Nuclear forces and their impact on structure, reactions and astrophysics

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Ohio State University

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Lectures for Week 3

- **M.** Many-body problem and basis considerations (as); Many-body perturbation theory (rjf)
- **T.** Neutron matter and astrophysics (as); MBPT + Operators (rjf)
- **W.** Operators + Nuclear matter (rjf); Student presentations
- **Th.** Impact on (exotic) nuclei (as); Student presentations
- **F.** Impact on fundamental symmetries (as); From forces to density functionals (rjf)

Outline

Some references for today (and many-body EFT)

Skyrme Hartree-Fock as density functional theory

Density Matrix Expansion

NUCLEI and UNEDF SciDAC projects

Some references (and others cited therein)

- "Toward ab initio density functional theory for nuclei," J.E. Drut, rjf, L. Platter, arXiv:0906.1463
- "EFT for DFT" by rjf, arXiv:nucl-th/0702040v2
- "Effective Field Theory and Finite Density Systems" by rjf, G. Rupak, and T. Schäfer, arXiv:0801.0729
- Online scanned notes from a 2003 course by rjf and Achim `http://www.physics.ohio-state.edu/~ntg/880/`
  - From path integrals to EFT for many-body systems, with lots of detail (e.g., spin sums, symmetry factors, . . .)
  - Also some homework problems and solutions
  - username: `physics` password: `880.05`
- Online scanned notes from a 2009 course by rjf and Joaquin Drut called "EFT, RG, and Computation" `http://www.physics.ohio-state.edu/~ntg/880_2009/`
  - username: `physics` password: `880.05`

Table 1. *Physical Review* Articles with more than 1000 Citations Through June 2003

Publication	# cites	Av. age	Title	Author(s)
PR **140**, A1133 (1965)	3227	26.7	Self-Consistent Equations Including Exchange and Correlation Effects	W. Kohn, L. J. Sham
PR **136**, B864 (1964)	2460	28.7	Inhomogeneous Electron Gas	P. Hohenberg, W. Kohn
PRB **23**, 5048 (1981)	2079	14.4	Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems	J. P. Perdew, A. Zunger
PRL **45**, 566 (1980)	1781	15.4	Ground State of the Electron Gas by a Stochastic Method	D. M. Ceperley, B. J. Alder
PR **108**, 1175 (1957)	1364	20.2	Theory of Superconductivity	J. Bardeen, L. N. Cooper, J. R. Schrieffer
PRL **19**, 1264 (1967)	1306	15.5	A Model of Leptons	S. Weinberg
PRB **12**, 3060 (1975)	1259	18.4	Linear Methods in Band Theory	O. K. Anderson
PR **124**, 1866 (1961)	1178	28.0	Effects of Configuration Interaction of Intensities and Phase Shifts	U. Fano
RMP **57**, 287 (1985)	1055	9.2	Disordered Electronic Systems	P. A. Lee, T. V. Ramakrishnan
RMP **54**, 437 (1982)	1045	10.8	Electronic Properties of Two-Dimensional Systems	T. Ando, A. B. Fowler, F. Stern
PRB **13**, 5188 (1976)	1023	20.8	Special Points for Brillouin-Zone Integrations	H. J. Monkhorst, J. D. Pack

PR, Physical Review; PRB, Physical Review B; PRL, Physical Review Letters; RMP, Reviews of Modern Physics.

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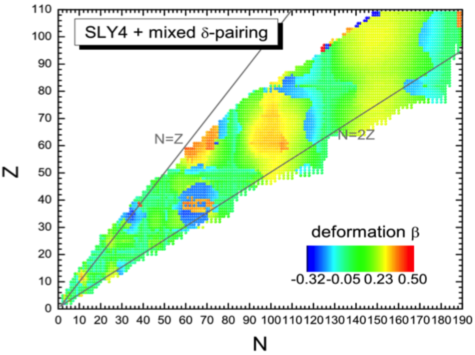
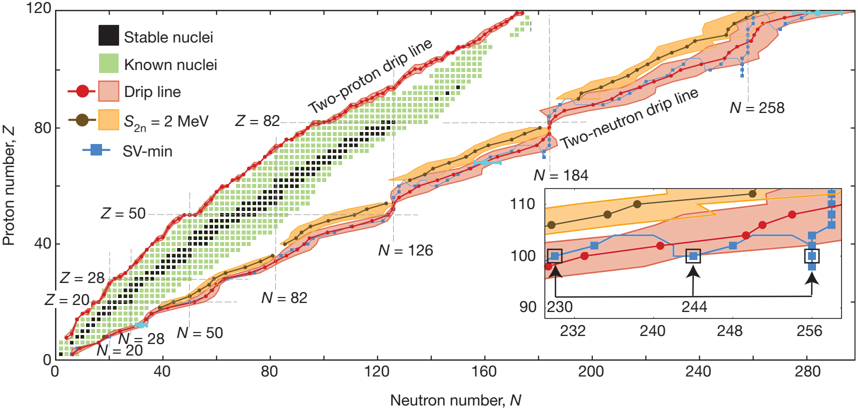
Large-scale mass table calculations [M. Stoitsov et al.]

- One Skyrme functional ($\sim$10–20 parameters) describes all nuclei from few-body to superheavies
- 9,210 nuclei in less than one day on ORNL Jaguar (Cray XT4)
- New developments as part of UNEDF and NUCLEI SciDAC projects
- Recently developed: optimization and correlation analysis tools



"The limits of the nuclear landscape"

J. Erler et al., Nature **486**, 509 (2012)



- Proton and neutron driplines predicted by Skyrme EDFs
  - Total: 6900 ± 500 nuclei with $Z \leq 120$ (≈ 3000 known)
  - Estimate systematic errors by comparing models

Skyrme energy functionals

- Minimize $E = \int d\mathbf{x}\,\mathcal{E}[\rho(\mathbf{x}), \tau(\mathbf{x}), \mathbf{J}(\mathbf{x}), \ldots]$ (for $N = Z$):

$$\mathcal{E}[\rho, \tau, \mathbf{J}] = \frac{1}{2M}\tau + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^{2+\alpha} + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)(\nabla\rho)^2 - \frac{3}{4}W_0\rho\nabla\cdot\mathbf{J} + \frac{1}{32}(t_1 - t_2)\mathbf{J}^2$$

  - where $\rho(x) = \sum_i |\psi_i(x)|^2$ and $\tau(x) = \sum_i |\nabla\psi_i(x)|^2$ (and $\mathbf{J}$)

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- Skyrme Kohn-Sham equation from functional derivatives:

$$\left(-\nabla\frac{1}{2M^*(\mathbf{x})}\nabla + U(\mathbf{x}) + \frac{3}{4}W_0\nabla\rho\cdot\frac{1}{i}\nabla\times\boldsymbol{\sigma}\right)\psi_i(\mathbf{x}) = \epsilon_i\,\psi_i(\mathbf{x}) ,$$

$U = \frac{3}{4}t_0\rho + (\frac{3}{16}t_1 + \frac{5}{16}t_2)\tau + \cdots$ and $\frac{1}{2M^*(\mathbf{x})} = \frac{1}{2M} + (\frac{3}{16}t_1 + \frac{5}{16}t_2)\rho$

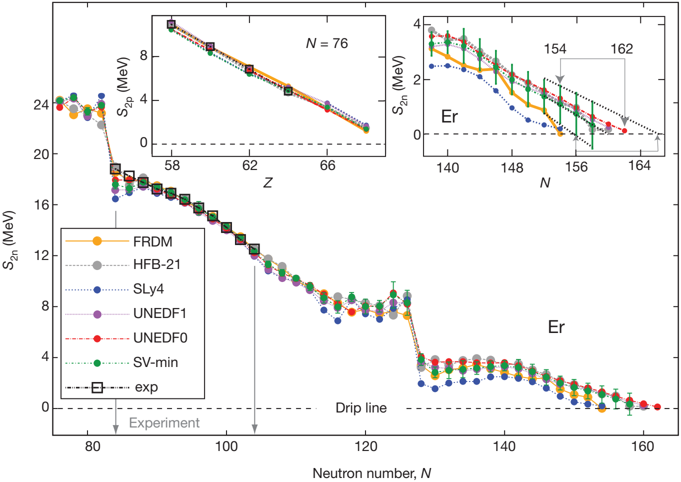
- Iterate until ψ_i's and ϵ_i's are self-consistent
- In practice: other densities, pairing is very important (HFB), projection needed, ...

Issues with empirical EDF's

- Density dependencies might be too simplistic
- Isovector components not well constrained
- No (fully) systematic organization of terms in the EDF
- Difficult to estimate theoretical uncertainties
- What's the connection to many-body forces?
- Pairing part of the EDF not treated on same footing
- and so on . . .

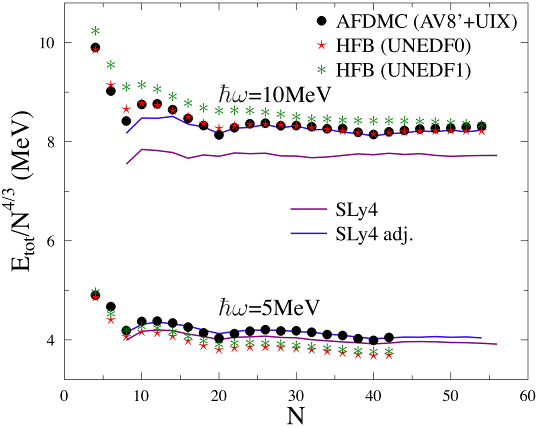
$\Longrightarrow$ Turn to microscopic many-body theory for guidance

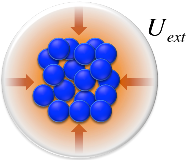
"The limits of the nuclear landscape"



- Two-neutron separation energies of even-even erbium isotopes
  - Compare different functionals, with uncertainties of fits
  - Dependence on neutron excess poorly determined (cf. driplines)

Impact of forces: Use *ab initio* pseudo-data





- Put neutrons in a harmonic oscillator trap with $\hbar\omega$ (cf. cold atoms!)
- Calculate exact result with AFDMC [S. Gandolfi, J. Carlson, and S.C. Pieper, Phys. Rev. Lett. 106, 012501 (2011)] (or with other methods)
- UNEDF0 and UNEDF1 functionals improve over Skyrme SLy4!

Teaser: Comparing Skyrme and natural, pionless Functionals

- Textbook Skyrme EDF (for $N = Z$) $[\rho = \langle\psi^\dagger\psi\rangle, \tau = \langle\nabla\psi^\dagger\cdot\nabla\psi\rangle]$

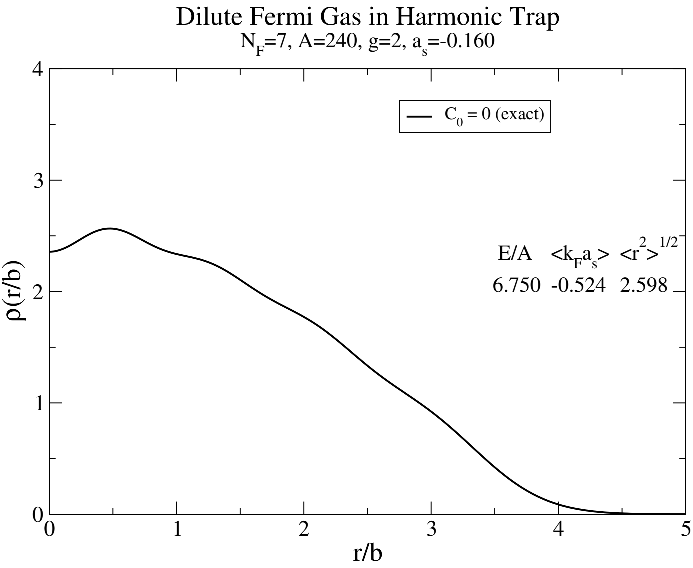
$$E[\rho,\tau,\mathbf{J}] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8}t_0\rho^2 + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)(\nabla\rho)^2 - \frac{3}{4}W_0\rho\nabla\cdot\mathbf{J} + \frac{1}{16}t_3\rho^{2+\alpha} + \cdots \right\}$$

- Natural, pionless $\rho\tau\mathbf{J}$ energy density functional for $\nu = 4$

$$E[\rho,\tau,\mathbf{J}] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8}C_0\rho^2 + \frac{1}{16}(3C_2 + 5C_2')\rho\tau + \frac{1}{64}(9C_2 - 5C_2')(\nabla\rho)^2 - \frac{3}{4}C_2''\rho\nabla\cdot\mathbf{J} + \frac{c_1}{2M}C_0^2\rho^{7/3} + \frac{c_2}{2M}C_0^3\rho^{8/3} + \frac{1}{16}D_0\rho^3 + \cdots \right\}$$

- Same functional as dilute Fermi gas with $t_i \leftrightarrow C_i$?
  - Is Skyrme missing non-analytic, NNN, long-range (pion), (and so on) terms? (But NDA works: C_i's are natural!)
  - Isn't this a "perturbative" expansion?

Pionless EFT in a trap as ab initio DFT (see refs.)



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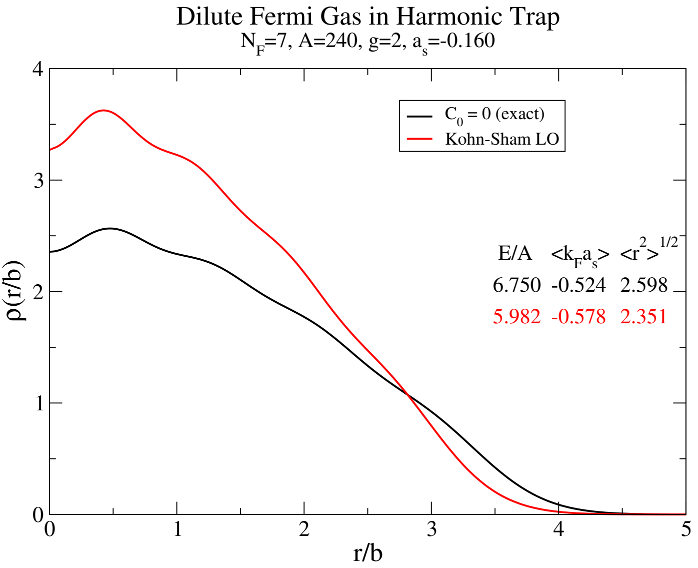

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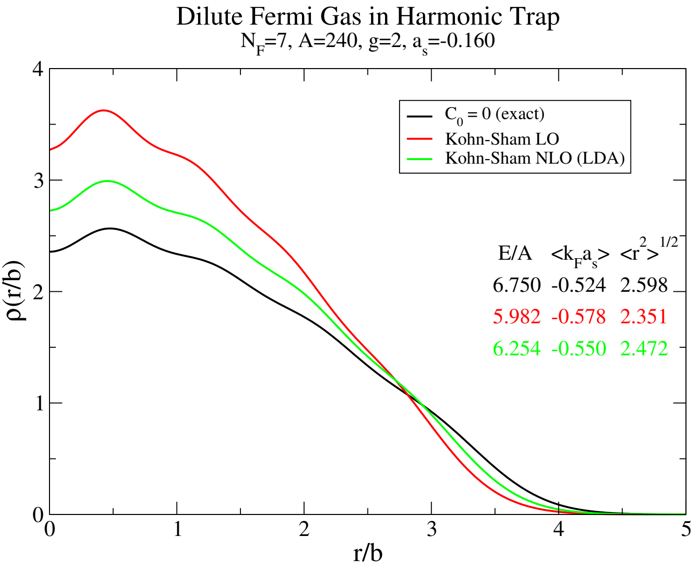

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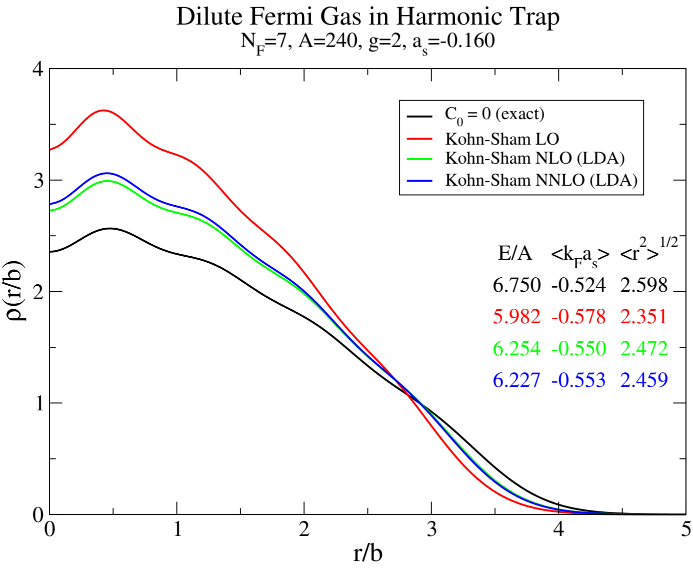
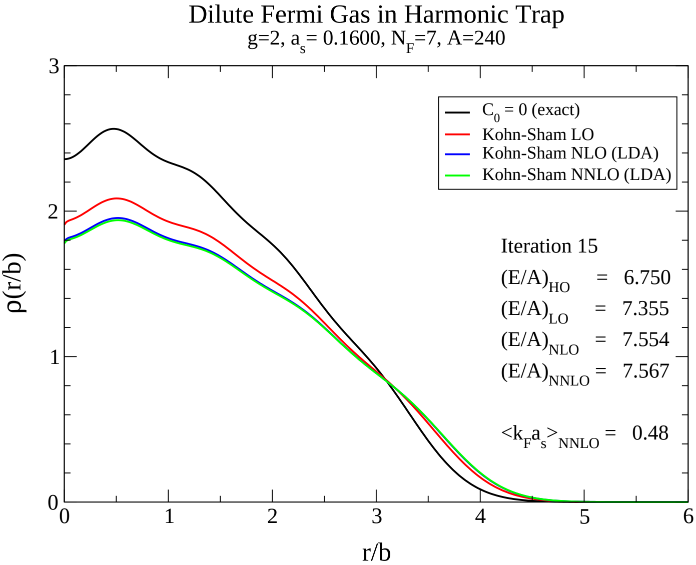


Other Examples [nucl-th/0212071]



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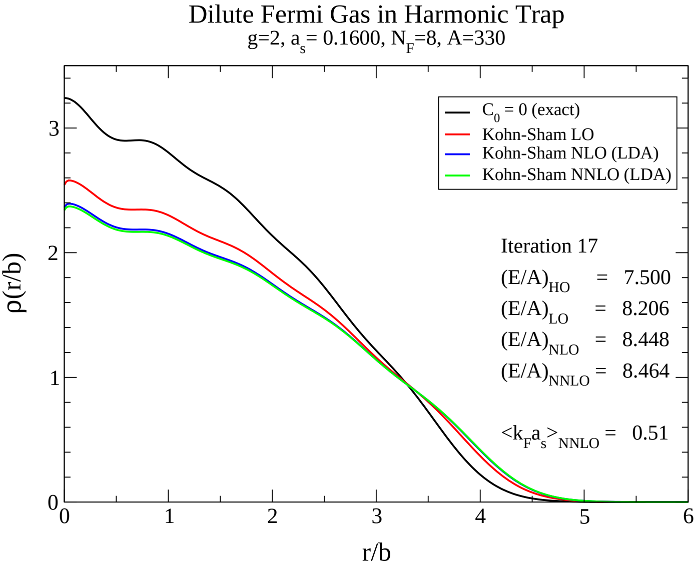

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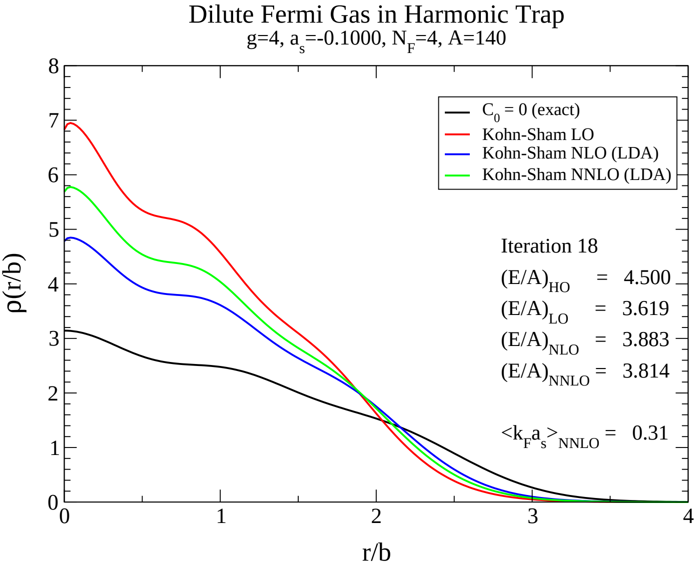

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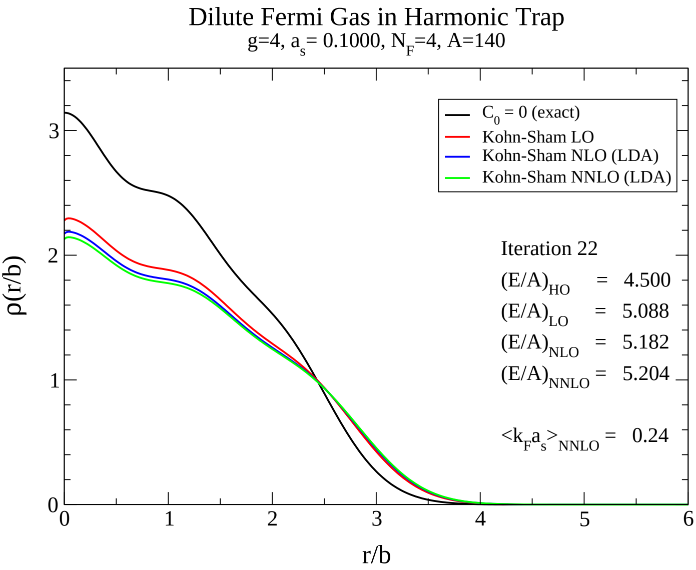

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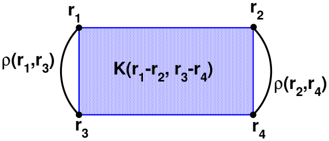
Density matrix expansion revisited [Negele/Vautherin]

- Dominant MBPT contributions can be put into form

$$\langle V \rangle \sim \int d\mathbf{R}\, d\mathbf{r}_{12}\, d\mathbf{r}_{34}\, \rho(\mathbf{r}_1, \mathbf{r}_3) K(\mathbf{r}_{12}, \mathbf{r}_{34}) \rho(\mathbf{r}_2, \mathbf{r}_4)$$



  - finite range and non-local resummed vertices K (+ NNN)

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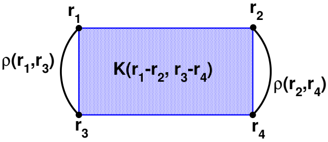
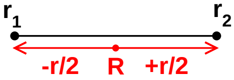


  - finite range and non-local resummed vertices K (+ NNN)
- DME: Expand KS ρ in local operators w/factorized non-locality

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\epsilon_\alpha \le \epsilon_{\rm F}} \psi^\dagger_\alpha(\mathbf{r}_1)\psi_\alpha(\mathbf{r}_2) = \sum_n \Pi_n(\mathbf{r}) \langle \mathcal{O}_n(\mathbf{R}) \rangle$$



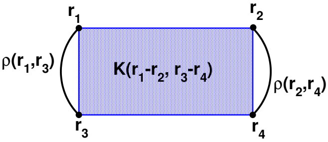
with $\langle \mathcal{O}_n(\mathbf{R}) \rangle = \{\rho(\mathbf{R}), \nabla^2\rho(\mathbf{R}), \tau(\mathbf{R}), \cdots\}$ maps $\langle V \rangle$ to Skyrme-like EDF!

- Adds density dependences, isovector, ... missing in Skyrme

Density matrix expansion revisited [Negele/Vautherin]

- Dominant MBPT contributions can be put into form

$$\langle V \rangle \sim \int d\mathbf{R}\, d\mathbf{r}_{12}\, d\mathbf{r}_{34}\, \rho(\mathbf{r}_1, \mathbf{r}_3) K(\mathbf{r}_{12}, \mathbf{r}_{34}) \rho(\mathbf{r}_2, \mathbf{r}_4)$$



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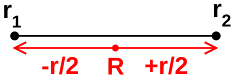


with $\langle \mathcal{O}_n(\mathbf{R}) \rangle = \{\rho(\mathbf{R}), \nabla^2\rho(\mathbf{R}), \tau(\mathbf{R}), \cdots\}$ maps $\langle V \rangle$ to Skyrme-like EDF!

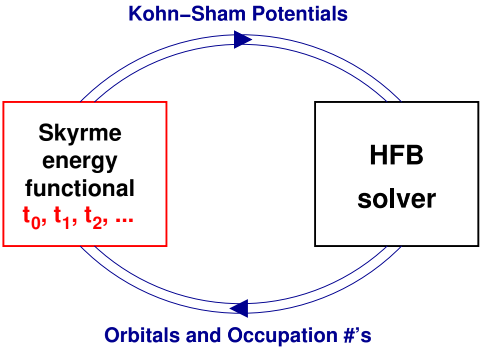
- Adds density dependences, isovector, . . . missing in Skyrme
- Original DME expands about nuclear matter (k-space + NNN)

$$\rho(\mathbf{R}+\mathbf{r}/2, \mathbf{R}-\mathbf{r}/2) \approx \frac{3j_1(sk_{\mathrm{F}})}{sk_{\mathrm{F}}}\rho(\mathbf{R}) + \frac{35 j_3(sk_{\mathrm{F}})}{2sk_{\mathrm{F}}^3}\left(\frac{1}{4}\nabla^2\rho(\mathbf{R}) - \tau(\mathbf{R}) + \frac{3}{5}k_{\mathrm{F}}^2\rho(\mathbf{R}) + \cdots\right)$$

Adaptation to Skyrme HFB Implementations

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

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



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

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

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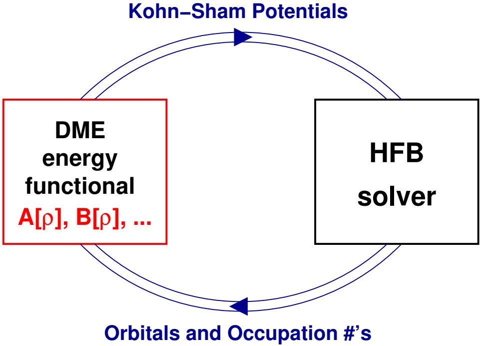

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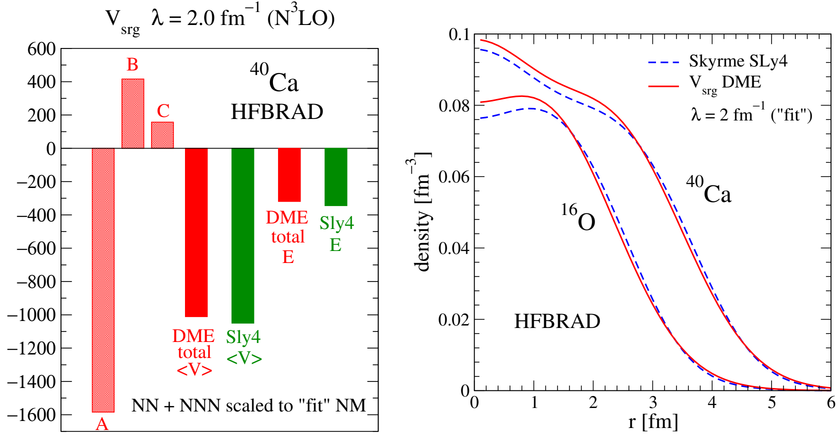
Does it work yet? (Is DME good enough?)

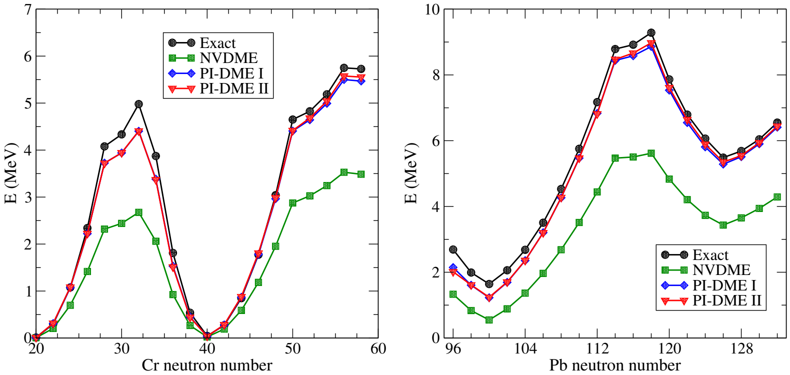
- Try tuned nuclear matter with low-momentum NN/NNN



- Do densities look like nuclei from Skyrme EDF's? (Yes!)
- Are the error bars competitive yet? (No! 1 MeV/A off in ^{40}Ca)

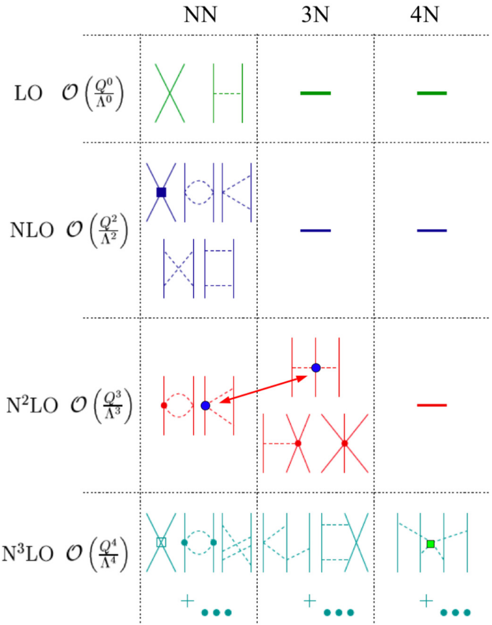
Improved DME for pion exchange [Gebremariam et al.]

- Phase-space averaging for finite nuclei (symmetries, sum rules)
- Focus on long-range interactions $\Longrightarrow$ pion exchange in NN and NNN from chiral effective field theory (χEFT)
- Tests are very promising [arXiv:0910.4979]:



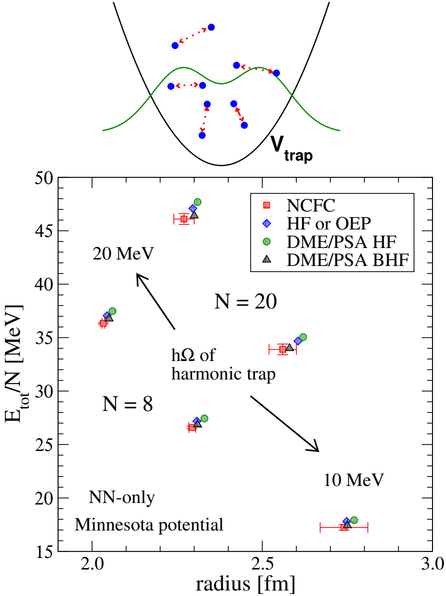
Long-range chiral EFT $\Longrightarrow$ enhanced Skyrme

- Add long-range (π-exchange) contributions in the density matrix expansion (DME)
  - NN/NNN through N^{2}LO [Gebremariam et al.]
- Refit Skyrme parameters
- Test for sensitities and improved observables (e.g., isotope chains) [ORNL]
- Spin-orbit couplings from 2π 3NF particularly interesting
- Can we “see” the pion in medium to heavy nuclei?

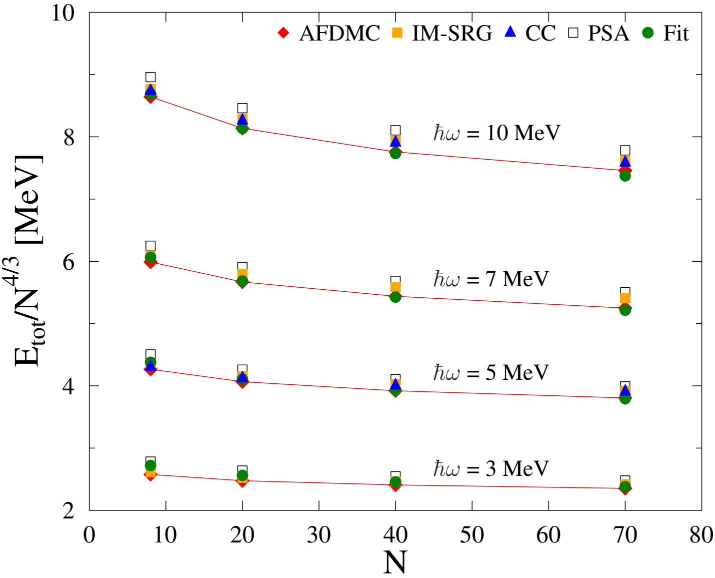


Hybrid DFT: Merge chiral EFT and Skyrme

- Include long-range pion physics via density matrix expansion (DME/PSA)
- Refit short-range physics in Skyrme EDF form
- Validate against ab initio NCFC calculations [Maris]
- Controlled tests for neutrons in trap $\Longrightarrow$ constraints on neutron-rich nuclei
  - NUCLEI/UNEDF collaboration
  - Tests with simplified interaction promising!



Hybrid DFT: on-going work with neutron drops



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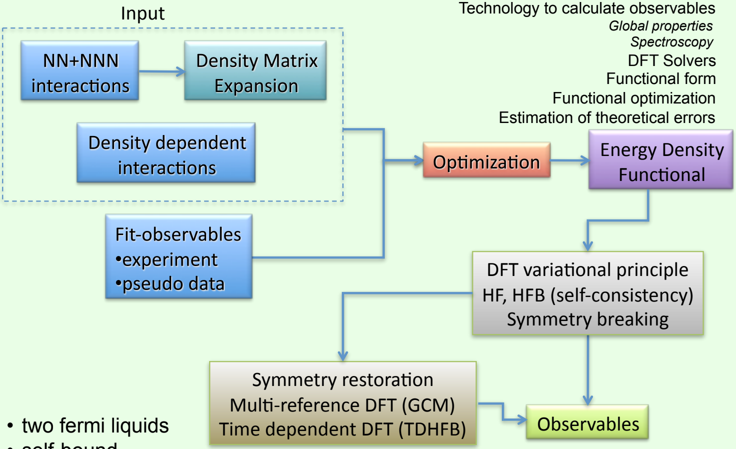
DFT for nuclei [UNEDF and NUCLEI projects]

Nuclear Density Functional Theory and Extensions

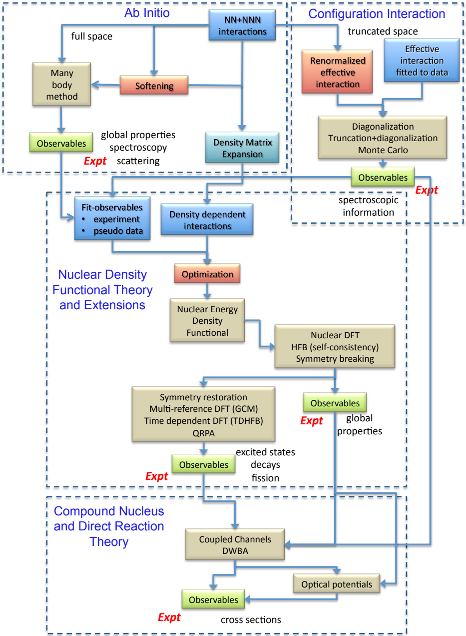


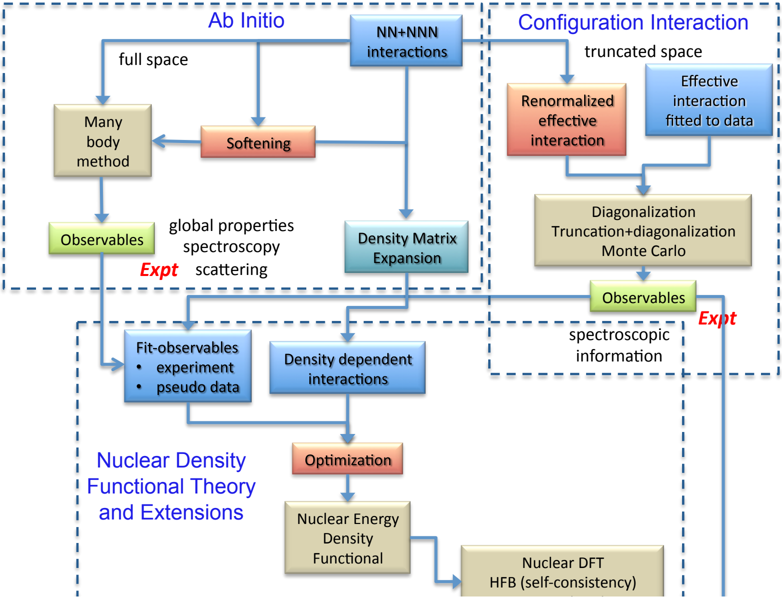
- two fermi liquids
- self-bound
- superfluid (ph and pp channels)
- self-consistent mean-fields
- broken-symmetry generalized product states

- Direct comparison with experiment
- Pseudo-data for reactions and astrophysics

- SciDAC-2 UNEDF project
- Universal Nuclear Energy Density Functional
- Collaboration of physicists, applied mathematicians, and computer scientists
- US funding but international collaborators also
- See unedf.org for highlights!

New SciDAC-3 NUCLEI project:
NUclear Computational
Low-Energy Initiative
(see computingnuclei.org)




Ab Initio
NN+NNN interactions
full space
Many body method
Softening
Observables
global properties
spectroscopy
Expt
scattering
Density Matrix Expansion
Configuration Interaction
truncated space
Renormalized effective interaction
Effective interaction fitted to data
Diagonalization
Truncation+diagonalization
Monte Carlo
Observables
Expt
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Optimization
Nuclear Density Functional Theory and Extensions
Nuclear Energy Density Functional
Nuclear DFT
HFB (self-consistency)

Interaction with computer science experts

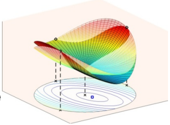
"Derivative-free Optimization for Density Functional Calibration" - Moré & Wild, ANL

ASCR- Applied Mathematics Highlight

Objectives

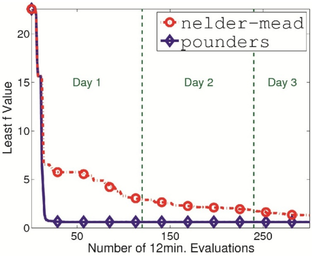
- **Develop optimization algorithms for calibrating UNEDF energy density functionals (EDFs) to selected experimental observables**
- **Exploit the mathematical structure of this calibration problem**
- **Enable sensitivity analysis**

Impact



- **Provide UNEDF with properly optimized functionals for wide classes of nuclei and diverse physical observables**
- **New computational tools for calibrating large scale computer simulations for applications outside of UNEDF project**
- **New statistical tools for providing uncertainty quantification and error analysis, and new experimental data assessment**

POUNDERS obtains better solutions faster



Progress / Accomplishments 2010

- New code, POUNDERS, yields substantial computational savings over alternative algorithms
- Enables fitting of complex EDFs -- previous optimizations required too many evaluations to obtain desirable features
- Using the resulting EDF parameterization, *UNEDF0,* the entire nuclear mass table was computed
- "Nuclear Energy Density Optimization." M. Kortelainen, T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. Stoitsov, and S. Wild. Physical Review C **82**, 024313 (2010).

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