Non-empirical energy density functionals

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Outline

1) Renormalization group methods

2) Microscopically-constrained Skyrme functionals

3) Other efforts towards non-empirical functionals
Λ / Resolution dependence of nuclear forces

with high-energy probes: quarks+gluons

Effective theory for NN, 3N, many-N interactions and electroweak operators: resolution scale/Λ-dependent

\[ H(\Lambda) = T + V_{NN}(\Lambda) + V_{3N}(\Lambda) + V_{4N}(\Lambda) + \ldots \]

Λ >> m_π, k_F in typical interactions

# of sp states for A-body ~ Λ^3A

Strong correlations, non-perturbative
Why large $\Lambda$’s are complicated: ab initio DFT

Ab initio DFT (OEP/effective action) corresponds to MBPT with

$$H = (T + U) + (V - U) = H_{KS} + H_1$$

Want freedom to chose $U$ such that corrections to density beyond $H_{KS}$ vanish

Large $\Lambda V_{NN}$ strongly couples low/high $k$

coupling persists even with $G$ matrix resummation $\implies$ non-perturbative in $G$ and convergence of hole-line expansion strongly depends on $U$
2 Types of Renormalization Group Transformations

“$V_{\text{low } k}$”
integrate-out high $k$ states
preserves observables for $k < \Lambda$

“Similarity RG”
eliminate far off-diagonal coupling
preserves “all” observables

Very similar consequences despite differences in appearance
(low and high momentum decoupled)
RG-Improved Convergence in ab-initio calculations

SKB, Furnstahl, Maris, Schwenk, Vary (2008)

Li-6 diagonalization in HO basis

$10^3$ states for $N_{max} = 2$

versus

$10^7$ states for $N_{max} = 10$

Helium Halo Nuclei

Bacca et al. (2009)

Ab-initio calculations of heavier nuclei accessible...
Towards including 3N interactions in medium mass nuclei

normal-ordered 0-, 1- and 2-body parts of 3N interaction dominate

residual 3N interaction can be neglected: very promising

coupled-cluster calculations of closed-shell nuclei
Perturbative Nuclear Matter with chiral EFT + RG?

HF bound and saturates, converged at $\approx 2$nd order MBPT
3N drives saturation, theoretical error bands

Empirical saturation lies in theoretical error bands w/out fine-tuning
Is a solution to a 50 year old problem in reach?
Promising for a microscopic nuclear Density Functional Theory (DFT)?
The Similarity Renormalization Group
Wegner, Glazek and Wilson

Unitary transformation on an initial $H = T + V$

$$H_\lambda = U(\lambda) H U^\dagger(\lambda) \equiv T + V_\lambda$$

$\lambda =$ continuous flow parameter

Differentiating with respect to $\lambda$:

$$\frac{dH_\lambda}{d\lambda} = [\eta(\lambda), H_\lambda]$$

with

$$\eta(\lambda) \equiv \frac{dU(\lambda)}{d\lambda} U^\dagger(\lambda)$$

Engineer $\eta$ to do different things as $\lambda \Rightarrow 0$

$$\eta(\lambda) = [G_\lambda, H_\lambda]$$

$$G_\lambda = T \Rightarrow H_\lambda \text{ driven towards diagonal in } k - \text{ space}$$

$$G_\lambda = PH_\lambda P + QH_\lambda Q \Rightarrow H_\lambda \text{ driven to block—diagonal}$$

\[\vdots\]
Normal Ordered Hamiltonians

\[ H = \sum t_i a_i^\dagger a_i + \frac{1}{4} \sum V_{ijkl}^{(2)} a_i^\dagger a_j^\dagger a_l a_k + \frac{1}{36} \sum V_{ijklmn}^{(3)} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l \]

Normal-order w.r.t. some reference state \( \Phi \) (e.g., HF):

\[ H = E_{vac} + \sum f_i N(a_i^\dagger a_i) + \frac{1}{4} \sum \Gamma_{ijkl} N(a_i^\dagger a_j^\dagger a_l a_k) + \frac{1}{36} \sum W_{ijklmn} N(a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l) \]

\[ E_{vac} = \langle \Phi | H | \Phi \rangle \]

\[ f_i = t_{ii} + \sum_h \langle ih | V_2 | ih \rangle n_h + \frac{1}{2} \sum_{hh'} \langle ihh' | V_3 | ihh' \rangle n_h n_{h'} \]

\[ \Gamma_{ijkl} = \langle ij | V_2 | kl \rangle + \sum_h \langle ijh | V_3 | klh \rangle n_h \]

\[ W_{ijklmn} = \langle ijk | V_3 | lmn \rangle \quad \langle \Phi | N(\cdots) | \Phi \rangle = 0 \]

0-, 1-, 2-body terms contain some 3NF effects thru density dependence => Efficient truncation scheme for evolution of 3N?
In-medium SRG for Infinite NM and closed-shell nuclei

• Normal order H w.r.t. fermi sea
• Choose SRG generator to eliminate “energy off-diagonal” pieces

\[ \lim_{s \to \infty} \Gamma_{od}(s) = 0 \]

\[ \langle 12 | \Gamma_{od} | 34 \rangle = 0 \text{ if } f_{12} = f_{34} \]

\[ \eta = [\hat{f}, \hat{\Gamma}] \]

• Truncate flow equations to 2-body normal-ordered operators
  - dominant parts of induced many-body forces included implicitly

\[ H(\infty) = E_{vac}(\infty) + \sum f_i(\infty) N(a_i^\dagger a_i) + \frac{1}{4} \sum \Gamma_{d}(\infty)_{ijkl}N(a_i^\dagger a_j^\dagger a_l a_k) \]

\[ E_{vac}(\infty) \rightarrow E_{gs} \]

\[ f_k(\infty) \rightarrow \epsilon_k \text{ (fully dressed s.p.e.)} \]

\[ \Gamma_d(\infty) \rightarrow f(k', k) \text{ (Landau q.p. interaction)} \]

Microscopic realization of SM ideas: dominant MF + weak A-dependent NN_{eff}
Some observations

1) \( \frac{d}{ds} \langle H \rangle_0 \leq 0 \) for monotonic \( f_k \)
   correlations weakened, HF picks up more binding with increasing \( s \).

2) pp channel + 2 ph channels treated on equal footing

3) Intrinsically non-perturbative

4) no unlinked diagrams (size extensive, etc.)

5) “3rd-order exact” a-la CCSD

6) Extension to effective operators/Shell model possible
In-medium SRG for nuclei \textsuperscript{13} 

Comparable to CCSD(T) in closed shell nuclei

Promising method to calculate shell model valence $H_{\text{eff}}/O_{\text{eff}}$
Correlations “adiabatically” summed into $H(\lambda)$

$\kappa_F = 1.35 \text{ fm}^{-1}$

$N^3 \text{LO}(500)$

$\lambda \text{ [fm}^{-1}\text{]}

$E/A$ [MeV]

$E_0$

$E_{\text{BHF}}$ (in-medium SRG)

$E_{\text{BHF}}$ (free-space SRG)

$E_{\text{MBPT}(2)}$

$h\omega = 30 \text{ MeV}$

$e_{\text{max}} = 2$

$e_{\text{max}} = 3$

$e_{\text{max}} = 4$

$e_{\text{max}} = 5$

$\text{INM}$

$^4\text{He}$

$\text{Useful for ab initio DFT? Shell model?}$
Accomplishments of Phenomenological Energy Functionals

2N separation energies, Quadrupole and BE2 values, Fission energy surfaces, mass tables in a day, plus many other impressive feats

BUT...
Limitations of Existing Energy Functionals (Predictability)

- Uncontrolled extrapolations away from known data
- Theoretical error-bars?

[Graphs showing two-neutron separation energies and binding energy in Sn isotopes]

[J. Sadoudi, T. D., unpublished]
What’s missing in phenomenological EDFs?

- Density dependencies too simplistic
- Isovector components not well constrained
- No way to estimate theoretical uncertainties
- What’s the connection to many-body forces?

Turn to microscopic many-body theory for guidance, aided by the simplifications enabled by RG-evolved interactions

[www.unedf.org](http://www.unedf.org)
Local Skyrme-like Functionals from RG-evolved Interactions

Dominant MBPT contributions to bulk properties take the form

$$\langle V \rangle \sim \text{Tr}_1 \text{Tr}_2 \int d\mathbf{R} \, dr_{12} \, dr_{34} \, \rho(r_1, r_3) \, K(r_{12}, r_{34}) \, \rho(r_2, r_4) \, + \, \text{NNN} \, \cdots$$

K is either free-space interaction (HF) or resummed in-medium vertex (BHF)

Written in terms on non-local quantities
- density matrices and s.p. propagators
- finite range interaction vertex $K$

Connection to $E = E[\rho]$ is not obvious!
Density Matrix Expansion Revisited (Negele and Vautherin)

Expand of DM in local operators w/factorized non-locality

\[
\langle \Phi | \psi^\dagger (\mathbf{R} - \frac{1}{2} \mathbf{r}) \psi (\mathbf{R} + \frac{1}{2} \mathbf{r}) | \Phi \rangle = \sum_n \Pi_n (k_F r) \langle \mathcal{O}_n (\mathbf{R}) \rangle
\]

\[
\langle \mathcal{O}_n (\mathbf{R}) \rangle = [\rho (\mathbf{R}), \nabla^2 \rho (\mathbf{R}), \tau (\mathbf{R}), \mathbf{J} (\mathbf{R}), \ldots]
\]

Dependence on local densities/currents now manifest

\[
\langle V_2 \rangle \sim \sum_{n,m} \int d\mathbf{R} \mathcal{O}_n (\mathbf{R}) \mathcal{O}_m (\mathbf{R}) \int d\mathbf{r} \Pi_n (k_F r) \Pi_m (k_F r) V_2 (r)
\]

\[
\sim \sum_t \int d\mathbf{R} \left\{ C_t^{\rho \rho} \rho_t^2 + C_t^{\rho \tau} \rho_t \tau_t + C_t^{\rho \Delta \rho} \rho_t \Delta \rho_t + C_t^{J J} J_t^2 + C_t^{J \nabla \rho} J_t \nabla \rho_t \ldots \right\}
\]

Skyrme-like EDF with density-dependent couplings dominated by long-range pion-physics
Prescriptions for $\Pi_n$-functions

Phase space averaging (PSA-DME) (Gebremariam et al. arXiv:0910.4979)

$$\rho(\vec{r}_1, \vec{r}_2) = e^{i \vec{r} \cdot \vec{k}} e^{\frac{\vec{r}}{2} \cdot (\vec{\nabla}_1 - \vec{\nabla}_2) - i \vec{r} \cdot \vec{k}} \rho(\vec{r}_1, \vec{r}_2) \bigg|_{\vec{r}_1 = \vec{r}_2 = \vec{R}}$$

Average the non-locality operator over local momentum distribution $g(\vec{R}, \vec{k})$ and expand exponentiated gradients

$$\rho(\vec{r}_1, \vec{r}_2) \approx \int d^3 \vec{k} \ g(\vec{R}, \vec{k}) e^{i \vec{k} \cdot \vec{r}} \sum_{n=0}^{2} \frac{1}{n!} \left\{\vec{r} \cdot \left(\frac{\vec{\nabla}_1 - \vec{\nabla}_2}{2} - i \vec{k}\right)\right\}^n \rho(\vec{r}_1, \vec{r}_2) \bigg|_{\vec{r}_1 = \vec{r}_2 = \vec{R}}$$

Easy to build in physics associated with surface effects in finite fermi systems

Crucial to accurately describe spin-vector part of OBDM
Prescriptions for $\Pi_n$-functions

Negele and Vautherin (NV-DME)
Truncated Bessel expansion of non-locality operator
Sufficient for spin-unsaturated nuclei only

Why it fails: no phase space averaging done for spin-vector part
Improved Vector PSA-DME

anisotropy of $g(R,k)$ in the spatial surface
(Bulgac et al.)
Inclusion of finite fermi phase space effects crucial for **quantitative** agreement

• completely parameter-free

Can now apply modified DME with confidence
to spin-unsaturated systems
Including Long Range Chiral EFT in Skyrme-like EDFs

\[ V_{EFT} = V_{ct}(\Lambda) + V_{1\pi} + V_{2\pi} + \cdots \]

Each EDF coupling function splits into 2 terms

1) \textbf{\textit{\Lambda-dependent}} Skyrme-like coupling constants (short-distance)

2) \textbf{\textit{\Lambda-independent}} coupling functions from “universal” pion physics

\[ C'_t^{\rho\tau} \Rightarrow C'_t^{\rho\tau}(\Lambda; V_{ct}) + C'_t^{\rho\tau}[k_F(R); V_{\pi}] \]

\text{From contact terms in EFT/RG V’s} \hspace{4cm} \text{From pion exchanges} \hspace{4cm} \text{Etc…}

Suggests a microscopically-improved Skyrme phenomenology

Add pion-exchange couplings to existing Skyrmes and refit constants using guidance from EFT (naturalness, etc.)
Gameplan - Include pion physics in Skyrme EDFs and refit

- Include DME coupling functions from finite-range NN and NNN chiral EFT thru N2LO

- Refit the Skyrme coupling constants (EFT constraints => naturalness)

- Look for improved observables and for sensitivities

- Can we “see” the pion as in NN phase shift analyses

Expect interesting spin-orbit consequences (NN vs NNN)

in progress w/ ORNL group (Stoitsov et al.)
New development: DME for chiral NNN force (N2LO)

- Expect interesting spin-orbit/tensor couplings from TPE

\[ V_c(q_1, q_2, q_3) \sim \frac{\sigma_1 \cdot q_1 \sigma_2 \cdot q_2}{(q_1^2 + m_n^2)(q_2^2 + m_n^2)} F_{123}^{\alpha\beta} \tau_1^\alpha \tau_2^\beta + \text{perms} \]

\[ F_{123}^{\alpha\beta} \equiv \delta_{\alpha\beta} \left[ -4 \frac{c_1 m_n^2}{f^2} + 2 \frac{c_3}{f^2} q_1 \cdot q_2 \right] + \frac{c_4}{f^2} \epsilon^{\alpha\beta\gamma} \tau_3^\gamma \sigma_3 \cdot (q_1 \times q_2) \]

Empirical EDFs (Skyrme, Gogny,...) spin-orbit coupling is density independent => appropriate for NN spin-orbit forces (short range)

This is a mismatch since microscopic NNN interactions are long-range (DME ==> strong density dependent \( J \cdot \nabla \rho \) couplings)

Complexity explodes ==> Automated symbolic tools developed (Gebremariam et al) will be available at www.unedf.org
\[ \varepsilon^{CR1,2x} = \int d\tau \left\{ C^0_7^{\rho_0^3} \rho_0^3(\tau) + C^0_7^{\rho_0^2} \rho_0^2(\tau) \rho_1^2(\tau) + C^0_7^{\rho_0^1 \xi_1^1} \rho_0(\tau) \rho_1(\tau) \xi_1^1(\tau) \\
+ C^0_7^{\rho_0^3} \rho_0^3(\tau) \Delta \rho_0(\tau) + C^0_7^{\rho_0^1 \Delta \rho_1} \rho_0(\tau) \rho_1(\tau) \Delta \rho_1(\tau) + C^0_7^{\rho_0^3 \xi_0^2} \rho_0(\tau) \xi_0^2(\tau) \\
+ C^0_7^{\rho_1^2 \xi_0^2} \rho_1^2(\tau) \xi_0^2(\tau) + C^0_7^{\rho_0^1 \xi_1^1} \rho_0(\tau) \rho_1(\tau) \xi_1^1(\tau) + C^0_7^{\rho_0^3 \xi_0^1} \rho_0(\tau) \xi_0^1(\tau) \\
+ C^0_7^{\rho_0^1 \xi_1^1} \rho_0(\tau) \xi_1^1(\tau) \tilde{J}_0(\tau) \cdot \tilde{J}_0(\tau) + C^0_7^{\rho_1^1 J_0 J_1} \rho_1(\tau) \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) + C^0_7^{\rho_0^1 J_1} \rho_0(\tau) \tilde{J}_1(\tau) \cdot \tilde{J}_1(\tau) \\
+ C^0_7^{\rho_0^3 \nabla J_0} \tilde{J}_0(\tau) \cdot \tilde{J}_0(\tau) \cdot \tilde{J}_0(\tau) + C^0_7^{\rho_0^1 \nabla J_1 \nabla J_1} \tilde{J}_1(\tau) \cdot \tilde{J}_1(\tau) \cdot \tilde{J}_1(\tau) + C^0_7^{\rho_0^1 J_0 \nabla J_1 J_1} \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) \cdot \tilde{J}_1(\tau) \\
+ C^0_7^{\rho_0^1 J_0 J_1} \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) + C^0_7^{\rho_0^1 J_0 J_1} \Delta \rho_1(\tau) \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) + C^0_7^{\rho_0^1 J_0 J_1} \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) \\
+ C^0_7^{\rho_0^1 J_0 J_1} \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) + C^0_7^{\rho_0^3 \nabla J_0} \rho_0(\tau) \tilde{J}_0(\tau) (\tilde{J}_0(\tau))^2 + C^0_7^{\rho_0^3 J_0 J_1 \nabla J_1} \rho_0(\tau) \tilde{J}_1(\tau) \cdot \Delta \tilde{J}_0(\tau) \\
+ C^0_7^{\rho_0^1 J_0 J_1} \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) + C^0_7^{\rho_0^1 J_0 J_1} \Delta \rho_1(\tau) \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) + C^0_7^{\rho_0^1 J_0 J_1} \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) \\
+ C^0_7^{\rho_0^1 J_0 J_1} \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) + C^0_7^{\rho_0^3 \nabla J_0 J_0} \rho_0(\tau) \tilde{J}_0(\tau) \cdot \tilde{J}_0(\tau) + C^0_7^{\rho_0^1 J_0 J_1} \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) \\
+ C^0_7^{\rho_0^1 J_0 J_1} \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) + C^0_7^{\rho_0^3 \nabla J_0 J_1 J_1} \rho_1(\tau) \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) \cdot \tilde{J}_1(\tau) + C^0_7^{\rho_0^3 J_0 J_1 J_1} \rho_0(\tau) \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) \cdot \tilde{J}_1(\tau) \\
+ C^0_7^{\rho_0^1 J_0 J_1 J_1} \rho_1(\tau) \tilde{J}_0(\tau) \cdot \tilde{J}_1(\tau) \cdot \tilde{J}_1(\tau) + C^0_7^{\rho_0^1 J_0 J_1 J_1} \rho_0(\tau) \tilde{J}_1(\tau) \cdot \Delta \tilde{J}_1(\tau) \right\} . \] 

(91)

\[ + 4 \text{ other classes of similar terms} \]

Looks ugly (or beautiful, depending on your view), but a regular structure emerges:

\[ C^{ijk}[u] \xi_i \xi_j \xi_k, \quad u \equiv \frac{k_F(R)}{m_\pi} \quad (\text{note: } u \text{ is NOT small}) \]

\[ C^{ijk}[u] = C^{ijk}_1[u] + C^{ijk}_2[u] \ln(1 + 4u^2) + C^{ijk}_3[u] \arctan(2u), \]

\[ C^{ijk}[u] = \text{rational polynomial} \]
Some examples (Gebremariam, SKB, Duguet 2010)

Comparison of EDF w/pions to Skyrme couplings w/tensor force

density dependence controlled by longest range component

\[ \rho^{7/3}, \rho^{4/3}, \rho^{2/3}, \frac{1}{\rho^{2/3}} \log(1 + c \rho^{2/3}), \ldots \]
Moral: Simple many-body theory + current understanding of underlying NN + NNN interactions tells us Skyrme is way too simple.

First exploratory calculations in progress w/M. Stoitsov et al. using the extended EDF (implemented in HFBRAD and HFBTHO)

Mathematica nb’s with 2N/3N DME couplings available at www.unedf.org
Other efforts developing non-empirical EDFs

**Non-empirical pairing functional** *(Duguet, Lesinski, Hebeler, Schwenk)*

Build first $\Sigma^q$ and $\Delta^q$ at lowest-order in $V_{NN}$ and $V_{NNN}$ (RG-evolved)

- $v^{pp}$: microscopically built from $V_{NN}$ and $V_{NNN}$
- $v^{ph}$: semi-empirical from constrained Skyrme EDF ($m^* \approx 0.7\, m$)

Low-rank separable expansion good at low $\Lambda$

Almost as cheap as local pairing EDF calculations
With $V_{\text{low } k} + V_{\text{coulomb}} + \text{approximate NNN}$


$\Delta_{q, \text{exp}}^{(3)}$ versus $\Delta_{q, \text{th}}^{(3)}$

- $\Delta_{q}^{(3)}$ decreased by 20% with slight isovector trend ($|V_{qq(q)}^{1S_0}| > |V_{qq(q)}^{1S_0}|$)
- Leave $\sim 20 - 30\%$ for coupling to (collective) fluctuations

Next: Beyond 1st order (Gorkov 2nd-order, In-medium SRG), local approx’s
Other efforts developing non-empirical EDFs

DME functional vs. ab initio (SKB, Furnstahl, Platter)

Start from the same H and compare with no adjustments

This was pre-PSADME improvements and implementation of exact Hartree. Worth revisiting!
Other efforts developing non-empirical EDFs

DME beyond $\nabla^2$ (Carlsson, Dobaczewski, arXiv:1003.2543)

New “Damped Taylor” DME gives dramatic improvements with higher order gradients

Solves the problem of exploding # of parameters with higher $\nabla$
Summary

• RG methods simplify nuclear many-body calculations
  - faster convergence, more perturbative, low k “universality”
  - empirical NM saturation within theoretical errors

• In-medium SRG
  - Normal-ordering => simple way to evolve many-body operators
  - analogous to CC; diagonalize many-body problems
  - non-perturbative path for shell model and possible ab-initio DFT

• Microscopic connections to DFT now possible
  - explicit inclusion of long-distance chiral EFT physics via the density matrix expansion (microscopic guidance for density dependence, isovector and spin-orbit properties, etc.)