EFT for nuclear DFT: Looking for help

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Frontiers in Nuclear Physics
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Key question #2:
Can successful, but model dependent, many-body methods, such as density functional approaches, be transformed into predictive EFTs, allowing for model-independent investigations of the limits of nuclear stability?

Outline

Motivations for considering nuclear DFT as an EFT

Extensions of nuclear EDFs using EFT ideas

Nuclear DFT as effective action

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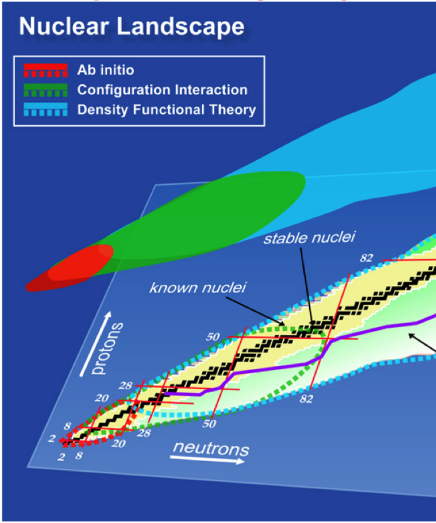
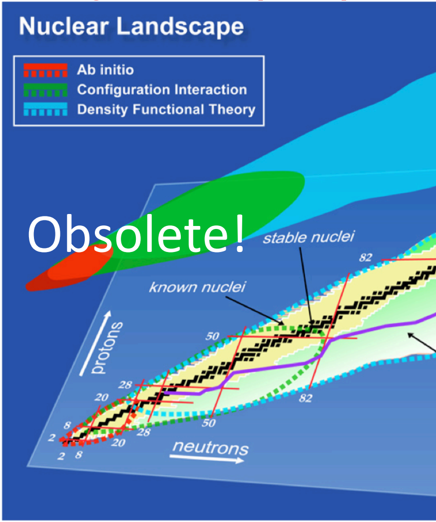
Explosion of many-body methods using microscopic input



- Ab initio (new and enhanced methods; microscopic NN+3NF)
- Shell model (usual: empirical inputs)
- Density functional theory

Explosion of many-body methods using microscopic input

- Ab initio (new and enhanced methods; microscopic NN+3NF)
  - Stochastic: GFMC/AFDMC; lattice EFT
  - Diagonalization: IT-NCSM
  - Non-linear eqs: coupled cluster
  - Flow equations: IM-SRG
  - Self-consistent Green's function
  - Many-body perturbation theory
- Shell model (usual: empirical inputs)
  - Effective SM interactions from coupled cluster, IM-SRG
- Density functional theory
  - Microscopic input, e.g., DME



Boundaries are continually pushed; e.g., α–α scattering and properties of Calcium isotopes and ...

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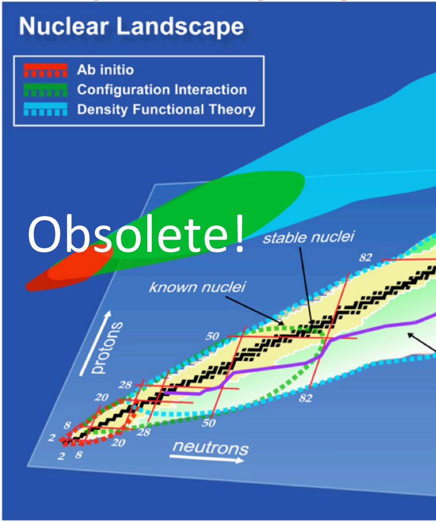
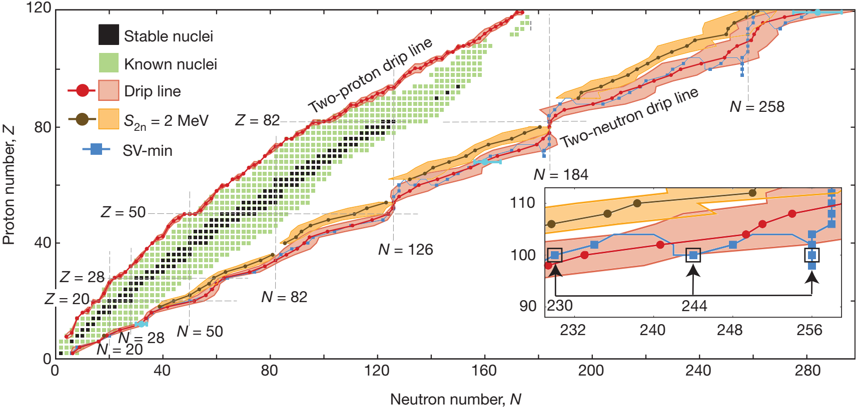
  - Bottom-up EFT?



Boundaries are continually pushed; e.g., α–α scattering and properties of Calcium isotopes and . . .

"The limits of the nuclear landscape" ⟶ full mass table

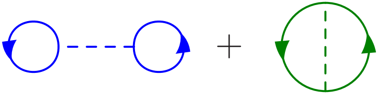
J. Erler et al., Nature **486**, 509 (2012)



- Proton and neutron driplines predicted by Skyrme EDFs
  - Total: 6900 $\pm$ 500 nuclei with $Z \leq 120$ ($\approx$ 3400 known)
  - Systematic errors estimated by comparing models
  - Computationally efficient (but still a HPC problem)

Bestiary of [universal] nuclear energy functionals

- Nonrelativistic [HFB] functionals
  - Skyrme — local densities and ∇s
  - Gogny — finite range Gaussians
  - Fayans — self-consistent FFS



- Relativistic [covariant Hartree + pairing = RHB] functionals
  - RMF — meson fields (generalized Walecka model)
  - point coupling Lagrangian

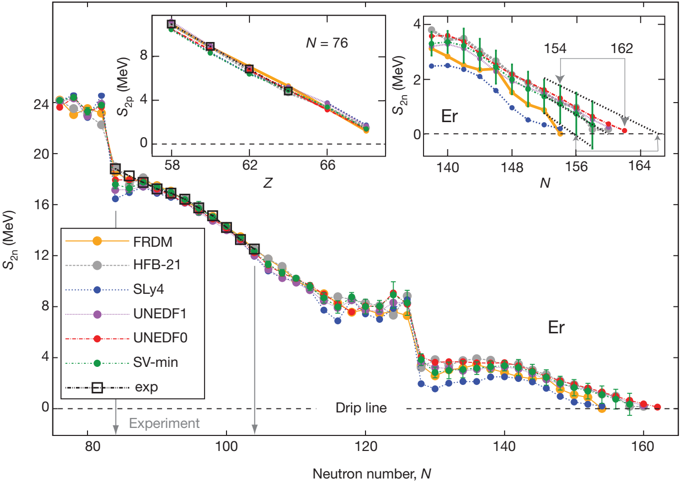
1. Repeat cycle until stops changing (self-consistent):

   densities $\rho_i \to$ potential that minimizes energy $E[\rho_i] \to$ s.p. states $\to \rho_i$

   Densities (or density matrices) from single-particle wave functions
   Includes pairing densities, i.e., $\langle\psi_i\psi_j\rangle$ as well as $\langle\psi_i^\dagger\psi_j\rangle$
2. [Restore symmetries, beyond mean-field correlations, . . .]
3. Evaluate observables (masses, radii, β-decay, fission . . .)

Frequently interpreted as Kohn-Sham density functional theory

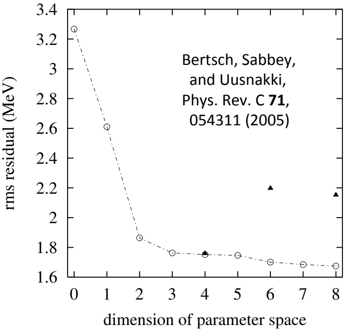
"The limits of the nuclear landscape"

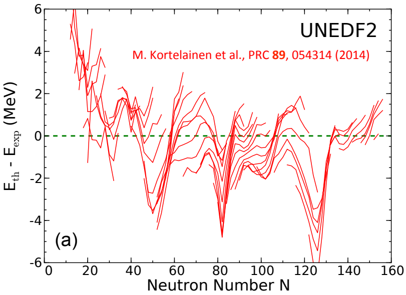


- Two-neutron separation energies of even-even erbium isotopes
  - Compare different functionals, with uncertainties of fits
  - Dependence on neutron excess poorly determined (cf. driplines)

State-of-the-art Skyrme EDFs

- Is there a limit to improvement of Skyrme rms energy residual?
- Recently many advances by UNEDF/NUCLEI, FIDIPRO, and others to improve/test EDFs
- Extra observables and ab initio calculations in neutron drops for constraints (e.g., on isovector)
- Sophisticated fit and correlation analysis implies the EDF is not limited by the parameter fitting
- But still don't beat the energy barrier (and not nearly as good energy rms as mass models)
- $\Longrightarrow$ limit of Skyrme EDF strategy?





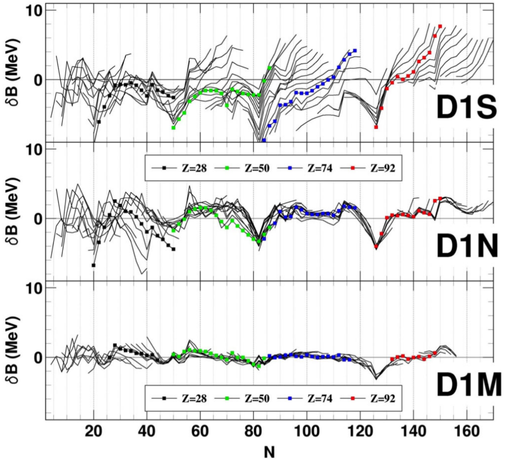
Gogny HFB as a mass model: State-of-the-art

$$V(1,2) = \sum_{j=1,2} e^{-\frac{(r_1-r_2)^2}{\mu_j^2}} \left(W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau\right) \qquad \{\mu_j\} = \{0.5, 1.0\}\,\text{fm}$$

$$+ t_0(1 + x_0 P_\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2)\rho(\bar{\mathbf{r}})^\alpha + iW_{LS}\overleftarrow{\nabla}_{12}\delta(\mathbf{r}_1 - \mathbf{r}_2) \times \overrightarrow{\nabla}_{12} \cdot (\vec{\sigma}_1 + \vec{\sigma}_2)$$

Goriely et al., Eur. Phys. J. A **52**, 202 (2016)

- $\approx$ 14 parameters
- quadrupole correlations included self-consistently
- D1M: $\delta B_{rms} = 0.8$ MeV for 2353 masses
- $\sigma \approx 0.65$ MeV for 2064 β-decay energies
- radii, giant resonances and fission properties
- SNM: $k_F \approx 1.34\,\text{fm}^{-1}$, $a_v \approx -16$ MeV

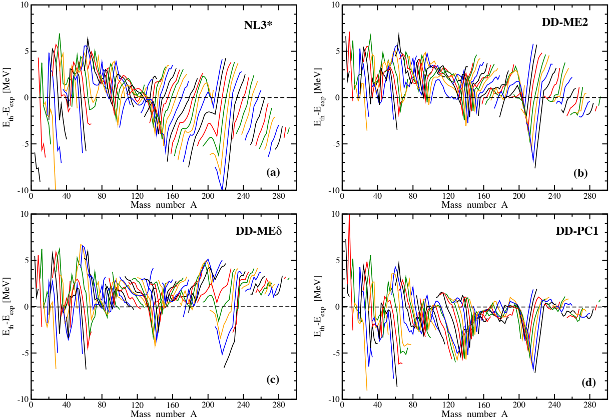


Covariant EDFs: Relativistic mean-field models

$$\mathcal{L} = \bar{\psi}\left[\gamma\cdot(i\partial - g_\omega\omega - g_\rho\boldsymbol{\rho}\cdot\boldsymbol{\tau} - eA) - m - g_\sigma\sigma\right]\psi + \frac{1}{2}(\partial\sigma)^2 - \frac{1}{2}m_\sigma\sigma^2 - \frac{1}{3}g_2\sigma^3 - \frac{1}{4}g_3\sigma^4 - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2\omega^2 - \frac{1}{4}\boldsymbol{R}_{\mu\nu}\boldsymbol{R}^{\mu\nu} + \frac{1}{2}m_\rho^2\boldsymbol{\rho}^2 - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}$$

Agbemava et al., Phys. Rev. C **89**, 054320 (2014)

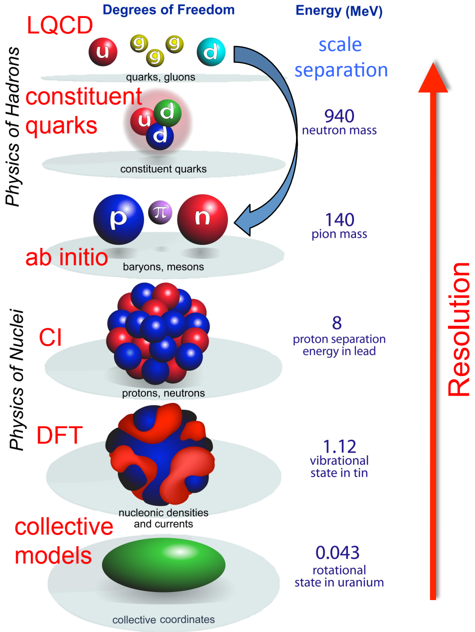
- RHB formalism
- different $\mathcal{L}$s used
- 6–8+ fit parameters (+ pairing parameters)
- beyond mean-field not included
- $\delta B_{rms} \approx 2$–3 MeV for 835 masses
- SNM: $k_F \approx 1.31\,\text{fm}^{-1}$, $a_v \approx -16.1$ MeV



Motivations for doing better than empirical EDFs

- Apparent model dependence (systematic errors?)
- Extrapolations to driplines, large *A*, high density are uncontrolled
- Breakdown and failure mode is unclear:
  e.g., *should* EDFs work to the driplines?
- More accuracy wanted for r-process: is this even possible?
- What observables? Coupling to external currents? $0\nu\beta\beta$ m.e.?
- Connect to nuclear EFTs (and so to QCD)?
- . . .

Hierarchy of nuclear degrees of freedom



Laundry list of nuclear EFTs

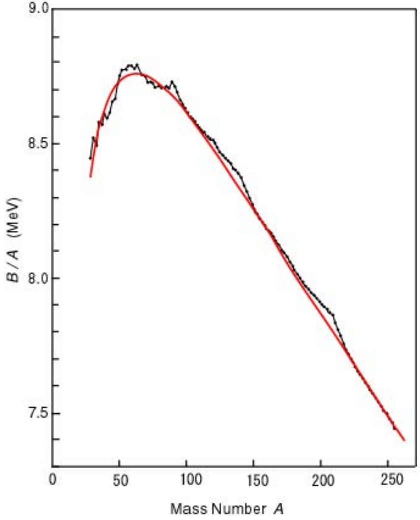
- Chiral EFT: nucleons, [Δ's,] pions; [HO basis]
- Pionless EFT: nucleons only (low-energy few-body) or nucleons and clusters (halo)
- EFT for deformed nuclei: systematic collective dofs (Papenbrock, Coello Pérez, Weidenmueller)
- EFT at Fermi surface (Landau-Migdal theory): quasi-nucleons

Where does DFT fit in?

Liquid drop model: SEMF (bulk properties) $(A = N + Z)$

$$E_B(N,Z) = a_v A - a_s A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_{\rm sym} \frac{(N-Z)^2}{A} + \Delta$$

- Many predictions! Implies $A \to \infty$ limit of nuclear matter (with $e \to 0$) $\Longrightarrow$ saturation point
- Rough numbers: $a_v \approx 16\,$MeV, $a_s \approx 18\,$MeV, $a_C \approx 0.7\,$MeV, $a_{\rm sym} \approx 28\,$MeV
- Nuclear radii: $R \approx (1.2\,\text{fm})A^{1/3}$
- Pairing $\Delta \approx \pm 12/\sqrt{A}\,$MeV (even-even/odd-odd) or 0 [or $43/A^{3/4}$ MeV or …]
- More detailed mass formulas include shell effects, etc.



Questions to address about EFT for DFT

- What are the relevant degrees of freedom? Symmetries?
  [Can we have quasiparticles in the bulk?]
- Power counting: what is our expansion? Breakdown scale?
- Is there an RG argument to apply? (cf. scale toward Fermi surface)
- How should the EFT be formulated? Effective action?
  How do I think about parameterizing a density functional?
- How can we implement/expand about liquid drop physics?
- How do we reconcile the different EDF representations?
- Dealing with zero modes — can we adapt methods for gauge theories (for constraints)?
- Can we implement such an EFT without losing the favorable computational scaling of current nuclear EDFs?

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Motivations for considering nuclear DFT as an EFT

Extensions of nuclear EDFs using EFT ideas

Nuclear DFT as effective action

Skyrme energy functionals (original motivation: G-matrix)

- 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 (zero modes), beyond mean-field correlations, ...

What is learned from comparing Skyrme and dilute EDFs?

- Skyrme energy density functional (for $N = Z$ and without pairing)

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

where $\rho(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2$, $\tau(\mathbf{r}) = \sum_i |\nabla\psi_i(\mathbf{r})|^2$, ...

- Systematic dilute LDA $\rho\tau\mathbf{J}$ EDF (4 species, short-range only)

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

- 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? Can we simply extend it?
  - Does a “perturbative” low-density expansion make sense?

Still more questions for EDFs

- Are density dependencies too simplistic? How do you know?
- How should we organize possible terms in the EDF?
- Where are the pions? Where is chiral symmetry?
- What is the connection to many-body forces?
- How do we estimate *a priori* theoretical uncertainties?
- What is the theoretical limit of accuracy?
- and so on . . .

$\Longrightarrow$ Extend or modify EDF forms in (semi-)controlled way

$\Longrightarrow$ Use microscopic many-body theory for guidance

There are multiple paths to a nuclear EDF $\Longrightarrow$ What about EFT?

Some current strategies for nuclear EDFs using EFT

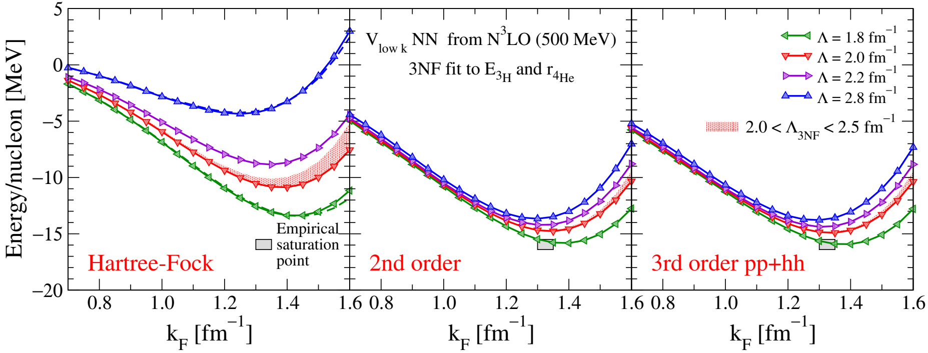
Extend or modify conventional EDF forms in (semi-)controlled ways

1. Long-distance chiral physics from an EFT expansion
   - Density matrix expansion (DME) applied to NN and NNN diagrams
   - [Re-fit residual Skyrme parameters and test description]
   - MBPT expansion justified by phase-space-based power counting
2. In-medium chiral perturbation theory [Munich group]
   - ChPT loop expansion becomes EOS expansion
   - Apply DME to get DFT functional
3. Extend existing functionals following EFT principles
   - Non-local regularized pseudo-potential [Raimondi et al., 1402.1556]
   - Optimize pseudo-potential to experimental data
   - Test with correlation analysis technology
4. RG evolution of effective action functional [Jens Braun et al.]

Here: can we develop bottom-up EFT using a QFT formulation?

Low resolution chiral EFT calculations of nuclear matter

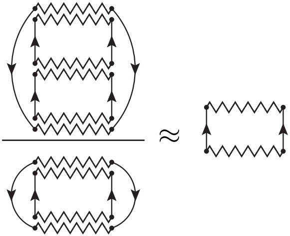
- Evolve NN by RG to low momentum, fit N^2LO NNN to $A = 3, 4$
- Predict nuclear matter in MBPT [Hebeler et al. (2011)]

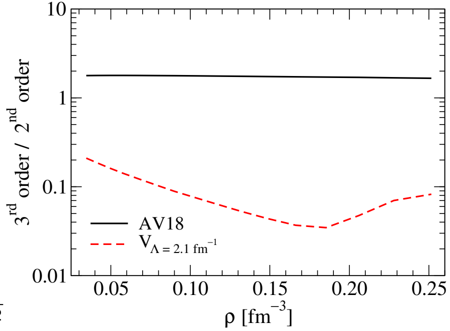


- Cutoff dependence at 2nd order significantly reduced
- 3rd order contributions are small (MBPT validated for PNM)
- Remaining cutoff dependence: many-body corrections, 4NF?

Effects of softening interactions in the nuclear medium

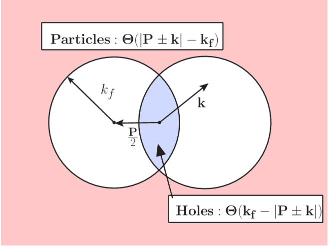
Separable estimate:

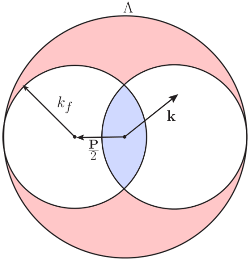




$$\frac{E_{\rm pp}^{(n+1)}}{E_{\rm pp}^{(n)}} \approx \frac{m^*}{m} \int \frac{d^3k}{(2\pi)^3}\, \overline{Q}(P_{\rm av}, k)\, \frac{\langle \mathbf{k}|V|\mathbf{k}\rangle}{k_{\rm av}^2 - k^2}$$

Phase space:





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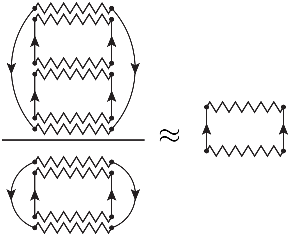

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Suppose $R \ll k_{\rm F}^{-1} \ll a$
and T-matrix has zero-energy pole:

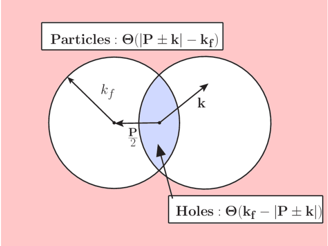
$$\langle \mathbf{p}|T|\mathbf{p}'\rangle = \frac{C_0 \langle \mathbf{p}|\eta\rangle\langle\eta|\mathbf{p}'\rangle}{1 - \int \frac{d^3k}{(2\pi)^3} \frac{\langle \mathbf{k}|V|\mathbf{k}\rangle}{E - \hbar^2 p^2/m}}$$

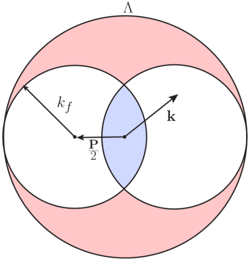
$\Longrightarrow C_0 \sim -2\pi^2/\Lambda$ and $R \propto \Lambda^{-1}$

$\Longrightarrow k_{\rm F} \ll \Lambda \Longrightarrow Q_{k_{\rm F}} \to 1$

$\Longrightarrow E_{\rm pp}^{(n+1)}/E_{\rm pp}^{(n)} \sim -1$

Phase space:

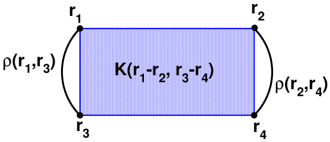




Density matrix expansion (DME) revisited [Negele/Vautherin]

- Dominant chiral EFT 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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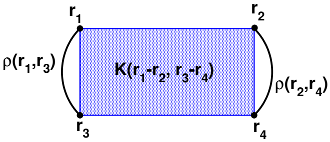

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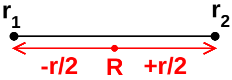
- DME: Expand KS ρ in local operators w/factorized non-locality

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



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!

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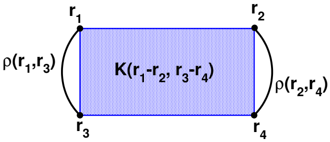

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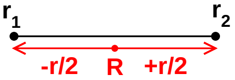


with $\langle \mathcal{O}_n(\mathbf{R})\rangle = \{\rho(\mathbf{R}), \nabla^2\rho(\mathbf{R}), \tau(\mathbf{R}), \cdots\}$ maps $\langle V\rangle$ to Skyrme-like EDF!

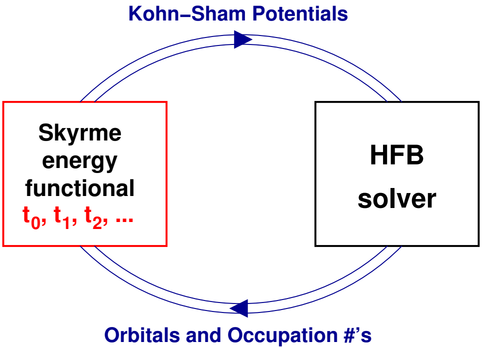
- Original DME expands about nuclear matter (k-space + NNN)

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

Adaptation of chiral EFT MBPT to Skyrme HFB form

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

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



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

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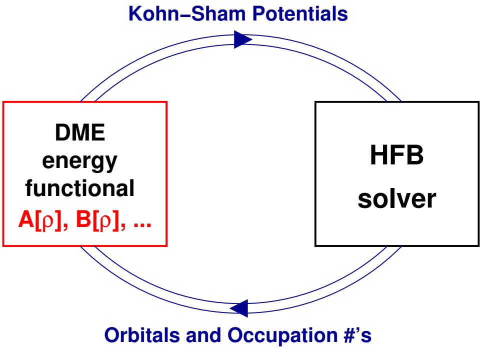

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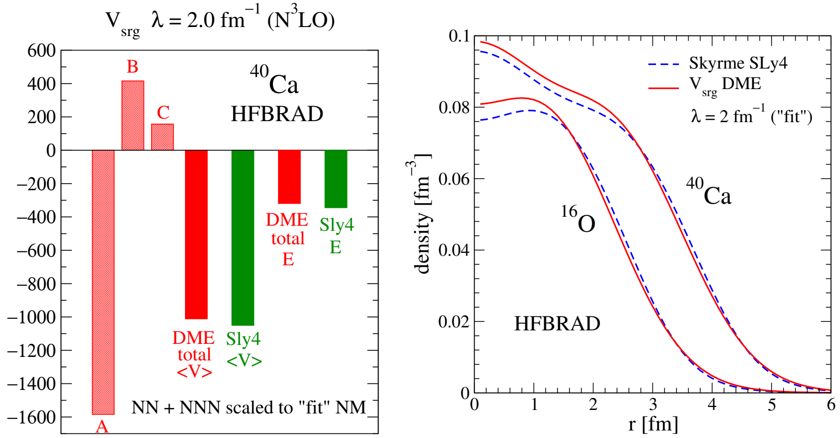
Full ab-initio: Is Negele-Vautherin DME good enough?

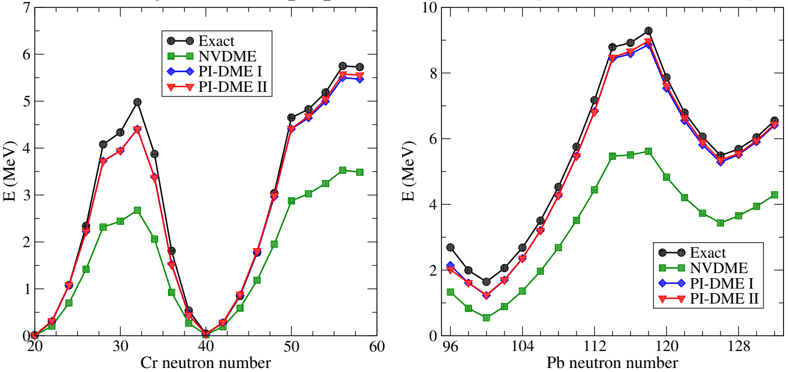
- Try best nuclear matter with RG-softened χ-EFT NN/NNN



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

Improved DME for pion exchange

- Phase-space averaging for finite nuclei [Gebremariam et al.]



- New developments [Alex Dyhdalo, OSU] : use local regulated NN + NNN
- Current gameplan [OSU + MSU + LLNL]: Can we see pions?
  - Add NN/NNN pion exchange through N^{2}LO
  - Optimized refit of Skyrme parameters for short-range parts
  - Assess global results *and* isotope chains (2π NNN)

Some current strategies for nuclear EDFs using EFT

Extend or modify conventional EDF forms in (semi-)controlled ways

1. Long-distance chiral physics from an EFT expansion
   - Density matrix expansion (DME) applied to NN and NNN diagrams
   - [Re-fit residual Skyrme parameters and test description]
   - MBPT expansion justified by phase-space-based power counting
2. In-medium chiral perturbation theory [Munich group]
   - ChPT loop expansion becomes EOS expansion
   - Apply DME to get DFT functional
3. Extend existing functionals following EFT principles
   - Non-local regularized pseudo-potential [Raimondi et al., 1402.1556]
   - Optimize pseudo-potential to experimental data
   - Test with correlation analysis technology
4. RG evolution of effective action functional [Jens Braun et al.]

Here: can we develop bottom-up EFT using a QFT formulation?

Effective theory for Nuclear EDFs

J. Dobaczewski, K. Bennaceur, F. Raimondi, J. Phys. G 39, 125103 (2012)

- Seek spectroscopic quality functional (including single-particle levels)
  - Consider non-ab-initio formulation but with firm theoretical basis
- Claim: resolution scale of chiral EFT is higher than needed
  - Rather than $k \lesssim 2m_\pi$ or $k_{\rm F}$, consider δk to dissociate a nucleon:
  $$\delta E_{\rm kin} = \hbar^2 k_{\rm F}\,\delta k/M \approx 0.25\hbar c\,\delta k \approx 8\,\text{MeV} \Longrightarrow \delta k \approx 32\,\text{MeV}/\hbar c$$
  - And describe nuclear excitations and shell-effects at the 1 MeV energy, which implies $\delta k \approx 4\,\text{MeV}/\hbar c$ and below
  - So from this perspective the pion is a *high-energy* dof

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- Strategy: expand “pseudopotential”, which specifies the EDF by folding with an uncorrelated Slater determinant, found self-consistently
  - Spirit of mean-field approaches (and technology)
  - Gives *full* functional within HF approximation (completeness?)
  - Self-interaction problem solved by deriving EDF in HF form

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  - And describe nuclear excitations and shell-effects at the 1 MeV energy, which implies $\delta k \approx 4\,\mathrm{MeV}/\hbar c$ and below
  - So from this perspective the pion is a *high-energy* dof
- Regulated zero-range interaction $\Longrightarrow$ introduces resolution scale
  - Gaussians smear away details of nuclear densities
  - Describe residual smooth variations within a controlled expansion
- Fit coupling constants to data with constraints (continuity equation)
  - Check for scale independence, convergence, and naturalness

Regularized pseudopotential: pionless-EFT-like expansion

- Central two-body regularized pseudopotential (also s.o. and tensor)

$$V(\mathbf{r}_1', \mathbf{r}_2'; \mathbf{r}_1, \mathbf{r}_2) = \sum_{i=1}^{4} \widehat{P}_i \widehat{O}_i(\mathbf{k}, \mathbf{k}') \delta(\mathbf{r}_1' - \mathbf{r}_1) \delta(\mathbf{r}_2' - \mathbf{r}_2) g_a(\mathbf{r}_1 - \mathbf{r}_2)$$

with operators $\widehat{P}_i$ (spin,isospin exchange), $\widehat{O}_i$ (derivative), $\mathbf{k}, \mathbf{k}'$ (relative momentum), while a sets the resolution scale:

$$g_a(\mathbf{r}) = \frac{1}{(a\sqrt{\pi})^3} e^{-r^2/a^2} \underset{a \to 0}{\longrightarrow} \delta(\mathbf{r})$$

- Simplified special case: If $\widehat{O}_i = \widehat{O}_i(\mathbf{k} + \mathbf{k}')$, then

$$V(\mathbf{r}) = \sum_{i=1}^{4} \widehat{P}_i \widehat{O}_i(\mathbf{k}) g_a(\mathbf{r}) = \sum_{i=1}^{4} \widehat{P}_i \sum_{n=0}^{n_{\max}} V_{2n}^{(i)} \nabla^{2n} g_a(\mathbf{r})$$

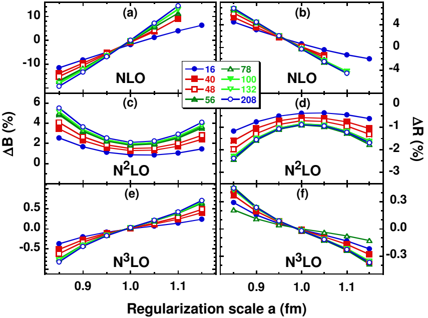
where $V_{2n}^{(i)}$ are the coupling constants to be fit

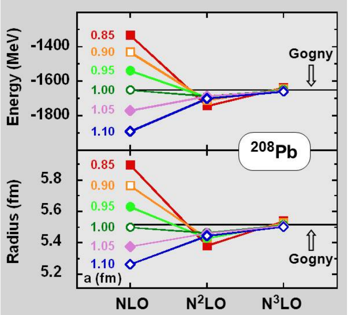
- EDF as functional of the one-body density matrix (cf. Gogny)

$$E_{\text{eff}}[\rho(\mathbf{r}, \mathbf{r}')] = \int d\mathbf{r} \int d\mathbf{r}' \, V(\mathbf{r} - \mathbf{r}')[\rho(\mathbf{r})\rho(\mathbf{r}') - \rho(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}', \mathbf{r})]$$

Does it work like an effective theory? Proof of principle

- Order-by-order convergence test against pseudo-data (from a Gogny functional)
  - factor of 4 at each order
  - can fine-tune couplings
- N^2LO regulator independent; N^3LO converged energy/radius
- Independence of the regulator scale *a* (i.e., flatness) and independent of reference nucleus
- Error plots vs. *A* shows convergence patterns
- Fixed $a = 0.85\,\text{fm}$; exponential decrease of constants with *n* with $\Lambda \approx 700\,\text{MeV}$





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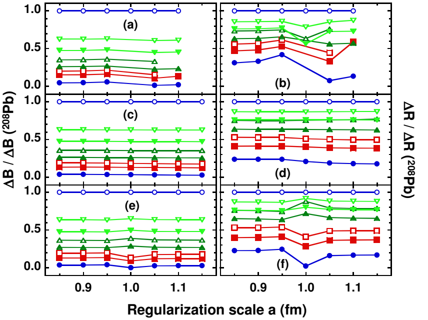

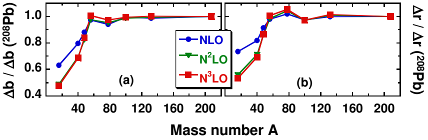

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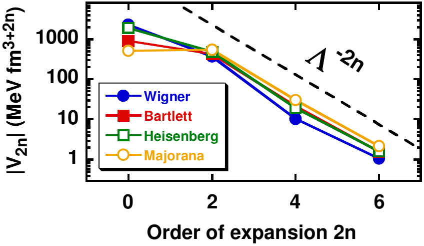
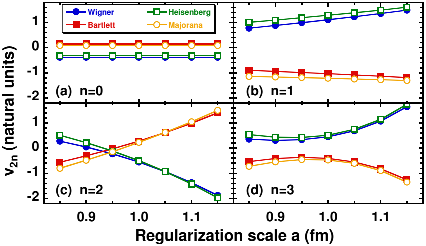




Naturalness in EDF coefficients as chiral signature?

Georgi (1993): f_π for strongly interacting fields; rest is $\Lambda_\chi \approx m_\rho$; $c_{lmn} \sim \mathcal{O}(1)$

$$\mathcal{L}_{\chi\,\mathrm{eft}} = c_{lmn} \left(\frac{N^\dagger N}{f_\pi^2 \Lambda_\chi}\right)^l \left(\frac{\pi}{f_\pi}\right)^m \left(\frac{\partial^\mu, m_\pi}{\Lambda_\chi}\right)^n f_\pi^2 \Lambda_\chi^2 \qquad f_\pi \sim 100\,\mathrm{MeV}$$

- Chiral NDA analysis for EDFs: [Friar et al., rjf et al.]

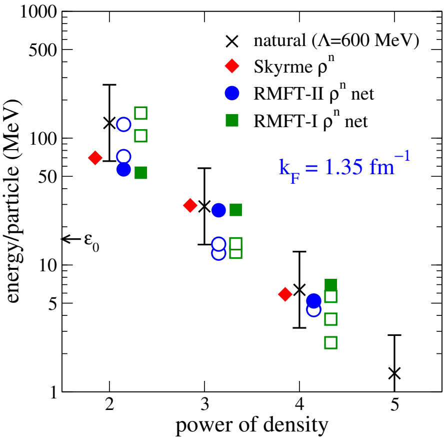
$$c \left[\frac{N^\dagger N}{f_\pi^2 \Lambda_\chi}\right]^l \left[\frac{\nabla}{\Lambda_\chi}\right]^n f_\pi^2 \Lambda_\chi^2$$

$$\Longrightarrow \quad \begin{array}{l} \rho \longleftrightarrow N^\dagger N \\ \tau \longleftrightarrow \nabla N^\dagger \cdot \nabla N \\ \mathbf{J} \longleftrightarrow N^\dagger \nabla N \end{array}$$

- Density expansion?

$$1000 \geq \Lambda_\chi \geq 500 \Longrightarrow \frac{1}{7} \leq \frac{\rho_0}{f_\pi^2 \Lambda_\chi} \leq \frac{1}{4}$$

- Also gradient expansion
- Applied to RMF, Skyrme EDFs



What does this tell us about accuracy limits?

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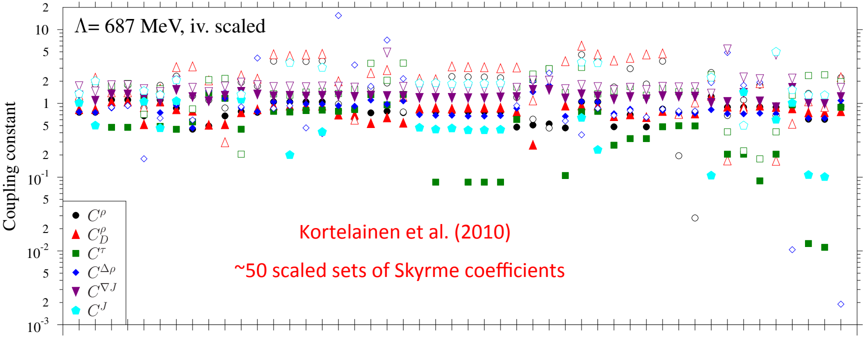
Check chiral naturalness for large set of Skyrme EDFs:



Looks like natural distribution $\Longrightarrow$ Does this mean pionful EFT is *needed*?

Some reasons to think EFT for nuclear DFT

- Folk theorem: Any successful low-energy phenomenology can be cast as [the leading order of] an EFT
- Five (or more) different representations all seem to work
  $\Longrightarrow$ build on common liquid drop systematics
- Works very well with simple calculations and few parameters
- (Some) EDFs look like momentum (and density?) expansions
- NDA phenomenology $\longrightarrow$ EDF constants seem to inherit underlying physics (e.g., chiral scales)
- . . .

Outline

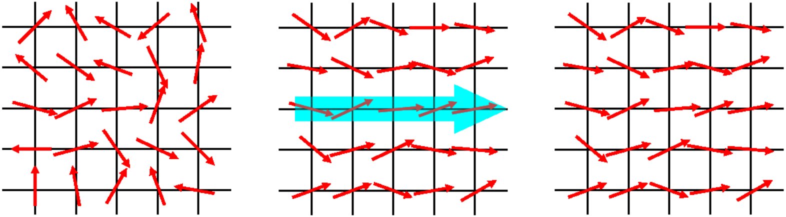
Motivations for considering nuclear DFT as an EFT

Extensions of nuclear EDFs using EFT ideas

Nuclear DFT as effective action

Effective actions and broken symmetries

- Natural framework for spontaneous symmetry breaking
  - e.g., test for zero-field magnetization M in a spin system
  - introduce an external field H to break rotational symmetry



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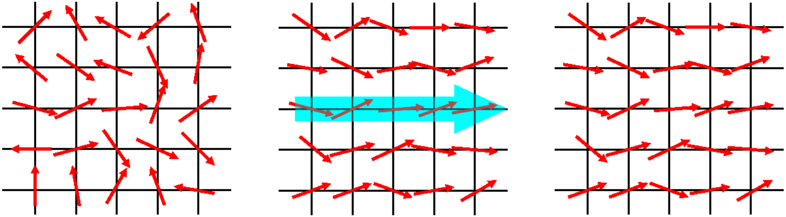


  - if $F[H]$ calculated perturbatively, $M[H=0]=0$ to all orders
  - Legendre transform Helmholtz free energy $F(H)$:

$$\text{invert} \quad M = -\partial F(H)/\partial H \quad \stackrel{H(M)}{\Longrightarrow} \quad \Gamma[M] = F[H(M)] + MH(M)$$

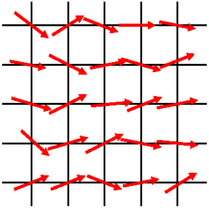
  - since $H = \partial\Gamma/\partial M \longrightarrow 0$, stationary points of $\Gamma \Longrightarrow$ ground state
- Can couple source "H" many ways (and multiple sources)

DFT and effective actions (Fukuda et al., Polonyi, ...)

- External field $\Longleftrightarrow$ Magnetization
- Helmholtz free energy $F[H]$
  $\Longleftrightarrow$ Gibbs free energy $\Gamma[M]$

Legendre transform $\Longrightarrow \Gamma[M] = F[H] + H\,M$

$$H = \frac{\partial\Gamma[M]}{\partial M} \xrightarrow[\text{state}]{\text{ground}} \left.\frac{\partial\Gamma[M]}{\partial M}\right|_{M_{\text{gs}}} = 0$$



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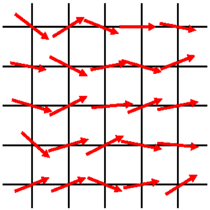


source magnet

Legendre transform $\Longrightarrow \Gamma[M] = F[H] + H\,M$

$$H = \frac{\partial\Gamma[M]}{\partial M} \xrightarrow[\text{state}]{\text{ground}} \left.\frac{\partial\Gamma[M]}{\partial M}\right|_{M_{\text{gs}}} = 0$$

- Partition function with sources J that adjust (any) densities:

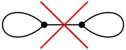
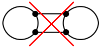
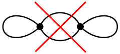
$$\mathcal{Z}[J] = e^{-W[J]} \sim \operatorname{Tr} e^{-\beta(\widehat{H} + J\,\widehat{\rho})} \quad \Longrightarrow \quad \text{e.g., path integral for } W[J]$$

- *Invert* to find $J[\rho]$ and Legendre transform from J to ρ:

$$\rho(\mathbf{x}) = \frac{\delta W[J]}{\delta J(\mathbf{x})} \quad \Longrightarrow \quad \Gamma[\rho] = W[J] - \int J\,\rho \quad \text{and} \quad J(\mathbf{x}) = -\frac{\delta\Gamma[\rho]}{\delta\rho(\mathbf{x})}$$

$\Longrightarrow \Gamma[\rho] \propto$ energy functional $E[\rho]$, stationary at $\rho_{\text{gs}}(\mathbf{x})$!

A bestiary of effective actions

- Couple source to local Lagrangian field, e.g., $J(x)\phi(x)$
  - $\Gamma[\varphi]$ where $\varphi(x) = \langle\phi(x)\rangle \Longrightarrow$ 1PI effective action 
  - Arises from fermion $\mathcal{L}$'s by introducing auxiliary (HS) fields
  - Can approximate with stationary phase $\Longrightarrow$ loop expansion
- Couple J to non-local composite op, e.g., $J(x,x')\phi(x)\phi(x')$
  - $\Gamma[G,\varphi] \Longrightarrow$ 2PI effective action [CJT] 
  - cf. Baym-Kadanoff conserving ("Φ-derivable") approximations
  - Often applied to hot, nonequilibrium QCD
- Source coupled to local composite operator, e.g., $J(x)\phi^2(x)$
  - 2PPI (two-particle-point-irreducible) effective action 
  - Kohn-Sham DFT from inversion method
  - Careful: new divergences arise (e.g., pairing)

Partition function in $\beta \to \infty$ limit [see Zinn-Justin]

- Consider Hamiltonian with time-independent source $J(\mathbf{x})$:

$$\widehat{H}(J) = \widehat{H} + \int J\,\widehat{\phi} \quad \text{or} \quad \widehat{H}(J) = \widehat{H} + \int J\,\psi^\dagger \psi$$

- *If* ground state is isolated (and bounded from below),

$$e^{-\beta \widehat{H}(J)} = e^{-\beta E_0(J)} \left[|0\rangle\langle 0|_J + \mathcal{O}\big(e^{-\beta(E_1(J) - E_0(J))}\big) \right]$$

- As $\beta \to \infty$, $\mathcal{Z}[J] \Longrightarrow$ ground state of $\widehat{H}(J)$ with energy $E_0(J)$

$$\mathcal{Z}[J] = e^{-W[J]} \sim \mathrm{Tr}\, e^{-\beta(\widehat{H} + J\,\widehat{\rho})} \Longrightarrow E_0(J) = \lim_{\beta \to \infty} -\frac{1}{\beta} \log \mathcal{Z}[J] = \frac{1}{\beta} W[J]$$

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- $\Gamma[\rho]$: expectation value of $\widehat{H}$ in ground state generated by $J[\rho]$

$$\frac{1}{\beta}\Gamma[\rho] = E_0(J) - \int J\,\rho = \langle\widehat{H} + J\,\widehat{\rho}\rangle_J - \int J\,\rho = \langle\widehat{H}\rangle_J \stackrel{J\to 0}{\longrightarrow} E_0$$

$$J(x) = -\frac{\delta\Gamma[\rho]}{\delta\rho(x)} \stackrel{J\to 0}{\longrightarrow} \left.\frac{\delta\Gamma[\rho]}{\delta\rho(x)}\right|_{\rho_{\mathrm{gs}}(\mathbf{x})} = 0 \quad \Longrightarrow \quad \text{variational } F_{\mathrm{HK}}[\rho]$$

Pairing in Kohn-Sham DFT [rjf, Hammer, Puglia, nucl-th/0612086]

- Add source j coupled to anomalous density:

$$Z[J,j] = e^{-W[J,j]} = \int D(\psi^\dagger\psi)\exp\Big\{-\int dx\,[\mathcal{L} + J(x)\,\psi_\alpha^\dagger\psi_\alpha + j(x)(\psi_\uparrow^\dagger\psi_\downarrow^\dagger + \psi_\downarrow\psi_\uparrow)]\Big\}$$

- Densities found by functional derivatives wrt J, j:

$$\rho(\mathbf{x}) = \left.\frac{\delta W[J,j]}{\delta v(\mathbf{x})}\right|_j, \qquad \phi(\mathbf{x}) \equiv \langle\psi_\uparrow^\dagger(\mathbf{x})\psi_\downarrow^\dagger(\mathbf{x}) + \psi_\downarrow(\mathbf{x})\psi_\uparrow(\mathbf{x})\rangle_{J,j} = \left.\frac{\delta W[J,j]}{\delta j(\mathbf{x})}\right|_J$$

- Find $\Gamma[\rho,\phi]$ from $W[J_0,j_0]$ by inversion $\quad(\Delta = \Delta_0 + \Delta_1 + \cdots)$
- Kohn-Sham system $\Longrightarrow$ short-range HFB with j_0 as gap

$$\begin{pmatrix} h_0(\mathbf{x}) - \mu_0 & j_0(\mathbf{x}) \\ j_0(\mathbf{x}) & -h_0(\mathbf{x}) + \mu_0 \end{pmatrix}\begin{pmatrix} u_i(\mathbf{x}) \\ v_i(\mathbf{x}) \end{pmatrix} = E_i\begin{pmatrix} u_i(\mathbf{x}) \\ v_i(\mathbf{x}) \end{pmatrix}$$

$$\text{where} \qquad h_0(\mathbf{x}) \equiv -\frac{\boldsymbol{\nabla}^2}{2M} + J_0(\mathbf{x})$$

- New renormalization counterterms needed (e.g., $\frac{1}{2}\zeta j^2$)

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Extend or modify conventional EDF forms in (semi-)controlled ways

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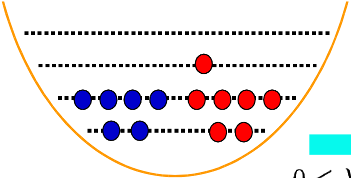
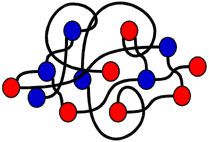
   - Apply DME to get DFT functional
3. Extend existing functionals following EFT principles
   - Non-local regularized pseudo-potential [Raimondi et al., 1402.1556]
   - Optimize pseudo-potential to experimental data
   - Test with correlation analysis technology
4. RG evolution of effective action functional [Jens Braun et al.]

Here: can we develop bottom-up EFT using a QFT formulation?

RG Approach to DFT [J. Braun et al., from Polonyi-Schwenk]





$0 \leqslant \lambda \leqslant 1$

Non-interacting fermions in background mean-field potential V at $\lambda = 0$

Gradually switch off background potential and turn on the microscopic interaction U as $\lambda \to 1$

$$S_{\lambda,1} = \int_\tau \int_x \psi^\dagger_\alpha(x) \left[\frac{\partial}{\partial \tau} - \frac{\nabla^2_{\mathbf{x}}}{2M} + (1-\lambda) V_{\lambda;\alpha}(\mathbf{x}) \right] \psi_\alpha(x)$$

$$S_{\lambda,2} = \frac{\lambda}{2} \int_\tau \int_x \int_{\tau'} \int_{x'} (\psi^\dagger \psi) \cdot U \cdot R_\lambda \cdot (\psi^\dagger \psi)$$

$$\Longrightarrow \quad Z_\lambda[J] \sim \int \mathcal{D}(\psi^\dagger \psi) e^{-S_\lambda + J\psi^\dagger\psi} \equiv e^{W_\lambda[J]}$$

- Latest: confine in box with $L \to \infty$ at end [Braun et al., arXiv:1606.04388]

$$\rho(\tau, x) = \frac{\delta W_\lambda[J]}{\delta J(\tau, x)} \quad \Longrightarrow \quad \Gamma_\lambda[\rho] = \sup_J \left\{ -W_\lambda[J] + \int_\tau \int_x J(\tau,x)\rho(\tau,x) \right\}$$

- 2PPI effective action gives HK functional: $E_\lambda[\rho] = \lim_{\beta\to\infty} \frac{1}{\beta} \Gamma_\lambda[\rho]$

What would a condensed matter theorist do?

From Atland and Simons “Condensed Matter Field Theory”:

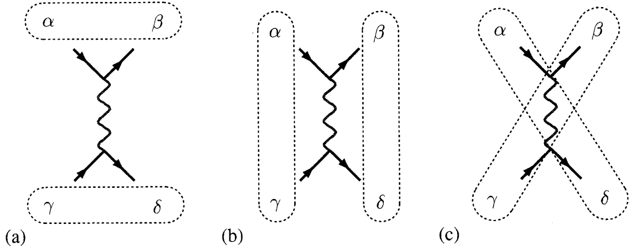


Figure 6.1 On the different channels of decoupling an interaction by Hubbard–Stratonovich transformation. (a) Decoupling in the “density” channel; (b) decoupling in the “pairing” or “Cooper” channel; and (c) decoupling in the “exchange” channel.

- May want to HS decouple in *all three* channels with $q \ll |p_i|$:

$$S_{\text{int}}[\overline{\psi}, \psi] \approx \frac{1}{2} \sum_{p,p',q} \Big(\overline{\psi}_{\sigma p} \psi_{\sigma p+q} V(\mathbf{q}) \overline{\psi}_{\sigma' p'} \psi_{\sigma' p'-q} - \overline{\psi}_{\sigma p} \psi_{\sigma' p+q} V(\mathbf{p}' - \mathbf{p}) \overline{\psi}_{\sigma' p'+q} \psi_{\sigma' p'}$$

$$- \overline{\psi}_{\sigma p} \overline{\psi}_{\sigma' -p+q} V(\mathbf{p}' - \mathbf{p}) \psi_{\sigma' p'} \psi_{\sigma' -p'+q} \Big)$$

Nuclei are self-bound $\Longrightarrow$ KS potentials break symmetries

- Conceptual issue: Is Kohn-Sham DFT well defined?
  - J. Engel: ground state density spread uniformly over space
  - Want DFT for *internal* densities
- Practical issue: what to do when KS potentials break symmetries?
  - Symmetry restoration with superposition of states:

$$|\psi\rangle = \int d\alpha\, f(\alpha)|\phi\alpha\rangle \implies \text{minimize wrt } f(\alpha)\text{, before or after } |\phi\rangle$$

  - Wave function method strategies for “center of mass” problem
    - isolate “internal” dofs, e.g., with Jacobi coordinates
    - work in HO Slater determinant basis for which COM decouples
    - work with internal Hamiltonian so that COM part factors
- How to accomodate within effective action DFT framework?
  - Zero-frequency modes $\Longrightarrow$ divergent perturbation expansion
  - Transformation to collective variables $\Longrightarrow$ work with overcomplete dof’s $\Longrightarrow$ system with constraints
  - Can we apply methods for gauge theories?

Zero modes: collective coordinates and functional integrals

- Possible approach: use BRST invariance
  - Add *more* fermionic variables (ghosts) so more overcomplete
  - Apparent complication is actually a simplification because in gauge systems there is a supersymmetry
  - Examples in the literature with applications to mechanical systems
  - E.g., Bes and Kurchan, “The treatment of collective coordinates in many-body systems: An application of the BRST invariance”
  - Can the procedure be adapted to DFT?

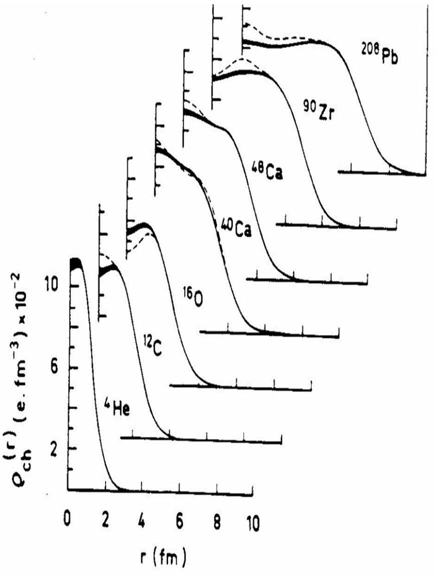
Questions to address about EFT for DFT

- What are the relevant degrees of freedom? Symmetries?
  [Can we have quasiparticles in the bulk?]
- Power counting: what is our expansion? Breakdown scale?
- Is there an RG argument to apply? (cf. scale toward Fermi surface)
- How should the EFT be formulated? Effective action?
  How do I think about parameterizing a density functional?
- How can we implement/expand about liquid drop physics?
- How do we reconcile the different EDF representations?
- Dealing with zero modes — can we adapt methods for gauge theories (constraints)?
- Can we implement such an EFT without losing favorable computational scaling?

What do (ordinary) nuclei look like?

- Charge densities of magic nuclei (mostly) shown
- Proton density has to be "unfolded" from $\rho_{\text{charge}}(r)$, which comes from elastic electron scattering
- Roughly constant interior density with $R \approx (1.1\text{–}1.2\,\text{fm}) \cdot A^{1/3}$
- Roughly constant surface thickness

$\Longrightarrow$ Like a liquid drop!



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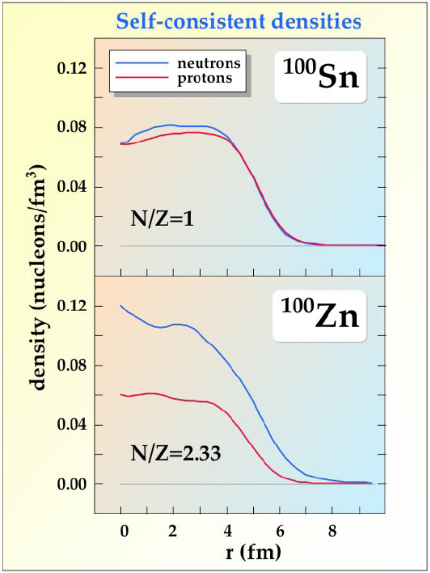
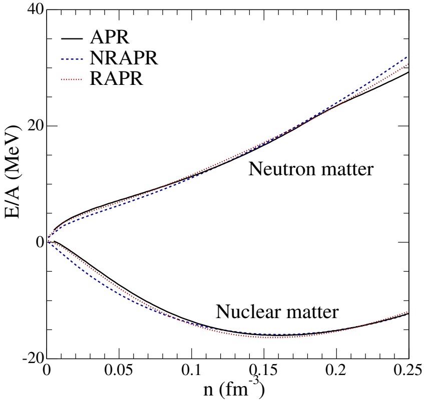


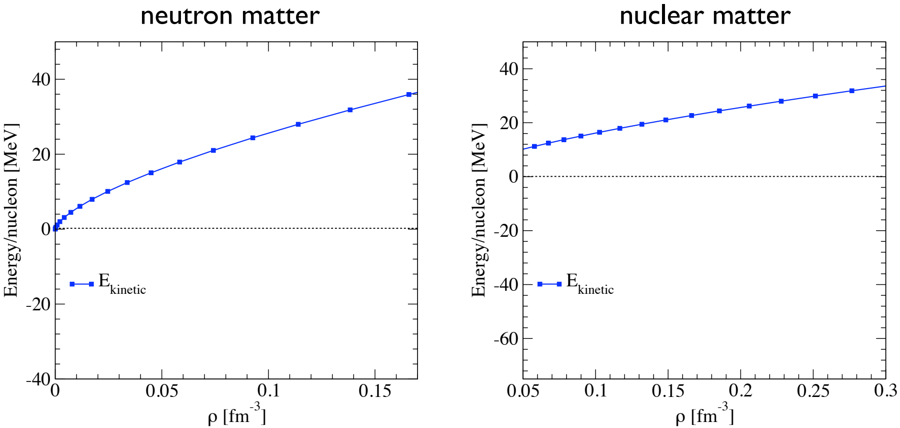
Nuclear and neutron matter energy vs. density

[Akmal et al. calculations shown]



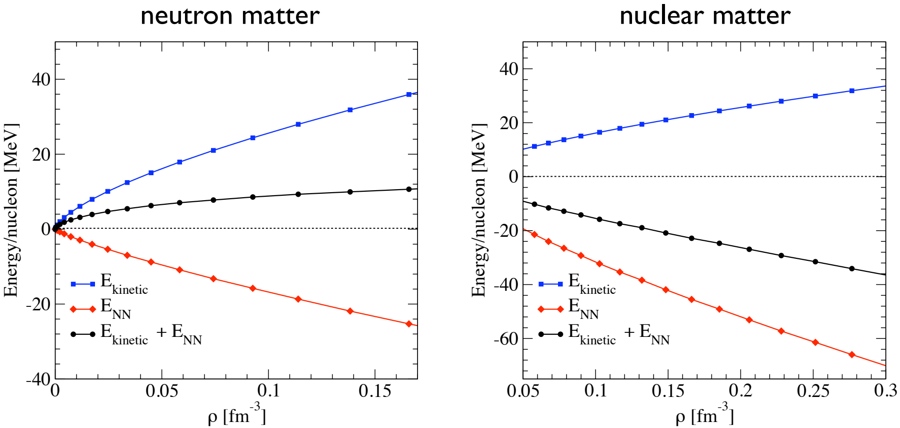
- Uniform with Coulomb turned off
- Density n (or often ρ)
- Fermi momentum $n = (\nu/6\pi^2)k_\mathrm{F}^3$
- Neutron matter ($Z = 0$) has positive pressure
- Symmetric nuclear matter ($N = Z = A/2$) saturates
- *Empirical* saturation at about $E/A \approx -16\,\mathrm{MeV}$ and $n \approx 0.17 \pm 0.03\,\mathrm{fm}^{-3}$

Hierarchy of contributions to infinite matter



- Large cancellation of kinetic and potential energy
- Chiral hierarchy of 2NF and 3NF up to saturation density

Hierarchy of contributions to infinite matter



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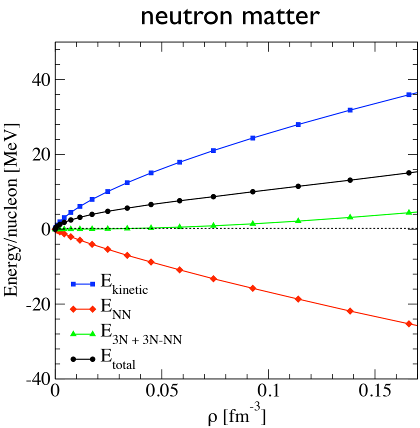

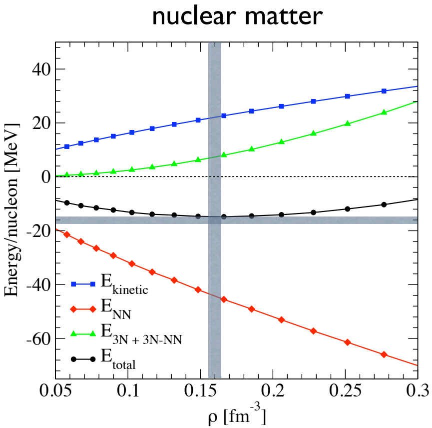

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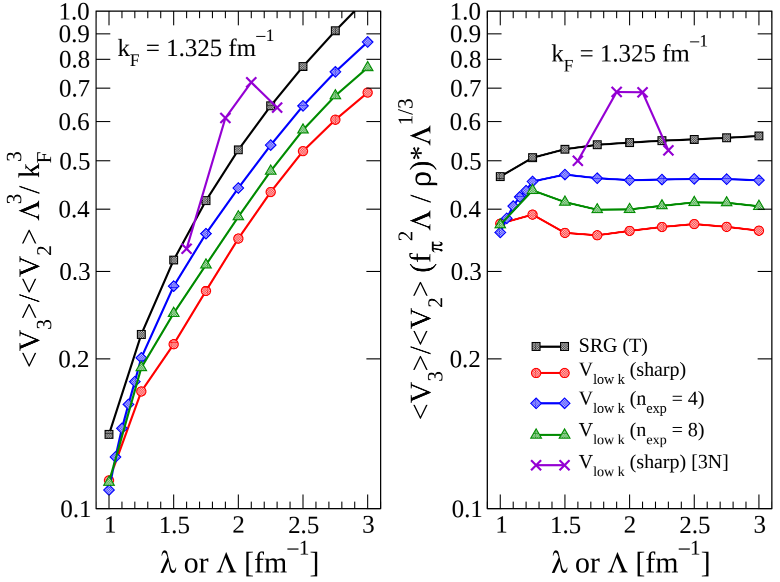
Scaling of $\langle V^{(3)} \rangle / \langle V^{(2)} \rangle$ in nuclear matter



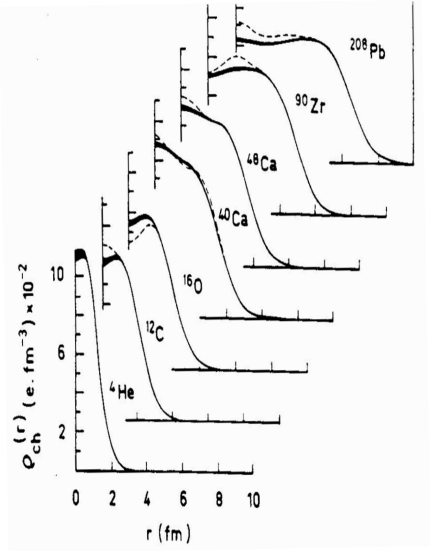
Density functional theory (DFT) as justification for energy density functional (EDF) approach

- Hohenberg-Kohn: There exists an energy functional $E_{v_{\rm ext}}[\rho]$ of $\rho(\mathbf{x})$ for external potential $v_{\rm ext}$:

$$E_{v_{\rm ext}}[\rho] = F_{\rm HK}[\rho] + \int d\mathbf{x}\, v_{\rm ext}(\mathbf{x})\rho(\mathbf{x})$$

Minimize $\Longrightarrow E_{gs}, \rho_{gs}$

- Useful if you can approximate the energy functional; suggests a hunting license for EDF's
- $F_{\rm HK}$ is *universal* (same for any external $v_{\rm ext}$), so should be able to add any $v_{\rm ext}$ we want!
- Kohn-Sham (KS) DFT: Introduce orbitals for $\rho(\mathbf{x})$



Unraveling the magic of DFT [Kutzelnigg (2008)]

- Wavefunction-based: for anti-symmetric A-body $|\Psi\rangle$, find $E_{gs} = \min_{\Psi} \langle\Psi|\widehat{H}|\Psi\rangle$ (CI, CC use a single-particle basis for $|\Psi\rangle$)
- DFT: fermion densities as basic variables
  - Common but misleading statements:

"All information about a quantum mechanical ground state is contained in its electron density ρ."

"The energy is completely expressible in terms of the density alone."

  - At odds with kinetic and interaction energies needing $(1, 2, \cdots)$–particle density matrices!

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  - At odds with kinetic and interaction energies needing $(1, 2, \cdots)$–particle density matrices!
- Key: WF formulation deals with *single, fixed Hamiltonian*, E stationary to density matrix (or Ψ) variations, not just $\rho(\mathbf{x})$
- DFT: Consider a *family* of Hamiltonians $\widehat{H}[v] \to E[v]$, then

$$F_{\mathrm{HK}}[\rho] = \min_{v}\{E[v] - \int d\mathbf{x}\, v(\mathbf{x})\rho(\mathbf{x})\} \quad \text{and}$$

$$E[v] = \min_{\rho}\{F[\rho] + \int d\mathbf{x}\, v(\mathbf{x})\rho(\mathbf{x})\} \equiv \min_{\rho}\{E_v[\rho]\}$$

Challenges for nuclear DFT (cf. Coulomb DFT)

- Difficult conventional nuclear Hamiltonians
  - Sources of non-perturbative physics for NN interaction
    1. Strong short-range repulsion (“hard core”)
    2. Iterated tensor interactions (e.g., from pion exchange)
    3. Near zero-energy bound states (e.g., deuteron)
  - Non-negligible many-body forces
- Non-trivial implementation issues
  - Essential role of pairing (so like HFB rather than HF)
  - Important long-range correlations
  - Some observables we want are not KS-DFT observables
  - We don’t have a v_{ext}!
  - Symmetry breaking in finite, self-bound systems (translation, rotation, number, . . .)
    $\Longrightarrow$ What about symmetry restoration?

Skyrme generalizations based on EFT principles

- Ability to use local densities based on short range of nuclear interactions compared to variations in local and non-local density matrix $\Longrightarrow$ use separation of scales

- Density functional

$$E = \int d^3\mathbf{r} \left[\frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_{\text{Skyrme}}(\rho_0, \rho_1, \tau_0, \tau_1, \mathbf{s}_0, \mathbf{s}_1, \ldots) + \mathcal{H}_{\text{Coul.}}(\rho_{\text{p}}) \right]$$

- Densities

$$\rho = \sum_i \varphi_i^\dagger \varphi_i, \qquad \tau = \sum_{i,\mu} (\nabla_\mu \varphi_i^\dagger)(\nabla_\mu \varphi_i), \qquad \mathbf{j},\ \mathbf{J} : \text{currents}$$

$$\mathbf{s}_\nu = \sum_i \varphi_i^\dagger \sigma_\nu \varphi_i, \quad \mathbf{T}_\nu = \sum_{i,\mu} (\nabla_\mu \varphi_i^\dagger) \sigma_\nu (\nabla_\mu \varphi_i), \quad \rho_0 = \rho_{\text{n}} + \rho_{\text{p}}, \quad \rho_1 = \rho_{\text{n}} - \rho_{\text{p}}, \ \ldots$$

- Strong interaction energy density $\mathcal{H}_{\text{Skyrme}}$

$$\begin{aligned}
\mathcal{H}_0^{\text{even}} &= C_0^\rho(\rho_0)\rho_0^2 + C_0^{\Delta\rho}\rho_0\Delta\rho_0 + C_0^\tau\rho_0\tau_0 + C_0^J\mathbf{J}_0^2 + C_0^{\nabla J}\rho_0\boldsymbol{\nabla}\cdot\mathbf{J}_0, \\
\mathcal{H}_1^{\text{even}} &= C_1^\rho(\rho_0)\rho_1^2 + C_1^{\Delta\rho}\rho_1\Delta\rho_1 + C_1^\tau\rho_1\tau_1 + C_1^J\mathbf{J}_1^2 + C_1^{\nabla J}\rho_1\boldsymbol{\nabla}\cdot\mathbf{J}_1, \\
\mathcal{H}_0^{\text{odd}} &= C_0^s(\rho_0)\mathbf{s}_0^2 + C_0^{\Delta s}\mathbf{s}_0\cdot\Delta\mathbf{s}_0 + C_0^{sT}\mathbf{s}_0\cdot\mathbf{T}_0 + C_0^j\mathbf{j}_0^2 + C_0^{\nabla j}\mathbf{s}_0\cdot(\boldsymbol{\nabla}\times\mathbf{j}_0), \\
\mathcal{H}_1^{\text{odd}} &= C_1^s(\rho_0)\mathbf{s}_1^2 + C_1^{\Delta s}\mathbf{s}_1\cdot\Delta\mathbf{s}_1 + C_1^{sT}\mathbf{s}_1\cdot\mathbf{T}_1 + C_1^j\mathbf{j}_1^2 + C_1^{\nabla j}\mathbf{s}_1\cdot(\boldsymbol{\nabla}\times\mathbf{j}_1).
\end{aligned}$$

- Expand in densities and gradients
- Includes time-odd fields $\Longrightarrow$ new domain to explore

Energy density functional for spherical nuclei (II)

We can write the N³LO spherical energy density as a sum of contributions from zero, second, fourth, and sixth orders:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_2 + \mathcal{H}_4 + \mathcal{H}_6,$$

where

$$\mathcal{H}_0 = C^0_{00} R_0 R_0,$$

$$\begin{aligned}\mathcal{H}_2 &= C^0_{20} R_0 \Delta R_0 + C^0_{02} R_0 R_2 \\ [0.5ex] &+ C^0_{11} R_0 \vec{\nabla}\cdot\vec{J}_1, + C^1_{01} \vec{J}_1^2,\end{aligned}$$

Energy densities $\mathcal{H}_0$ and $\mathcal{H}_2$ correspond, of course, to the standard Skyrme functional with $C^0_{00} = C^\rho$, $C^0_{20} = C^{\Delta\rho}$, $C^0_{02} = C^\tau$, $C^0_{11} = C^{\nabla J}$, and $C^1_{01} = C^{J1}$. At fourth order, the energy density reads

$$\begin{aligned}\mathcal{H}_4 &= C^0_{40} R_0 \Delta^2 R_0 + C^0_{22} R_0 \Delta R_2 \\ &+ C^0_{04} R_0 R_4 + C^2_{02} R_2 R_2 \\ &+ D^0_{22} R_0 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + D^2_{02} \sum_{ab} \overleftrightarrow{R}_{2ab} \overleftrightarrow{R}_{2ab} \\ &+ C^1_{21} \vec{J}_1 \cdot \Delta \vec{J}_1 + C^1_{03} \vec{J}_1 \cdot \vec{J}_3 \\ &+ D^1_{21} \vec{J}_1 \cdot \vec{\nabla}\left(\vec{\nabla}\cdot\vec{J}_1\right) \\ &+ C^0_{31} R_0 \Delta \left(\vec{\nabla}\cdot\vec{J}_1\right) + C^0_{13} R_0 \left(\vec{\nabla}\cdot\vec{J}_3\right) \\ &+ C^2_{11} R_2 \left(\vec{\nabla}\cdot\vec{J}_1\right) + D^2_{11} \sum_{ab} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{J}_{1b},\end{aligned}$$

At sixth order, the energy density reads

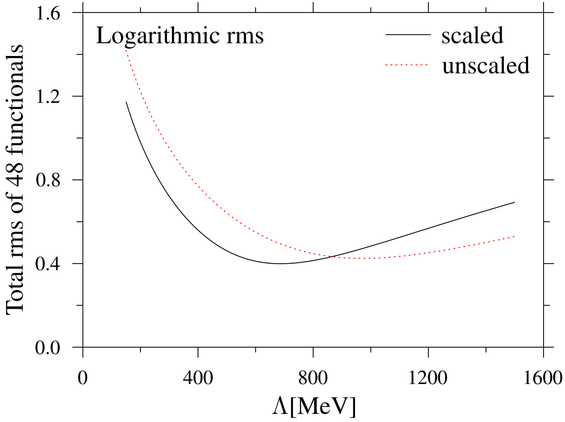
$$\begin{aligned}\mathcal{H}_6 &= C^0_{60} R_0 \Delta^3 R_0 + C^0_{42} R_0 \Delta^2 R_2 \\ &+ C^0_{24} R_0 \Delta R_4 + C^0_{06} R_0 R_6 \\ &+ C^2_{22} R_2 \Delta R_2 + C^2_{04} R_2 R_4 \\ &+ D^0_{42} R_0 \Delta \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + D^0_{24} R_0 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{4ab} \\ &+ D^2_{22} R_2 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + E^2_{22} \sum_{ab} \overleftrightarrow{R}_{2ab} \Delta \overleftrightarrow{R}_{2ab} \\ &+ F^2_{22} \sum_{abc} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{\nabla}_c \overleftrightarrow{R}_{2cb} + E^2_{04} \sum_{ab} \overleftrightarrow{R}_{2ab} \overleftrightarrow{R}_{4ab} \\ &+ C^1_{41} \vec{J}_1 \cdot \Delta^2 \vec{J}_1 + C^1_{23} \vec{J}_1 \cdot \Delta \vec{J}_3 \\ &+ C^1_{05} \vec{J}_1 \cdot \vec{J}_5 + C^3_{03} \vec{J}_3 \cdot \vec{J}_3 \\ &+ D^1_{41} \vec{J}_1 \cdot \Delta \vec{\nabla}\left(\vec{\nabla}\cdot\vec{J}_1\right) + D^1_{23} \vec{J}_1 \cdot \vec{\nabla}\left(\vec{\nabla}\cdot\vec{J}_3\right) \\ &+ E^1_{23} \sum_{abc} \vec{J}_{1a} \vec{\nabla}_b \vec{\nabla}_c \overleftrightarrow{J}_{3abc} + D^3_{03} \sum_{abc} \overleftrightarrow{J}_{3abc} \overleftrightarrow{J}_{3abc} \\ &+ C^0_{51} R_0 \Delta^2 \left(\vec{\nabla}\cdot\vec{J}_1\right) + C^0_{33} R_0 \Delta \left(\vec{\nabla}\cdot\vec{J}_3\right) \\ &+ C^0_{15} R_0 \left(\vec{\nabla}\cdot\vec{J}_5\right) + C^2_{31} R_2 \Delta \left(\vec{\nabla}\cdot\vec{J}_1\right) \\ &+ C^2_{13} R_2 \left(\vec{\nabla}\cdot\vec{J}_3\right) + C^4_{11} R_4 \left(\vec{\nabla}\cdot\vec{J}_1\right) \\ &+ D^0_{33} R_0 \sum_{abc} \vec{\nabla}_a \vec{\nabla}_b \vec{\nabla}_c \overleftrightarrow{J}_{3abc} + D^2_{13} \sum_{abc} \overleftrightarrow{R}_{2ab} \vec{\nabla}_c \overleftrightarrow{J}_{3abc} \\ &+ D^2_{31} \sum_{ab} \overleftrightarrow{R}_{2ab} \Delta \vec{\nabla}_a \vec{J}_{1b} + E^2_{13} \sum_{ab} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{J}_{3b} \\ &+ D^4_{11} \sum_{ab} \overleftrightarrow{R}_{4ab} \vec{\nabla}_a \vec{J}_{1b} \\ &+ E^2_{31} \sum_{ab} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{\nabla}_b \left(\vec{\nabla}\cdot\vec{J}_1\right).\end{aligned}$$

The energy densities above are given in terms of 50 coupling constants $C^{n'}_{mn}$, $D^{n'}_{mn}$, $E^{n'}_{mn}$, and $F^{n'}_{mn}$.

B.G. Carlsson *et al.*, C 78, 044326 (2008)

Naturalness revisited (M. Kortelainen et al.)

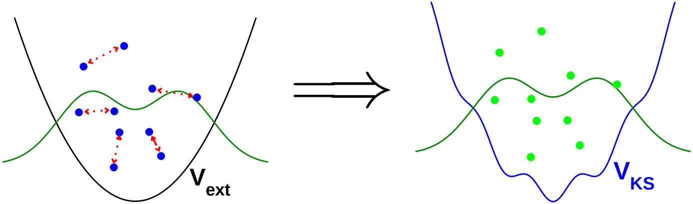
- Apply natural units scaling to 48 Skyrme functionals
- Look for optimal Λ by deviations from unity:



- $\Lambda \approx 600\,$MeV consistent with previous analysis

Construct $W[v]$ and then $\Gamma[\rho]$ order-by-order

- Need a diagrammatic *expansion* (e.g., MBPT or EFT)
- Inversion method $\Longrightarrow$ Split source $v(\mathbf{x}) = V_{\rm KS} + v_1 + v_2 + \cdots$
  - $V_{\rm KS}$ *chosen* to get $\rho(\mathbf{x})$ in noninteracting (Kohn-Sham) system:



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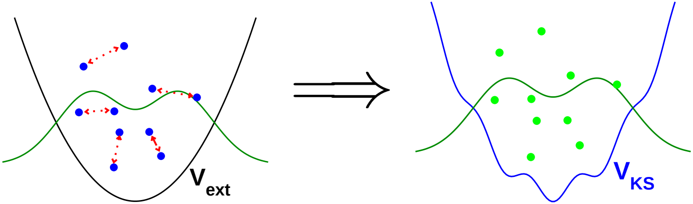

  - Orbitals $\{\psi_\alpha(\mathbf{x})\}$ in local potential $V_{\rm KS}([\rho], \mathbf{x})$

$$[-\nabla^2/2m + V_{\rm KS}(\mathbf{x})]\psi_\alpha = \varepsilon_\alpha \psi_\alpha \quad \Longrightarrow \quad \rho(\mathbf{x}) = \sum_{\alpha=1}^{A} |\psi_\alpha(\mathbf{x})|^2$$

  - Self-consistency from $v(\mathbf{x}) \to v_{\rm ext}(\mathbf{x}) \Longrightarrow V_{\rm KS}(\mathbf{x}) \propto \delta\Gamma_{\rm int}[\rho]/\delta\rho(\mathbf{x})$

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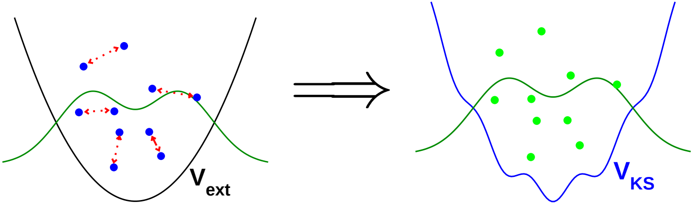

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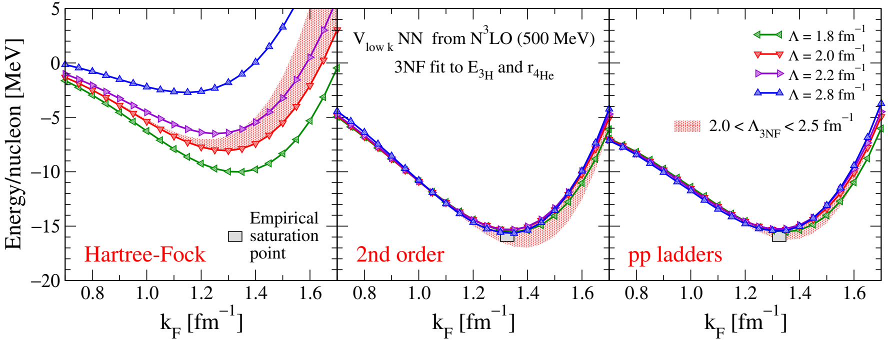
  - Self-consistency from $v(\mathbf{x}) \to v_{\rm ext}(\mathbf{x}) \Longrightarrow V_{\rm KS}(\mathbf{x}) \propto \delta\Gamma_{\rm int}[\rho]/\delta\rho(\mathbf{x})$
- Alternative: Do MBPT with single particle potential $U(\mathbf{x})$ and $H = (T + U) + (V - U + v_{\rm ext})$ and choose $U = V_{\rm KS}$ (no $\Delta\rho(\mathbf{x})$)

What is needed for ab initio Kohn-Sham DFT?

1. Need MBPT to work with tuned U $[H = (T + U) + (V - U)]$



   - (see new results from K. Hebeler et al.)
   - If convergence insensitive to $U \Longrightarrow$ choose so KS density exact

2. Need to calculate $V_{\text{KS}}(\mathbf{x})$ from $\delta E[\rho]/\delta\rho(\mathbf{x})$, etc. but diagrams depend non-locally on KS orbitals
   - Density matrix expansion (DME) $\Longrightarrow$ explicit densities
   - Use chain rule $\Longrightarrow$ "optimized effective potential" (OEP)

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

$\Uparrow$

5. Full orbital-based DFT from MBPT+. [E.g., RPA with Kohn-Sham orbitals.]
4. Hyper-GGA includes exact exchange energy density calculated with (occupied) orbitals.
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.]
2. Generalized gradient approximation (GGA) adds $\nabla\rho_\uparrow(\mathbf{r})$ and $\nabla\rho_\downarrow(\mathbf{r})$.
1. Local spin density approximation (LSDA) with $\rho_\uparrow(\mathbf{r})$ and $\rho_\downarrow(\mathbf{r})$ as ingredients.

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]

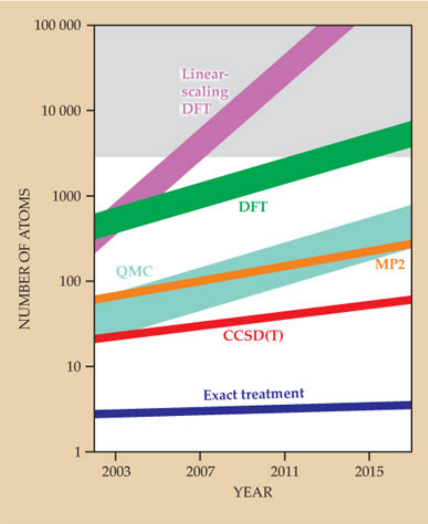
HEAVEN $\Longrightarrow$ UNEDF from NN$\cdots$N (QCD)

5. Full orbital-based DFT based on [lattice QCD $\Longrightarrow$] chiral EFT $\Longrightarrow$ $V_{\text{low }k}$.
4. Complete semi-local functional (e.g., DME) from chiral EFT $\Longrightarrow$ $V_{\text{low }k}$.
3. Long-range chiral NN and NNN $\Longrightarrow$ Π–DME $\Longrightarrow$ merged with Skyrme and refit.
2. Generalized Skyrme with $\nabla^n\rho(\mathbf{r})$, $\rho^\alpha(\mathbf{r})$, . . . with constraints (e.g., neutron drops)
1. Conventional Skyrme EDF's [e.g. SLY4].

- Developing 2.–5. in parallel!

Computational scaling for Coulomb systems

- Full configuration interaction (CI) grows exponentially with number N
- Coupled cluster CCSD(T) $\propto N^7$
- Quantum Monte Carlo (QMC) scales $\propto N^3$
- Density functional theory (DFT) scales $\propto N^3$ and linear scaling possible



M. Head-Gordon and E. Artacho
Physics Today, April 2008

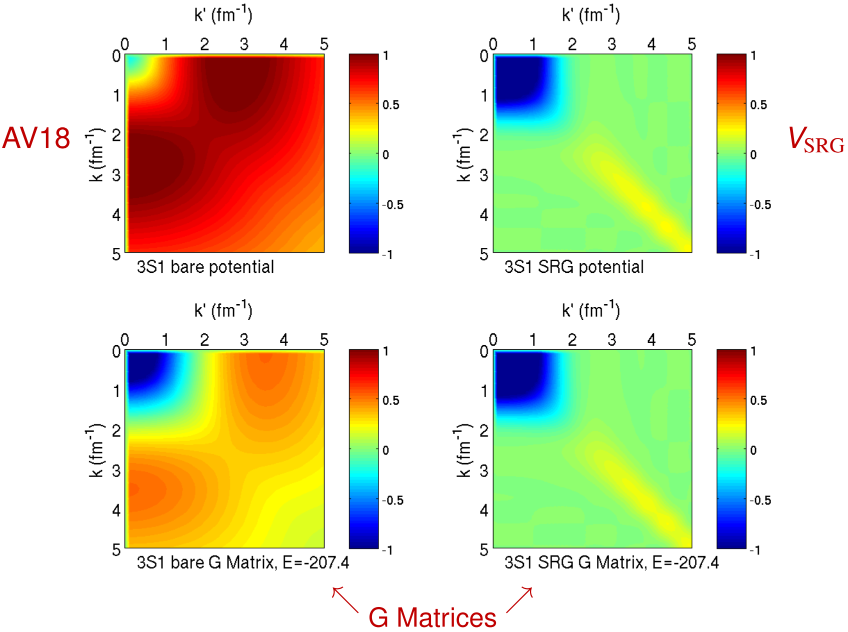
Historically: Microscopic EDF from G-Matrix

- G-matrix softens highly non-perturbative NN potentials
- Negele/Vautherin density matrix expansion (DME)
  $\Longrightarrow$ Skyrme-like EDF from G-matrix for Hartree-Fock
  - Semi-quantitatively successful
  - Empirical fits far superior $\Longrightarrow$ little further development
- Ab-initio DFT is possible from many-body perturbation theory (MBPT) if convergent and can tune single-particle potential U

$$H = \underbrace{(T + U)}_{\text{Kohn}-\text{Sham}} + (V - U)$$

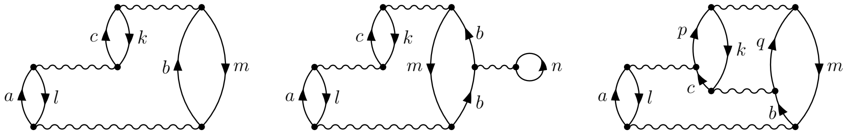
  - Need to be able to adjust U so density unchanged
  - Recent successes for Coulomb DFT
- But MBPT with G-matrix doesn't work (hole-line expansion)
- Use RG to soften: low-momentum potentials ($V_{\text{low}\,k}$, V_{SRG})
  - revisit hole-line expansion

Compare Potential and G Matrix: AV18 vs. V_{SRG}



Hole-Line Expansion Revisited (Bethe, Day, . . .)

- Consider ratio of fourth-order diagrams to third-order:



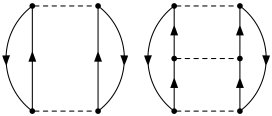
- "Conventional" G matrix still couples low-k and high-k
  - no new hole line $\Longrightarrow$ ratio $\approx -\chi(\mathbf{r}=0) \approx -1 \Longrightarrow$ sum all orders
  - add a hole line $\Longrightarrow$ ratio $\approx \sum_{n \le k_{\rm F}} \langle bn|(1/e)G|bn\rangle \approx \kappa \approx 0.15$
- Low-momentum potentials decouple low-k and high-k
  - add a hole line $\Longrightarrow$ still suppressed
  - no new hole line $\Longrightarrow$ also suppressed (limited phase space)
  - freedom to choose single-particle $U \Longrightarrow$ use for Kohn-Sham

$\Longrightarrow$ Ab initio MBPT and DFT can work!

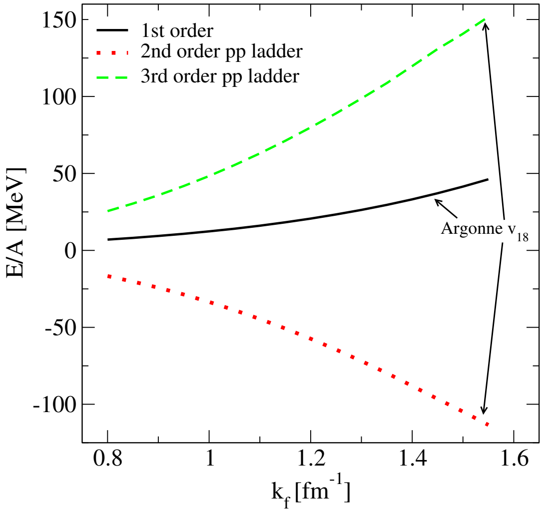
- (How do we get a Kohn-Sham $V_{\rm KS}(\mathbf{x})$ from even HF diagrams?)

Nuclear matter with NN ladders only [nucl-th/0504043]

- Brueckner ladders order-by-order



- Repulsive core $\Longrightarrow$ series diverges
- Usual solution: resum into G-matrix then do hole-line expansion



Nuclear matter with NN ladders only [nucl-th/0504043]

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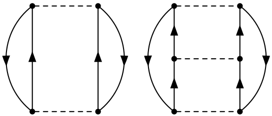
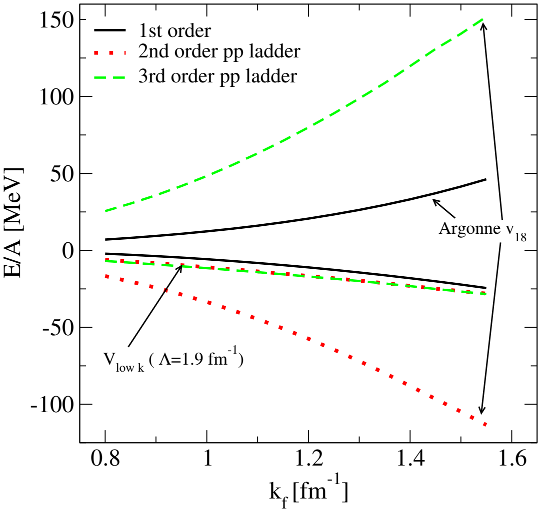
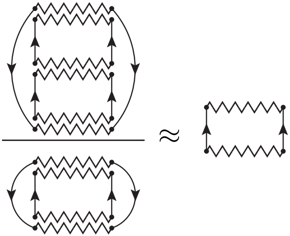


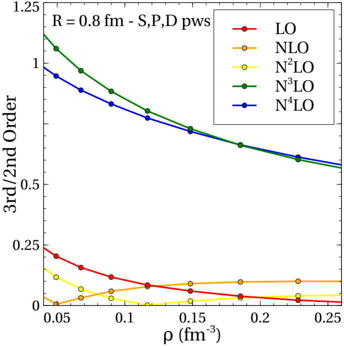
- Repulsive core $\Longrightarrow$ series diverges
- Usual solution: resum into G-matrix then do hole-line expansion
- $V_{\text{low}\,k}$ or V_{SRG} converges $\Longrightarrow$ KS DFT possible!
- Add 3-body fit to few-body binding



Effects of softening interactions in the nuclear medium

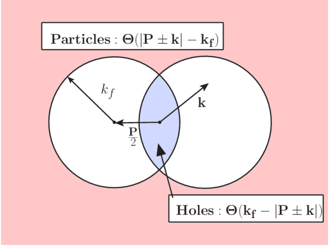
Separable estimate:

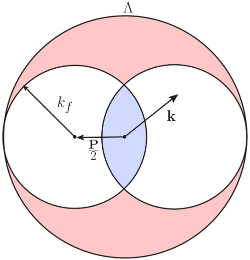




$$\frac{E^{(n+1)}_{\rm pp}}{E^{(n)}_{\rm pp}} \approx \frac{m^*}{m} \int \frac{d^3k}{(2\pi)^3}\, \overline{Q}(P_{\rm av}, k)\, \frac{\langle \mathbf{k}|V|\mathbf{k}\rangle}{k^2_{\rm av} - k^2}$$

Phase space:





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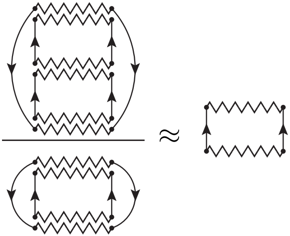

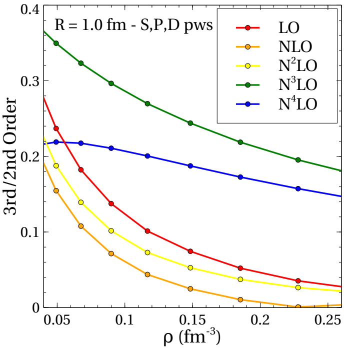

$$\frac{E_{\rm pp}^{(n+1)}}{E_{\rm pp}^{(n)}} \approx \frac{m^*}{m} \int \frac{d^3k}{(2\pi)^3}\, \overline{Q}(P_{\rm av}, k)\, \frac{\langle \mathbf{k}|V|\mathbf{k}\rangle}{k_{\rm av}^2 - k^2}$$

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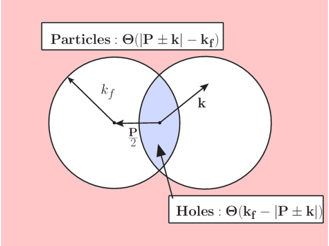

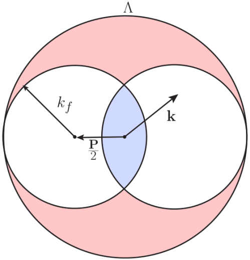

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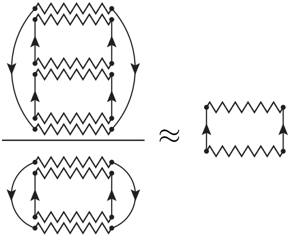

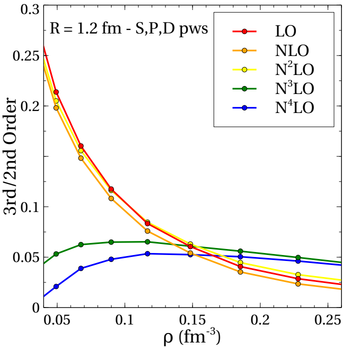

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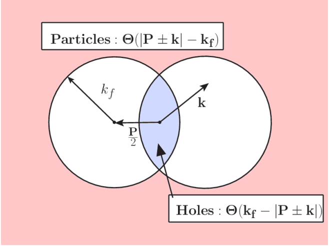
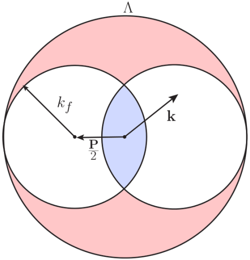
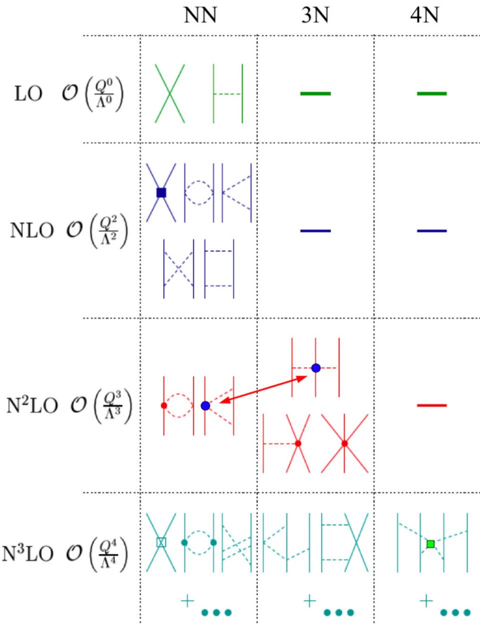




Long-range chiral EFT
$\Longrightarrow$ extended Skyrme

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



DME meets $V_{\mathrm{low}\,k}$ [Bogner, Furnstahl, Platter]

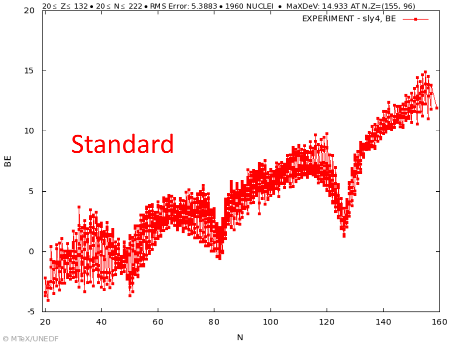
- $\mathcal{E} = \frac{1}{2M}\tau + A[\rho] + B[\rho]\tau + C[\rho]|\nabla\rho|^2 + \cdots$ in momentum space

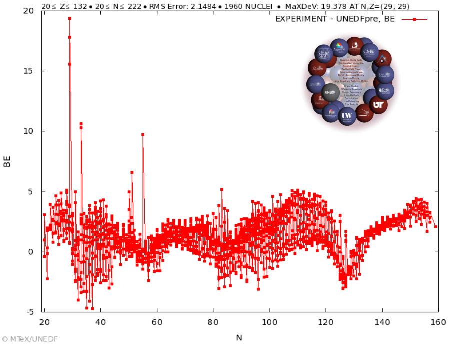
$$A[\rho] \sim k_{\mathrm{F}}^3 \sum_{lsj} \widehat{j}\,\widehat{t} \int_0^{k_{\mathrm{F}}} k^2\,dk\; V_{lsjt}(k,k)\,P_A(k/k_{\mathrm{F}}) \;+\; \{V_{3N}\} \;+\; \cdots$$

$$B[\rho] \sim k_{\mathrm{F}}^{-3} \sum_{lsj} \widehat{j}\,\widehat{t} \int_0^{k_{\mathrm{F}}} k^2\,dk\; V_{lsjt}(k,k)\,P_B(k/k_{\mathrm{F}}) \;+\; \{V_{3N}\} \;+\; \cdots$$

  - P_A, P_B are simple polynomials in k/k_{F}
  - See also DME applied to ChPT in nuclear medium (N. Kaiser et al., nucl-th/0212049, 0312059, 0406038)
- Three-body contributions from DME in Jacobi coordinates
- $C[\rho]$ is a two-dimensional integral over off-diagonal V
- Also spin-orbit, tensor, ...

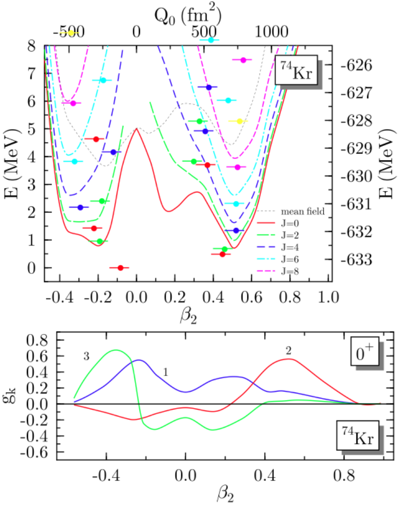
Novel optimization algorithms: Test case

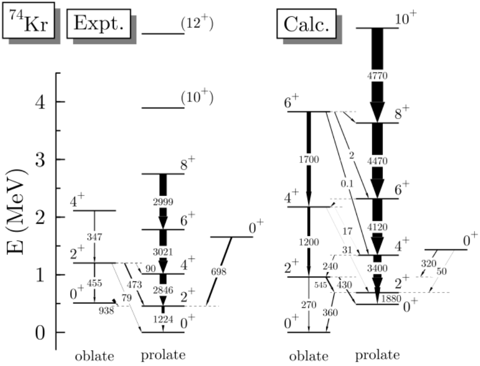




- left: Deviation between theoretical and experimental nuclear masses for the SLy4 Skyrme EDF using HFBTHO solver
- right: Same for UNEDFpre EDF parametrization
- Close to conventional Skyrme accuracy limit

Nuclear constrained calculations: GCM





- SLy6+density-dependent pairing
- There are no adjustable parameters. . .

Experiment: E. Clément *et al.* Phys. Rev. C75 (2007) 054313, A. Görgen *et al.* Eur. Phys. J. A26 (2005) 153

M. B., P. Bonche, P.-H. Heenen, Phys. Rev. C 74 (2006) 024312.

Nuclear constrained calculations:
Deformation energy surface