

# Ab-Initio Building Blocks for Nuclear DFT

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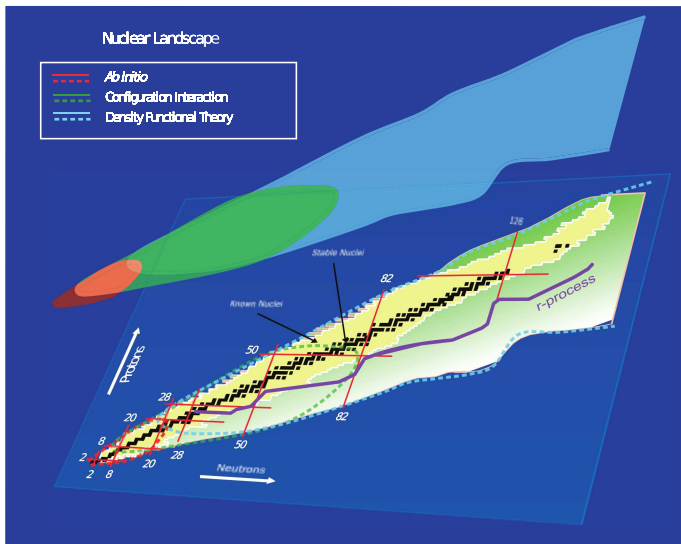
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UNEDF collaboration meeting  
MSU, June 22, 2011

## Nuclear structure: methods



# Outline

- 1 Kohn-Sham functional from coupled-cluster theory
  - Kohn-Sham DFT
  - Ab-initio inputs for nuclear functionals
- 2 First results
  - Potentials and densities
  - Single-particle energies
- 3 Summary

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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

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

- Kohn-Sham scheme

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

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

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# Ab-initio inputs for nuclear functionals

- Typically assume form of functional and fit parameters
  - Observables: cannot do better than experiment
  - ✓ Theoretical intermediates
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- 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 ( $^{48}\text{Ca}$ ,  $V_{\text{low } k}$   $\Lambda = 1.9$ )
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# Determining KS potentials

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

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

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

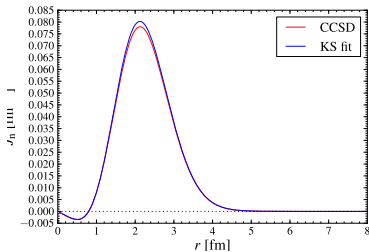
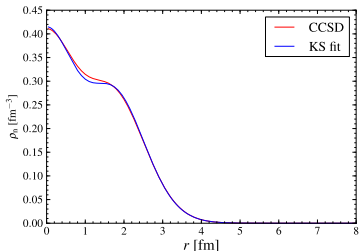
$$S^2 = \int \left( \frac{\rho_{KS} - \rho_{CCSD}}{\rho_{CCSD}} \right)^2 + \left( \frac{J_{KS} - J_{CCSD}}{|J_{CCSD}| + \epsilon} \right)^2 dr$$

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

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

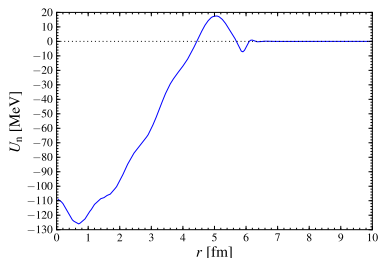
- On the same basis as the CC calculation

## Densities

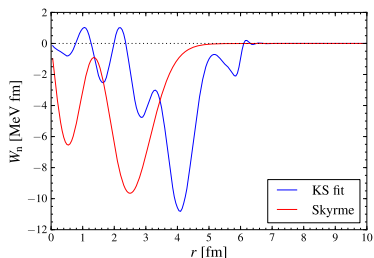


- Non-interacting V-representability not guaranteed for  $(\rho, J)$
- $J$  in KS depends only on  $f_{7/2}$  orbital (filled spin-orbit partners give 0)
- If intruder configurations in CC, will be difficult to reproduce

## Potentials

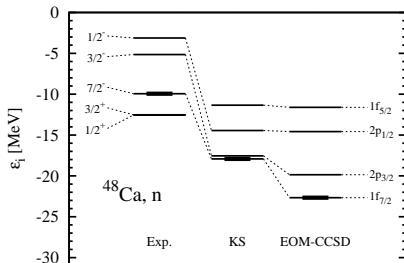
Central potential  $U$ 

Spin-orbit potential



# Single-particle energies

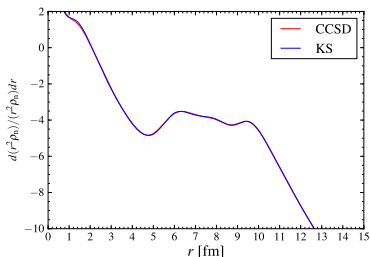
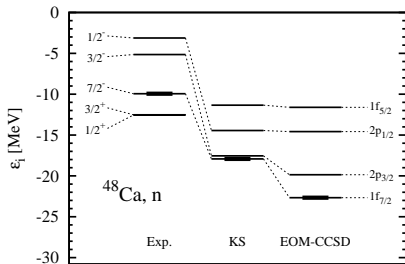
- $\varepsilon_i$ : eigenvalues of the KS potentials
- In principle, meaningless except the Fermi level (“DFT-Koopmans” theorem)
- Need good fit to asymptotic density AND correct exponential asymptotic behavior
- In practice, need to be close to exp. separation energies



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

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## 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:

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

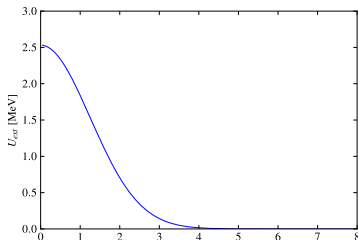
- Calculating second derivatives of  $E$  probes prefactors (Skyrme, Gogny...)

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

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

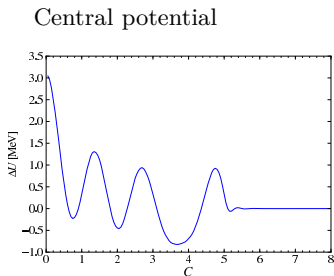
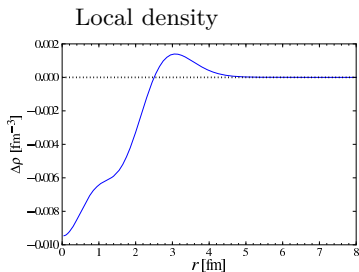
- Can assess whether proposed functional form is consistent with CC

- 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



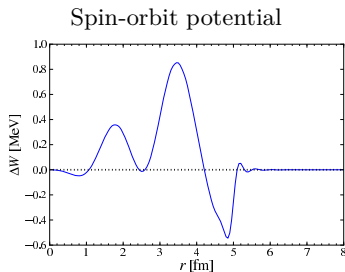
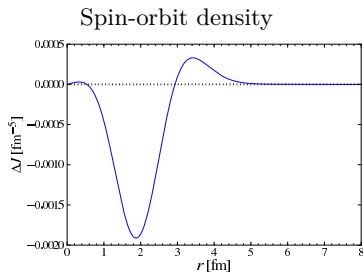
# Static Linear response (In progress)

## ■ Response of density to $U_{ext}$



# Static Linear response (In progress)

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



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

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## Summary and outlook

- Progress in many-body techniques and understanding of the nuclear  $\hat{H}$  allows to add meaningful 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 !