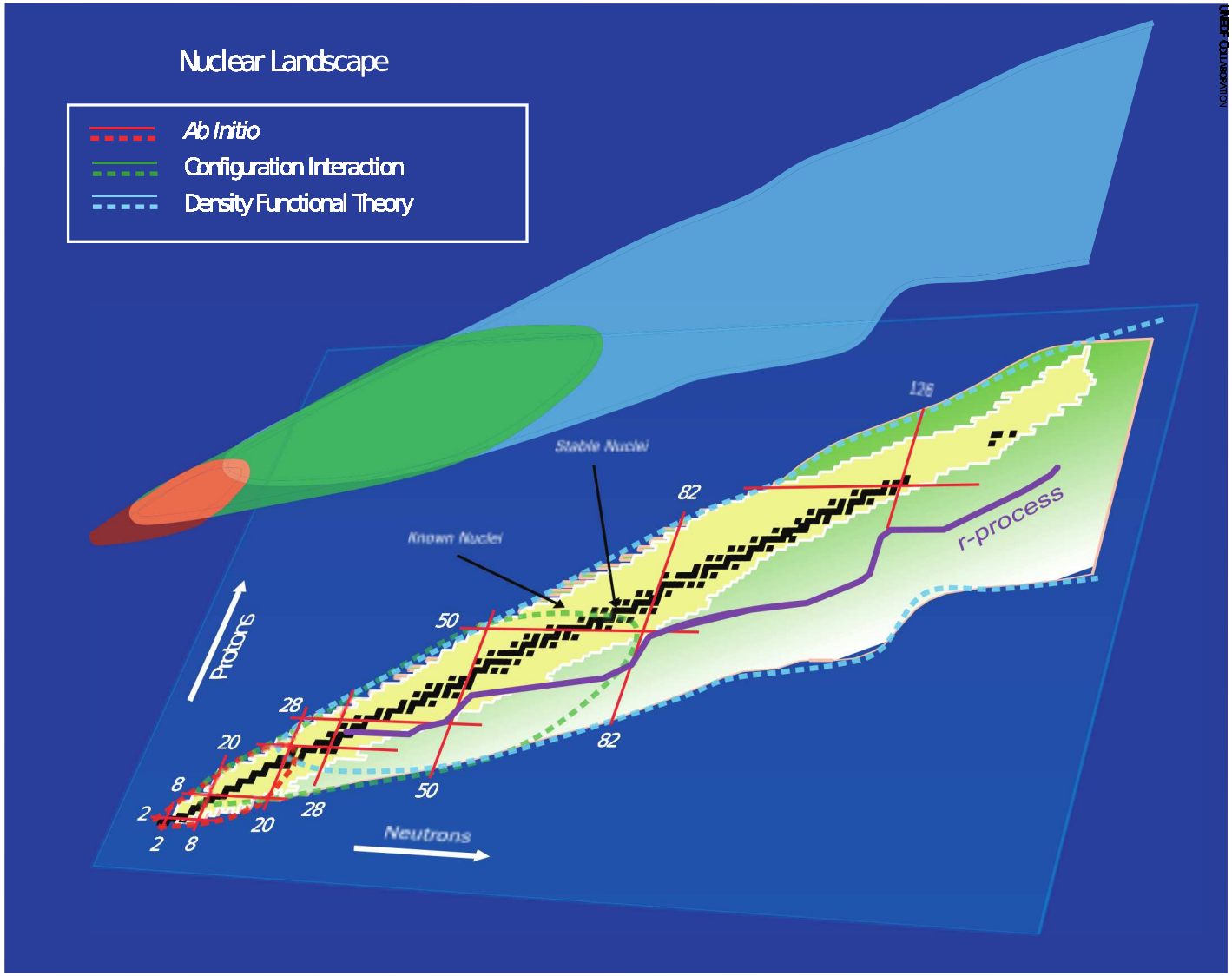
Nuclear structure: methods



Outline

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Kohn-Sham DFT

- Hohenberg-Kohn: there exists a functional of the density yielding the exact many-body energy of an interacting system

$$\begin{aligned}\mathcal{F}[U] &= \min_{\Phi} \left\langle \Phi \left| \hat{H} + \hat{U} \right| \Phi \right\rangle, \\ &= \min_{\Phi} \left[\left\langle \Phi \left| \hat{H} \right| \Phi \right\rangle + \int d^3\mathbf{r}\, U(\mathbf{r}) \rho_{\Phi}(\mathbf{r}) \right].\end{aligned}$$

$$\mathcal{E}[\rho] = \mathcal{F}[U] - \int d^3\mathbf{r}\, U(\mathbf{r}) \rho(\mathbf{r}),$$

- Kohn-Sham scheme

$$\mathcal{E}[\rho] = \mathcal{E}_T[\rho] + \mathcal{E}_{\rm KS}[\rho]$$

  - $\mathcal{E}_T[\rho]$: Exact functional of the non-interacting system
  - $\mathcal{E}_{\rm KS}[\rho]$: Interaction-correlation energy
  - KS replaces interacting system with non-interacting one in external potential

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Ab-initio inputs fur nuclear functionals

- Typically assume form of functional and fit parameters
- Observables: cannot do better than experiment
- ✔ Theoretical intermediates

- Use Kohn-Sham DFT (formulated for a trapped nucleus) mapped on CCSD
- Adequate for a doubly-magic nucleus
- Start from a g.s. CCSD calculation (^{48}Ca, $V_{\mathrm{low}\ k}$ $\Lambda = 1.9$)
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Determining KS potentials

- Zeroth order: ground state
- First order: KS fields U_{KS} and W_{KS}

$$U_{KS}(r) = \frac{\delta \mathcal{E}_{KS}[\rho, J]}{\delta \rho(r)} \qquad W_{KS}(r) = \frac{\delta \mathcal{E}_{KS}[\rho, J]}{\delta J(r)}$$

- Fit U_{KS} and W_{KS} such that CC g.s. densities are reproduced
- Let

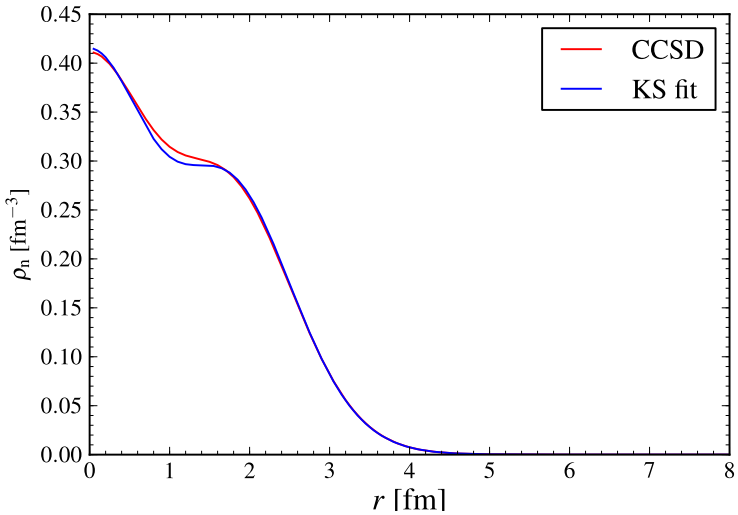
$$S^2 = \int \left(\frac{\rho_{\mathrm{KS}} - \rho_{\mathrm{CCSD}}}{\rho_{\mathrm{CCSD}}} \right)^2 + \left(\frac{J_{\mathrm{KS}} - J_{\mathrm{CCSD}}}{|J_{\mathrm{CCSD}}| + \epsilon} \right)^2 dr$$

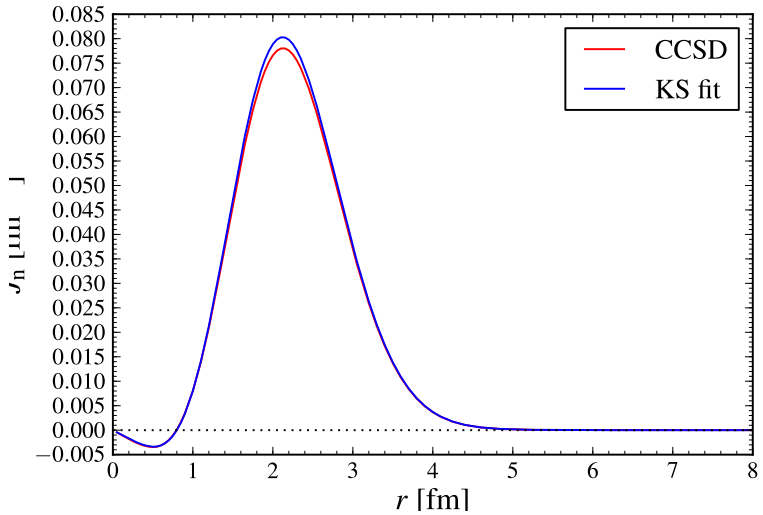
- Minimize w.r.t. U (central) and W (s.o.) fields
  - For a trial $(U(r), W(r))$, solve the KS equations, build densities

$$\left[-\frac{\hbar^2}{2m} \left(\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{\ell(\ell+1)}{r^2} \right) + U + W \frac{j(j+1) - \ell(\ell+1) - 3/4}{r} - \varepsilon_{n\ell j} \right] \varphi_{n\ell j} = 0$$

  - On the same basis as the CC calculation

Densities

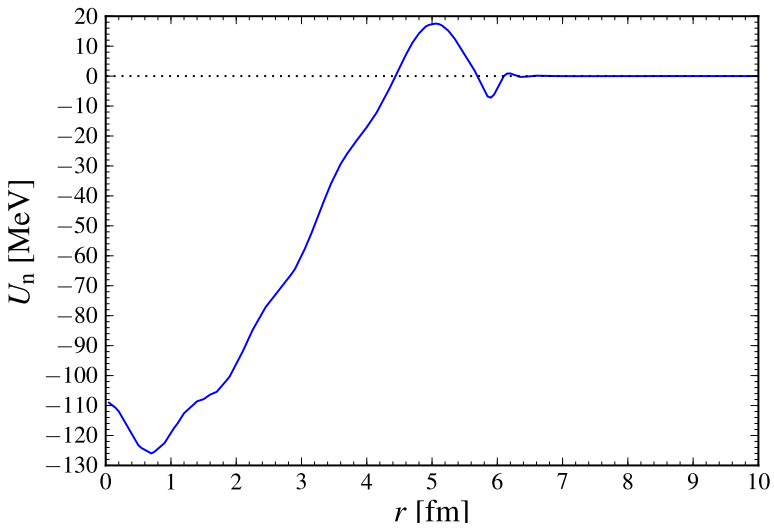




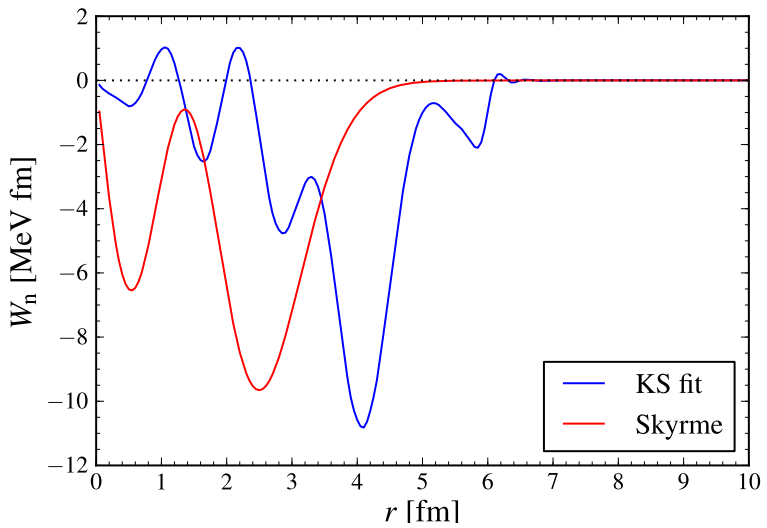
- Non-interacting V-representability not guaranteed for (ρ, J)
- J in KS depends only on $f_{7/2}$ orbital (filled spin-orbit partners give 0)
- If intruder configurations in CC, will be difficult to reproduce

Potentials

Central potential U

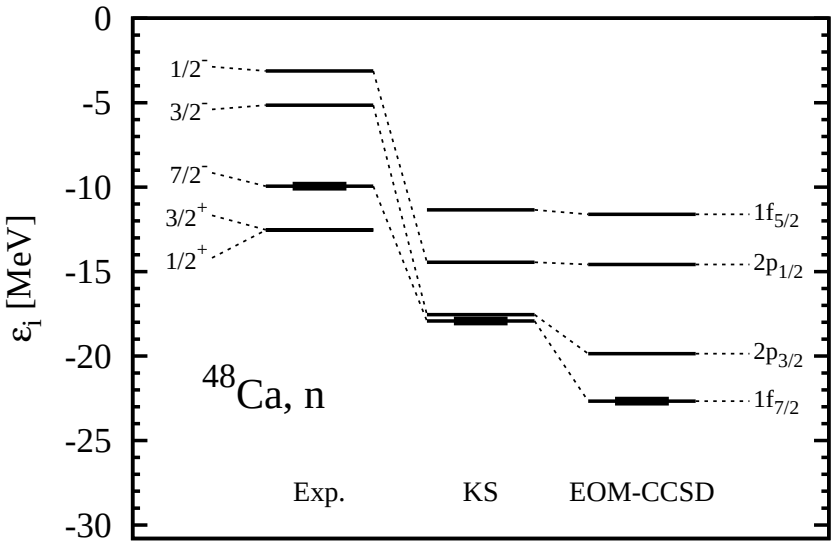


Spin-orbit potential



Single-particle energies

- ε_i: eigenvalues of the KS potentials
- In principle, meaningless except the Fermi level ("DFT-Koopmans" theorem)
- Need good fit to asymptotic density AND correct exponential asymptotic behavior
- In practice, need to be close to exp. separation energies



- 5 MeV disagreement - EOM-CC doesn't give true SPE or...

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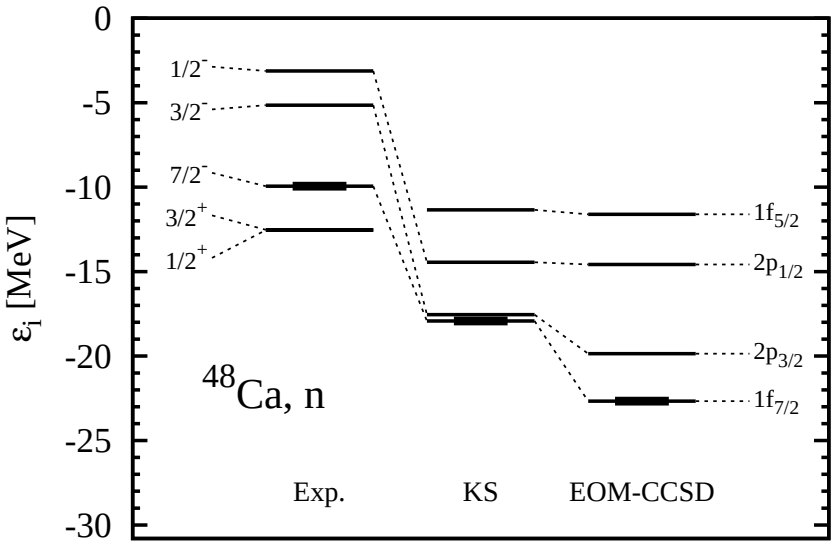

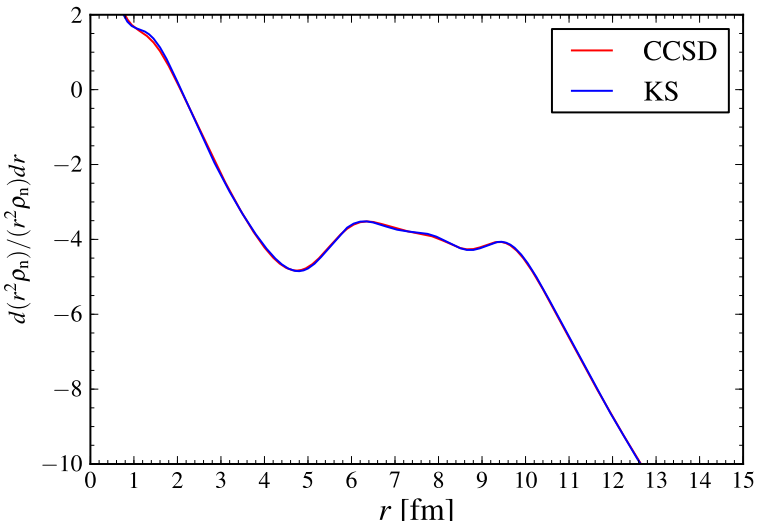

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Static Linear response (In progress)

- G.s. energy and fields give us a 1st-order expansion of $\mathcal{E}[\rho, J]$ around the minimum
- Second order: Why?
- Most proposed functionals are bilinear in densities:

$$\mathcal{E}[\rho,\tau,J] = \int d^3r\, d^3r' [v_1(r-r')\rho(r)\rho(r') + v_2(r-r')\rho(r)\tau(r') + ...]$$

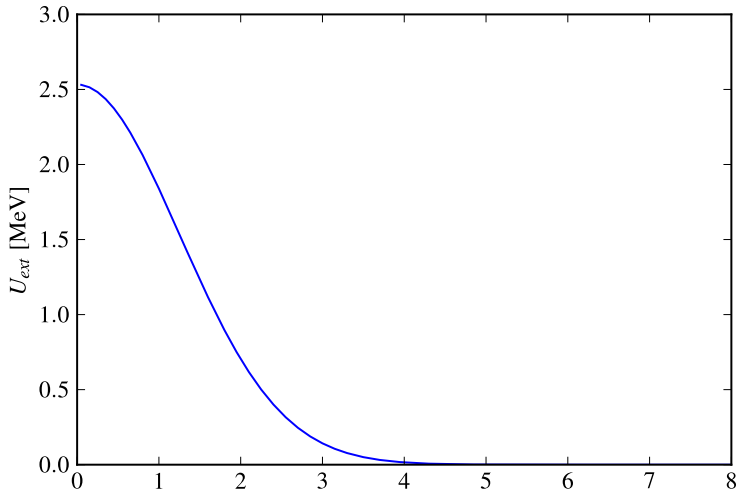
- Calculating second derivatives of E probes prefactors (Skyrme, Gogny...)

$$v_{KS}^{\rho\rho}(r,r') = \frac{\delta\mathcal{E}}{\delta\rho(r)\delta\rho(r')} = \frac{\delta U_{KS}(r')}{\delta\rho(r)}$$

$$v_{KS}^{JJ}(r,r') = \frac{\delta\mathcal{E}}{\delta J(r)\delta J(r')} = \frac{\delta W_{KS}(r')}{\delta J(r)}$$

- Can assess whether proposed functional form is consistent with CC

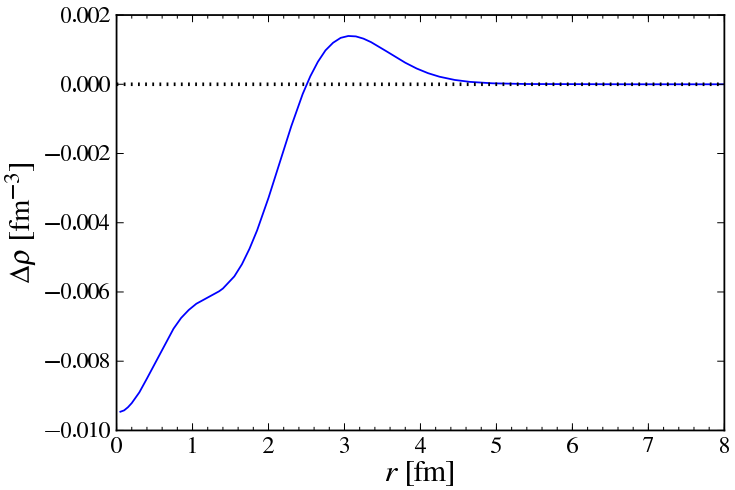
- Can't vary densities explicitly.
  - Application of external field U_{ext} induces a change in density
- Examine reaction of KS fields to multiple U_{ext}, W_{ext}
- Perform CC calculations in presence of external fields and repeat fits



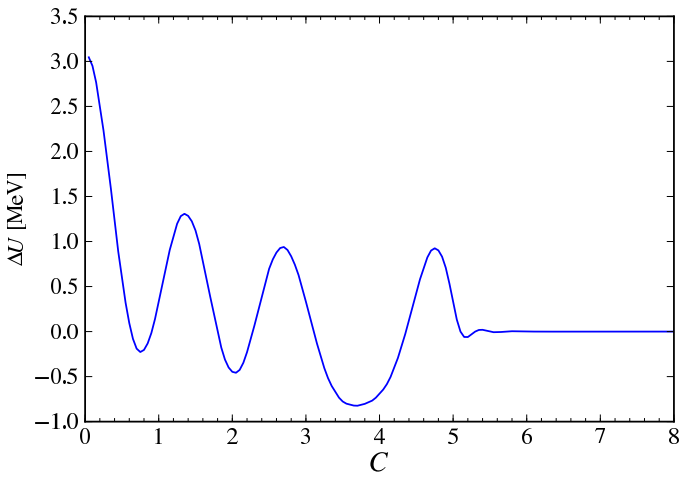
Static Linear response (In progress)

- Response of density to U_{ext}

Local density



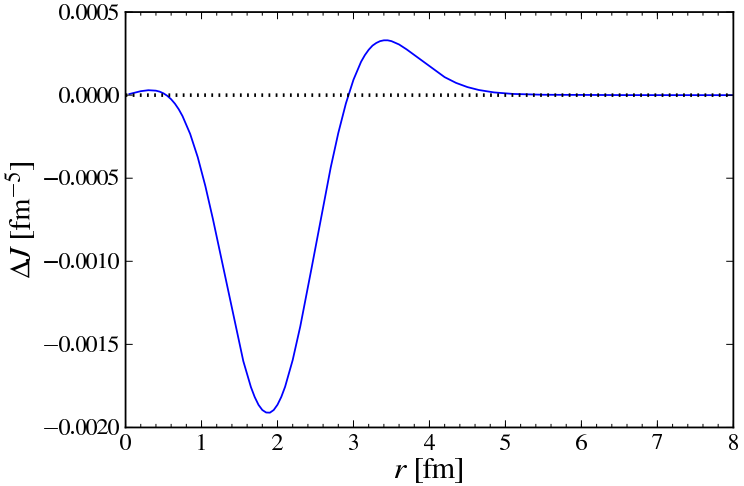
Central potential



Static Linear response (In progress)

- Response of spin-orbit density to W_{ext}

Spin-orbit density



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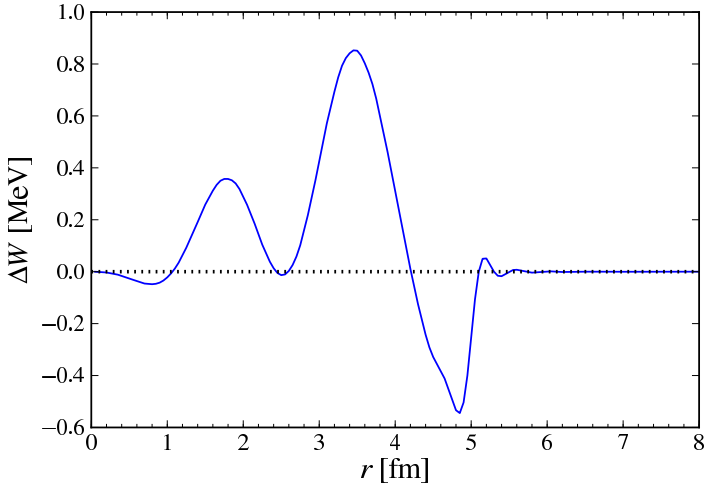

- Procedure seems to work - still need to calculate other derivatives

Outline

Summary and outlook

- Progress in many-body techniques and understanding of the nuclear $\hat{H}$ allows to add meaninful input to nuclear functionals
- Kohn-Sham DFT useful in establishing theory vs. theory comparison
- Issues may arise (V-representability, numerics) but technique is promising
- Work with intrinsic densities
- Perform further CC calculations with various external potentials to probe spatial response of KS fields to density variations
- Can also assume analytic functional form and fit parameters at level of potential instead of data
- Self-consistency check: should agree with CC g.s. energy

Thank you !