Ab Initio Nuclear DFT Progress Report

Year-3 Deliverables from Continuation Report

- Extend DME and validate against ab initio calculations.
  - low-*k* interactions: evolve, test, export evolved 3D 3NF;
  - improve and test nuclear matter on which DME relies;
  - upgrade and validate the DME implementation;
  - compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
- Develop and test a refit Skyrme functional including universal long-range DME parts.
- Develop orbital-based nuclear DFT (1D models $\Longrightarrow$ 3D).

Affiliated Ab Initio DFT Efforts

- Development of non-empirical pairing using $V_{\text{low}\,k}$

Jacob's Ladder: Coulomb DFT **[J. Perdew et al.]**

"And he [Jacob] dreamed, and behold a ladder set up on the earth, and the top of it reached to heaven . . . " [Genesis 28:12]

HEAVEN $\Longrightarrow$ Chemical Accuracy

$\Uparrow$

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3. Meta-GGA adds (some subset of) $\nabla^2\rho_\uparrow(\mathbf{r})$, $\nabla^2\rho_\downarrow(\mathbf{r})$, $\tau_\uparrow(\mathbf{r})$, and $\tau_\downarrow(\mathbf{r})$.
[Note: $\tau[\rho]$ is nonlocal; $\tau[\phi_i^{\mathrm{KS}}]$ is semi-local.]

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- "Non-empirical" functionals $\Longrightarrow$ constraints, not fits!

Jacob's Ladder: Nuclear DFT [arXiv:0906.1463]

"And he [Jacob] dreamed, and behold a ladder set up on the earth, and the top of it reached to heaven . . . " [Genesis 28:12]

HEAVEN $\Longrightarrow$ UNEDF from NN$\cdots$N (QCD)

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1. Conventional Skyrme EDF's [e.g. SLY4].

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1. Conventional Skyrme EDF's [e.g. SLY4].

- Each rung has sub-rungs!
- Parallel development of 2. – 5. (load balancing??)
- Add constraints (e.g., ab initio neutron drops)

UNEDF Interconnections for Ab Initio Functionals

Interactions

Chiral EFT

Bonn/Julich
(Epelbaum, Nogga)

Idaho/Salamanca
(Entem, Machleidt)

↓

Vlowk/SRG

OSU (Jurgenson)
MSU (Bogner)
TRIUMF (Schwenk,
Bacca, Hebeler)

Ab Initio WF Methods

CC: UT/ORNL (Hagen et al.)
TRIUMF (Bacca)
NCFC: ISU (Maris, Vary)
LLNL (Navratil et al.)

Ab Initio Functional + Nuclear Matter

OSU (Drut, Furnstahl, Platter)
MSU (Bogner, Gebremariam)
also Saclay/Lyon, TRIUMF

DFT Applications

UT/ORNL (Schunck, Stoitsov)
UW (Bertsch, Baroni)
Saclay (Duguet, Lesinski, ...)

Participant color key:

UNEDF
International collaborator
Outside UNEDF

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N3LO 3NF
Explicit Delta's
New 3NF fits
SRG 3NF evolution
In−medium SRG

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Ab Initio WF Methods
CC: UT/ORNL (Hagen et al.)
TRIUMF (Bacca)
NCFC: ISU (Maris, Vary)
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Wider range of nuclei
Full 3NF vs. dd 2NF
Ab Initio densities
External potentials

Tests of DME: energies, densities with same H
Vary 3NF, external potential parameters
Cutoff dependence as diagnostic

Ab Initio Functional + Nuclear Matter
OSU (Drut, Furnstahl, Platter)
MSU (Bogner, Gebremariam)
also Saclay/Lyon, TRIUMF

Tests of nuclear matter:
new fits, self−energies, ...
Improved 3NF for DME
Generalized DME
DFT from OEP/OPM

Long−range pion contributions
from NN and NNN DME
plus fit residual Skyrme in HFB code

DFT Applications
UT/ORNL (Schunck, Stoitsov)
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Saclay (Duguet, Lesinski, ...)

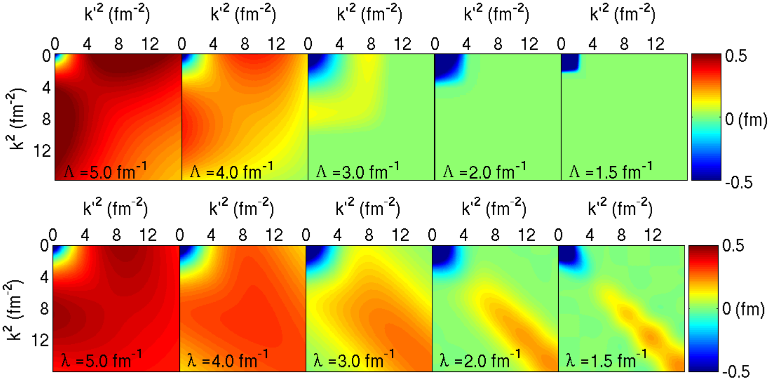
Systematics along
isotope chains, odd−even
Tests: spin−orbit splittings,
time−odd terms, ...
Non−empirical pairing functional

Progress on $V_{\text{low }k}$/SRG Interactions (since Aug. 2008)

OSU + MSU + TRIUMF + LLNL

$V_{\text{low }k}$:

SRG:

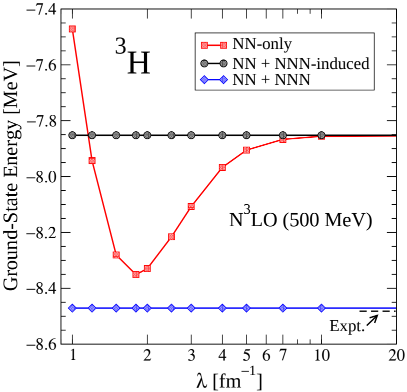


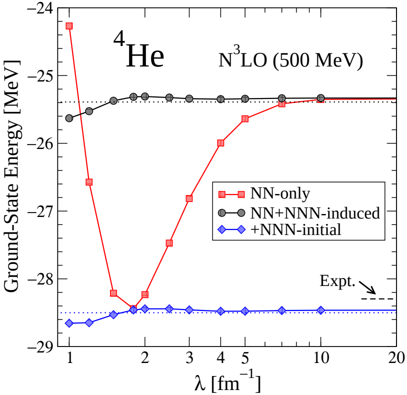
- Decoupling paper: E. Jurgenson et al., Phys. Rev. C **78**, 014003 (2008)
- SRG/$V_{\text{low }k}$ NN code available; ho matrix elements; new NNN fits
- Year 2–3 plan: SRG evolution of NNN (first 1D, then 3D)
- Or: In-medium SRG (Bogner), density-dependent NN (TRIUMF)

3D SRG Evolution with $T_{\rm rel}$ in a Jacobi HO Basis

E. Jurgenson, P. Navratil, rjf, arXiv:0905.1873

- Evolve in *any* basis [momentum space in progress by L. Platter]
  - Here: use anti-symmetric Jacobi HO basis from NCSM
  - directly obtain SRG matrix elements in HO basis
  - separate 3-body evolution not needed
- Compare 2-body only to full $2+3$-body evolution:





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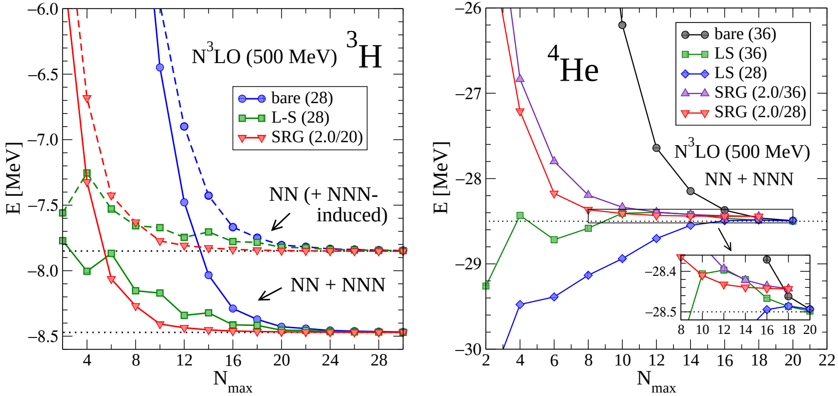
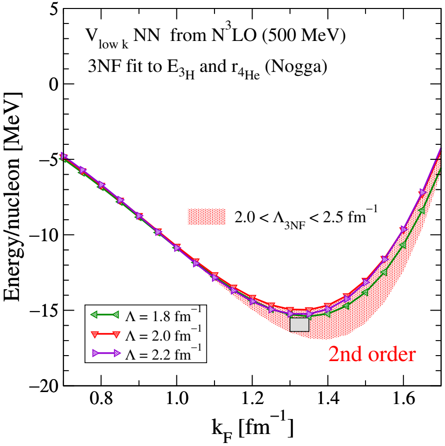
- Good convergence properties independent of 3-body:

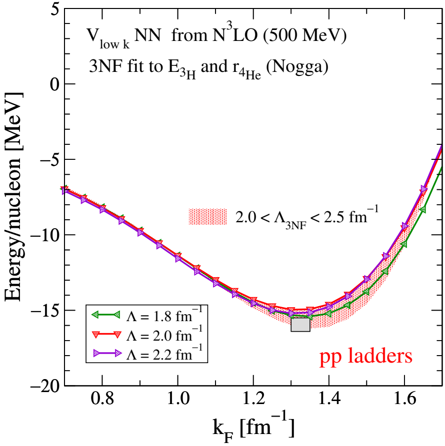


- HO matrix elements (to be) available for NCFC, CC, . . .
- Challenge: efficient (on-the-fly) conversion to m-scheme

Nuclear Matter Status [Bogner et al., arXiv:0903.3363]

- Use a chiral EFT to a given order (e.g., E/M N^3LO below); soften with RG (evolve to $\Lambda \approx 2\,\text{fm}^{-1}$ for ordinary nuclei)
  - NN interactions fully, NNN interactions (3NF) approximately
- Need CC calculation of nuclear matter to validate!



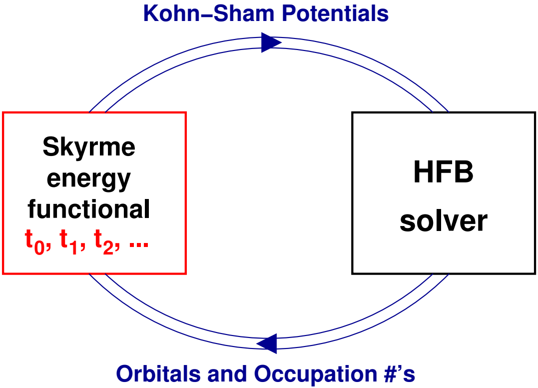


- Generate density functional using NV DME in *k*-space

Year 2: Adaptation to Skyrme HFB Code (HFBRAD)

$$\mathcal{E}_{Skyrme} = \frac{\tau}{2M} + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^{2+\alpha} + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)|\nabla\rho|^2 + \cdots$$

$$\Longrightarrow \ \mathcal{E}_{DME} = \frac{\tau}{2M} + A[\rho] + B[\rho]\tau + C[\rho]|\nabla\rho|^2 + \cdots$$



$$J_0(\mathbf{r}) = \frac{\delta E_{\rm int}[\rho]}{\delta\rho(\mathbf{r})} \quad \Longleftrightarrow \quad [-\frac{\nabla^2}{2m} - J_0(\mathbf{x})]\psi_\alpha = \varepsilon_\alpha \psi_\alpha \ \Longrightarrow \ \rho(\mathbf{x}) = \sum_\alpha n_\alpha |\psi_\alpha(\mathbf{x})|^2$$

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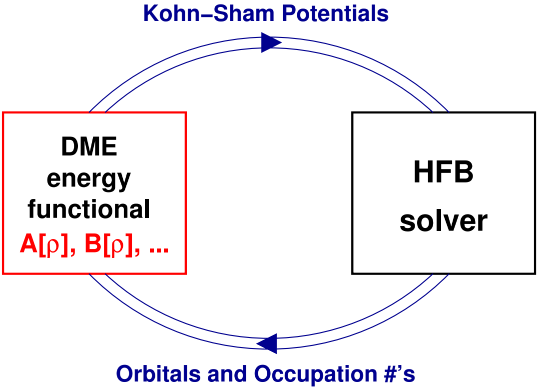

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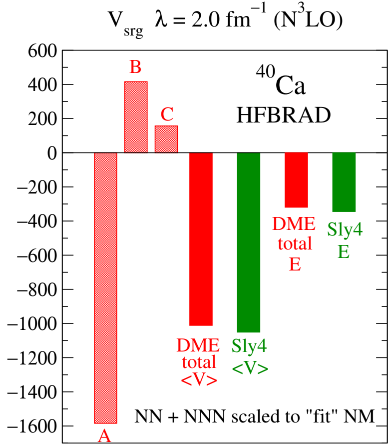
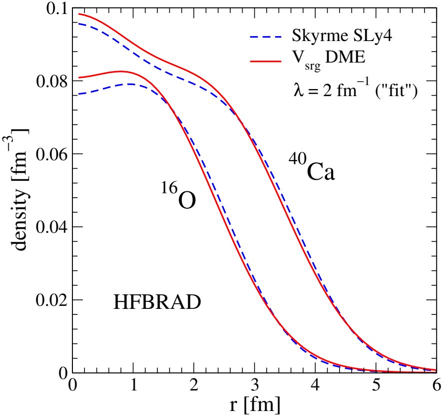
Validation of HFBRAD_DME Implementation

- Reproduces Skyrme results (with good accuracy)
- Possible issues: Sprung et al. test; $dC[\rho]/d\rho$ terms
- Try fine-tuned nuclear matter with low-momentum NN/NNN

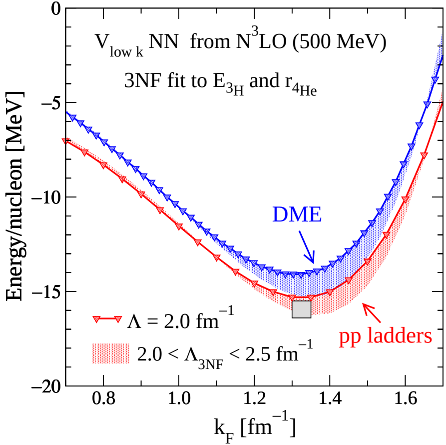


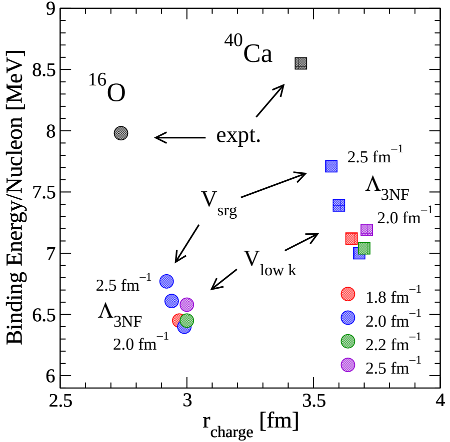


- Do densities look like nuclei from Skyrme EDF's? (Yes)

DME Nuclear Matter and Bulk Nuclei

- Use latest (unadjusted) nuclear matter calculations in DME
- Problem: DME approximations cost 1–1.5 MeV/nucleon binding even in nuclear matter



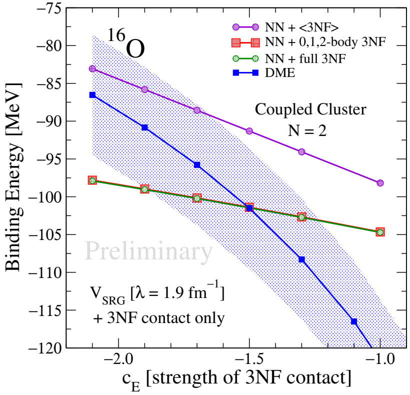


- Correct trends for nuclei (Coester line), but way underbound
- CC comparison calculations delayed because of 3NF

DFT Validation Against *Ab Initio* Calculations

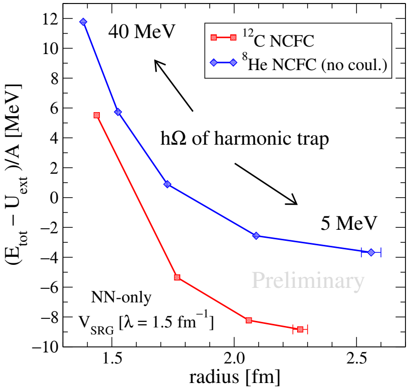
"Coester Lines"

- Compare systematics, e.g., by varying 3NF coupling in Hamiltonian



External Potentials

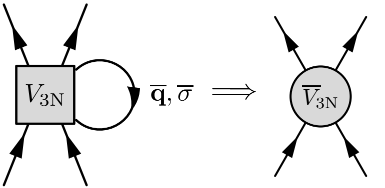
- DFT from response of energy to perturbation of densities
  $\Longrightarrow$ Apply external fields



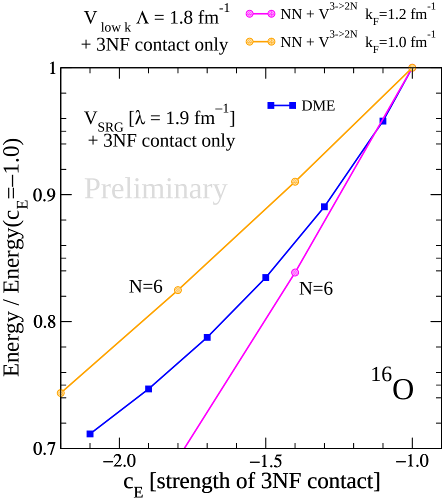
- Plan: Revisit c_E trends, neutron drops

Revisit Dependence on Contact 3NF (Preliminary!)

- Approximate the 3NF contribution by averaging 3rd particle at fixed $k_F \Longrightarrow$ effective NN (K. Hebeler)



- Applied to coupled cluster by S. Bacca $\Longrightarrow$ fast!
- Slope vs. c_E gives $\langle 3NF \rangle$
- Here: normalize to $c_E = -1$



What is the OEP?

- Density Functional Theory (Hohenberg-Kohn)

  "A density functional exists..."

- Kohn-Sham approach

  "The density functional can be optimized by solving a Schrödinger-like problem..."

  - If the functional is explicitly density-dependent we know how to do this:

    $$v_{KS}(\mathbf{r}) = \frac{\delta E_{int}[\rho]}{\delta \rho(\mathbf{r})}$$

  - But what happens if the functional depends explicitly on the KS orbitals and only implicitly on the density?

    (E.g. Hartree-Fock functional (!))

The DFT ladder in quantum chemistry

- LDA "Take the density-dependent energy of the uniform system and replace n with n(x)..."
  - Very easy to implement
  - Not very accurate
- GGA "Take the LDA and add gradient corrections..."
  - Great improvement over LDA
  - Has some difficult problems: Absence of negative ions, van der Waals forces, strong correlations...
- OEP "Allow for explicit orbital dependence ..."
  - Harder to implement, computationally more expensive
  - Allows for exact exchange, solves many of the GGA problems

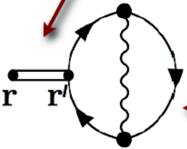
The OEP equation

- How do we determine $v_{KS}(\mathbf{r})$? Apply chain rule!

$$v_{KS}(\mathbf{r}) = \frac{\delta E_{int}[\varphi_i, \varepsilon_i]}{\delta \rho(\mathbf{r})} = \int d\mathbf{r}' \frac{\delta v_{KS}(\mathbf{r}')}{\delta \rho(\mathbf{r})} \sum_j \left\{ \int d\mathbf{r}'' \frac{\delta \varphi_j^\dagger(\mathbf{r}'')}{\delta v_{KS}(\mathbf{r}')} \frac{\delta E_{int}}{\delta \varphi_j^\dagger(\mathbf{r}'')} + \text{c.c.} + \frac{\delta \varepsilon_j}{\delta v_{KS}(\mathbf{r}')} \frac{\partial E_{int}}{\partial \varepsilon_j} \right\}$$

$$\frac{\delta E_{int}[\varphi_i, \varepsilon_i]}{\delta v_{KS}(\mathbf{r}')}$$

$v_{KS}(\mathbf{r})$



$$G_{s,j\sigma}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{k \neq j} \frac{\varphi_{k\sigma}(\mathbf{r}_1) \varphi_{k\sigma}^*(\mathbf{r}_2)}{\varepsilon_{j\sigma} - \varepsilon_{k\sigma}}$$

- Talman & Shadwick (1976):

  "What is the best multiplicative potential that minimizes the energy?"

  Minimization with subsidiary condition!

The OEP equation

- OEP integral equation

$$\int dx' \, Q(x,x') v_{\rm xc}(x') = \Lambda(x)$$

$$Q(x,x') = \sum_{j=1}^{N} \varphi_j^*(x') G_j(x',x) \varphi_j(x) + c.c.$$

$$\Lambda(x) = \sum_{j=1}^{N} \int dx' \; \varphi_j^*(x') u_{xc,j}(x') G_j(x',x) \varphi_j(x) + c.c.$$

Green's function

$$G_j(x',x) = \sum_{k \neq j} \frac{\varphi_k(x') \varphi_k^*(x)}{\varepsilon_j - \varepsilon_k}$$

Sum over occupied and unoccupied states!

Auxiliary potential

$$u_{xc,j}(x') = \frac{1}{\varphi_j^*(x')} \frac{\delta E_{int}}{\delta \varphi_j(x')}$$

The KLI approximation

Krieger, Li and Iafrate, Phys. Rev. A **45**, 101 (1992)

- Take the OEP equation and replace...

$$G_j(x',x) = \sum_{k\neq j} \frac{\varphi_k(x')\varphi_k^*(x)}{\varepsilon_j - \varepsilon_k} \quad \longrightarrow \quad \begin{aligned} G_j^{KLI}(x',x) &= \frac{1}{\varepsilon_j - \varepsilon_j^0} \sum_{k\neq j} \varphi_k(x')\varphi_k^*(x) \\ &= \frac{1}{\varepsilon_j - \varepsilon_j^0} \left[\delta(x-x') - \varphi_j(x')\varphi_j(x)\right] \end{aligned}$$

Is this a good approximation?

In practice it gives excellent results in the exchange-only limit.

- KLI equation

$$v_{xc}^{KLI}(r) = V_{SL}(r) + \sum_i \frac{n_i(r)}{n(r)} \left(\langle i | v_{xc}^{KLI} | i \rangle - \langle i | u_{xc,i} | i \rangle \right)$$

$$V_{SL}(r) = \sum_i \frac{n_i(r)}{n(r)} u_{xc,i}(r) \quad \longleftarrow \quad \text{Slater potential}$$

- Sum only over occupied states!
- Can be solved iteratively or directly!

The KLI approximation

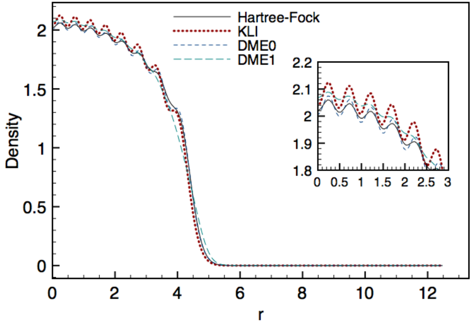
- Performance comparison

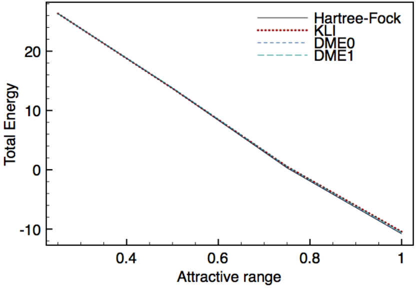
Table 2.2. Exchange-only ground-state energies of closed-subshell atoms: Self-consistent OPM results [48] versus KLI, LDA, PW91-GGA [30] and HF [49] energies (all energies in mhartree)

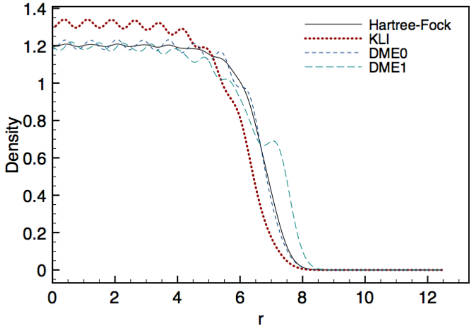
Atom	E_{tot}	$E_{tot} - E_{tot}^{OPM}$			
	OPM	KLI	LDA	GGA	HF
He	−2861.7	0.0	138.0	6.5	0.0
Be	−14572.4	0.1	349.1	18.2	−0.6
Ne	−128545.4	0.6	1054.7	−23.5	−1.7
Mg	−199611.6	0.9	1362.8	−0.5	−3.1
Ar	−526812.2	1.7	2294.8	41.2	−5.3
Ca	−676751.9	2.2	2591.8	25.7	−6.3
Zn	−1777834.4	3.7	3924.5	−252.6	−13.8
Kr	−2752042.9	3.2	5176.8	−18.4	−12.0
Sr	−3131533.4	3.6	5535.4	−8.8	−12.2
Pd	−4937906.0	4.5	6896.0	−65.2	−15.0
Cd	−5465114.4	6.0	7292.6	−31.9	−18.7
Xe	−7232121.1	6.1	8463.8	54.9	−17.3
Ba	−7883526.6	6.5	8792.5	15.7	−17.3
Yb	−13391416.3	10.0	10505.6	−852.4	−39.9
Hg	−18408960.5	9.1	13040.4	−221.5	−31.0
Rn	−21866745.7	8.5	14424.3	8.3	−26.5
Ra	−23094277.9	8.7	14807.2	0.5	−25.8
No	−32789472.7	12.9	17202.9	−373.1	−39.5

One-Dimensional Laboratory for OEP

- J. Drut, L. Platter, rjf
- Simple short-range repulsion and long-range attraction
- Warm-up for realistic problem
- With trap or self-bound
- Compare approximations (e.g., Hartree-Fock vs. KLI vs. DME vs. full OEP)



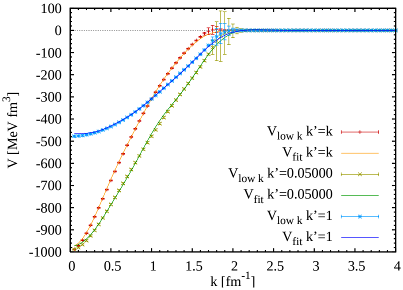


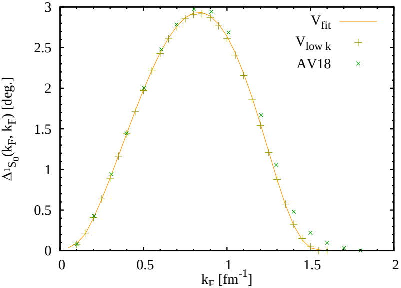


Non-Empirical Pairing Functional for Nuclei

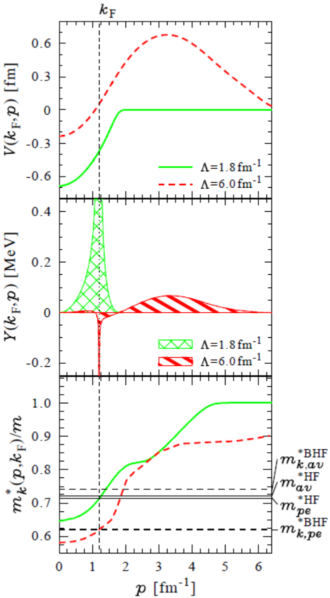
T. Duguet (Saclay); T. Lesinski (UT/ORNL), K. Bennaceur, J. Meyer (Lyon)

- Spherical code BSLHFB (T.L.)
  - spherical Bessel function basis
  - finite-range / non-local pairing interactions in EDF
  - separable $V_{\mathrm{low}\,k}(\Lambda)$ expansion
- Pairing at lowest order in NN (nuclear + Coulomb); no fits!
  - use $V_{\mathrm{low}\,k}$ at $\Lambda \approx 2\,\mathrm{fm}^{-1}$ as NN pairing interaction
  - Use SLY4 Skyrme for ph EDF with fixed $m_0^*/m = 0.7$
- Studied $m^*(k, k_{\mathrm{F}})$ for cutoffs Λ (K. Hebeler, T.D., T.L., A. Schwenk)
  - see arXiv:0904.3152
  - consistent ph/pp scales needed
  - $V_{\mathrm{low}\,k}$ ok with $m^*_{\mathrm{Skyrme}}(k_{\mathrm{F}})$





Analysis



- Consider matrix elements $V_{\Lambda=1.8/6}(k_F^n, p)$
- Write gap equation schematically as

$$\hat{\Delta}(k_F^n) \equiv \int dq\, Y(k_F^n, q)$$

Gap generated

- Around the Fermi surface for soft Λ
- Mainly at large momenta for hard Λ

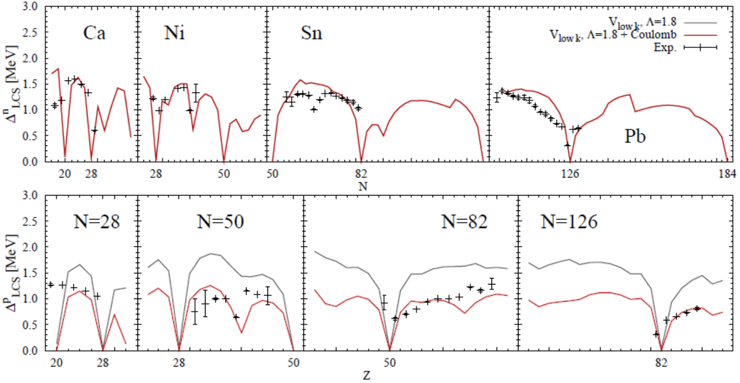
Effect of $m_\tau^*(k_F^\tau) = \text{constant}$ - 'pe' values here

- Good approx for soft Λ around k_F^n
- Bad approx for hard Λ at relevant $p \gtrsim 2\,\text{fm}^{-1}$

Pairing gaps from $v^{pp} = V_{NN} + V_{Coul}$

[T. Lesinski, T. Duguet, K. Bennaceur, J. Meyer, EPJA 40 (2009) 121]

- $\Delta^{(3)}_{exp}$(odd) versus Δ_{LCS}(even)

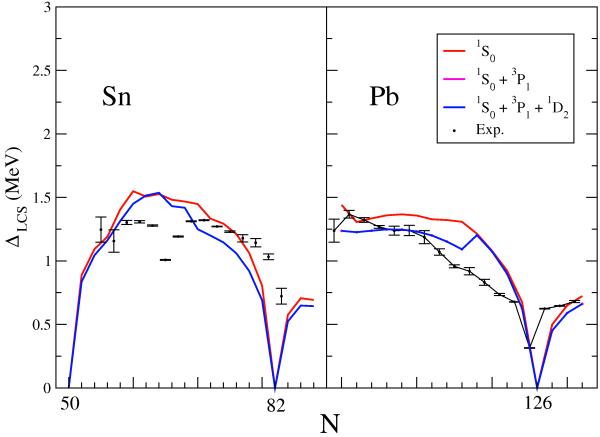


- Pairing gaps Δ^q are consistently close to experimental data
- Coulomb decreases Δ^p by $\sim 40\%$ to bring them close to experiment

Contribution from Higher Partial Waves

S. Baroni et al., “Partial wave contributions to pairing in nuclei” (soon)

- Several $L_{\rm rel}$ contribute to $J = 0$ pairing with $J = J_{\rm rel} + L_{\rm cm}$
- Time-reversal restricts to $^3P_1$ and $^1D_2$

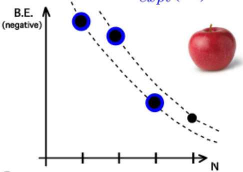


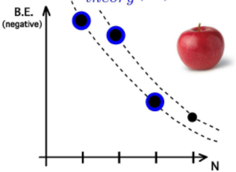
- Non-zero but limited repulsive effects from $^3P_1$ to the OEMS
- More pronounced effects on QP excitation spectrum

Comparing theoretical and experimental "pairing gaps"

- The good method

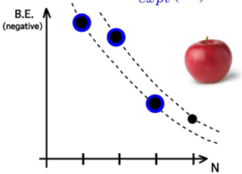
$\Delta^{(3)}_{expt}(N)$ vs $\Delta^{(3)}_{theory}(N)$

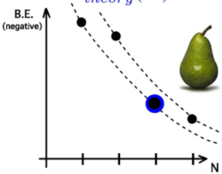




- The actual method

$\Delta^{(3)}_{expt}(N)$ vs $\Delta^{LCS}_{theory}(N)$



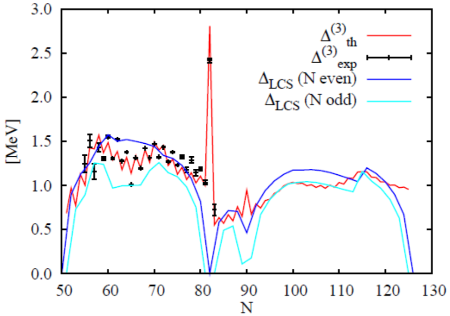


$\Delta^{(3)}_{\rm exp}(\text{odd})$ versus $\Delta_{\rm LCS}(\text{even})$ = Gap at ϵ_F in even N nucleus

Pairing gaps ($^1S_0$) and interplay with shell structure

[T. Lesinski, T. Duguet, K. Bennaceur, J. Meyer, in preparation]

- $\Delta^{(3)}_{\rm exp}(N)$ versus $\Delta^{(3)}_{\rm th}(N)$ (self-consistent qp filling approx)

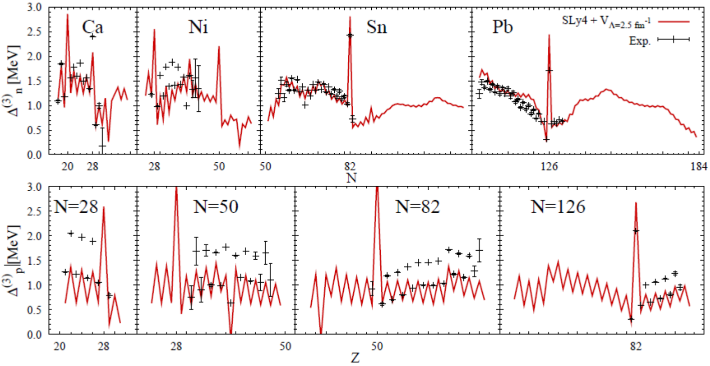


- $\Delta^{(3)}_{\rm th}(\text{odd}) \approx [\Delta_{\rm LCS}(\text{even}) + \Delta_{\rm LCS}(\text{odd})]/2$ [T. Duguet *et al.* PRC65 (2002)]
- Deepening around $N \approx 115$ arises from blocking of $\Delta_{\rm LCS}(\text{odd})$
- $\Delta^{(3)}$ well described close to $N = 82$ without LN, proj. or pairing vib.

Pairing gaps ($^1S_0$) and interplay with shell structure

[T. Lesinski, T. Duguet, K. Bennaceur, J. Meyer, in preparation]

- $\Delta^{(3)}_{exp}(N)$ versus $\Delta^{(3)}_{th}(N)$ (self-consistent qp filling approx)



- Neutron (proton) gaps consistent with (slightly lower than) experiment
- Access detailed interplay with shell structure

Other: Include chiral N^{2}LO 3NF [T. Lesinski] using 3rd particle averaging [K. Hebeler]; include p-h fluctuations [Baroni, Pastore et al.]

Ab Initio Nuclear DFT Progress Report

Year-3 Deliverables from Continuation Report

- Extend DME and validate against ab initio calculations.
  - low-*k* interactions: ✓evolve, ✓test, export evolved 3D 3NF;
  - ✓ improve and test nuclear matter on which DME relies;
  - ✓upgrade and validate the DME implementation;
  - compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
- ✓Develop and test a refit Skyrme functional including universal long-range DME parts.
- ✓ Develop orbital-based nuclear DFT (1D models $\Longrightarrow$ 3D).

Affiliated Ab Initio DFT Efforts

- ✓Development of non-empirical pairing using $V_{\text{low }k}$

Articles and Preprints Citing SCIDAC Support

- Published or Posted since Pack Forest 2008
  - "Decoupling in the similarity renormalization group for nucleon-nucleon forces," E.D. Jurgenson, S.K. Bogner, R.J. Furnstahl, R.J. Perry, Phys. Rev. C **78**, 014003 (2008)
  - "Density matrix expansion for low-momentum interactions," S.K. Bogner, R.J. Furnstahl, and L. Platter, Eur. Phys. J. **A39**, 219 (2009)
  - "Similarity renormalization group evolution of many-body forces in a one-dimensional model," E.D. Jurgenson and R.J. Furnstahl, Nucl. Phys. A **818**, 152 (2009)
  - "Nuclear matter from chiral low-momentum interactions," S.K. Bogner, R.J. Furnstahl, A. Nogga and A. Schwenk, arXiv:0903.3366 [nucl-th], submitted to PRL
  - "Evolution of nuclear many-body forces with the similarity renormalization group," E.D. Jurgenson, P. Navratil and R.J. Furnstahl, arXiv:0905.1873, submitted to PRL
  - "Toward ab initio density functional theory for nuclei," J.E. Drut, R.J. Furnstahl, and L. Platter, arXiv:0906.1463 [nucl-th], commissioned review for Prog. Part. Nucl. Sci.

Plans for Rest of Year 3 and Year 4 . . . (Part 1)

- NNN fits and tests
  - NNN project to interface $V_{\text{low}\,k}$ chiral EFT NNN with FCI
  - Test new fits with CC and FCI in larger nuclei (e.g., λ/Λ dependence)
- Evolving NNN with SRG
  - Harmonic oscillator matrix elements for input to NCFCs, CC
  - Understand 3D many-body power counting and use to estimate higher-body interactions; evolve operators
  - Momentum-space evolution of NNN
  - Validate 3NF fits vs. evolved 3NF
- Nuclear matter calculational extensions
  - Full 2nd order calculation with fit NNN (w/TRIUMF)
  - Asymmetric nuclear matter (just coding to finish)
  - Solve uniform matter with in-medium SRG
  - Explore coupled cluster for nuclear matter (UT/ORNL)

Plans for Rest of Year 3 and Year 4 . . . (Part 1)

- Nuclear matter studies
  - Complete and publish the G-matrix and BBG study
    $\Longrightarrow$ test power counting with numerical examples
  - Nonperturbativeness in the particle-hole channel
  - Pairing, e.g., in $^3S_1$
  - Nuclear/neutron matter with Jisp-16 (MSU/ISU)
  - 4NF from N^3LO chiral EFT at Hartree-Fock
- Validating (or invalidating) DME from $V_{\mathrm{low}\,k}$/SRG
  - Compare energies, ρ's to CC, NCFC with same Hamiltonian
    - Vary contact 3NF strength, full 3NF-fitted $V_{\mathrm{low}\,k}$/SRG
  - Compare in external potentials with NCFC, GFMC/AFMC
    - neutron drops
- Beyond DME
  - Continue 1D (3D) development of orbital based nuclear DFT
  - KLI approximations vs. full OEP
  - Model tests against DME; full comparison
  - Symmetry breaking, long-range correlations . . .