DFT and EFT: Recent developments and ideas

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Bridging nuclear ab-initio and energy density functional theories

October, 2017

Collaborators: S. Bogner (MSU), A. Dyhdalo (OSU), R. Navarro-Perez (LLNL), N. Schunck (LLNL), Y. Zhang (OSU) plus discussions with T. Papenbrock (UT) and many others

U.S. DEPARTMENT OF ENERGY
NUCLEI
Nuclear Computational Low-Energy Initiative
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Outline

Viewpoint: nuclear reduction and emergence

Progress report on new DME implementation

Nuclear DFT and effective actions (EFT)

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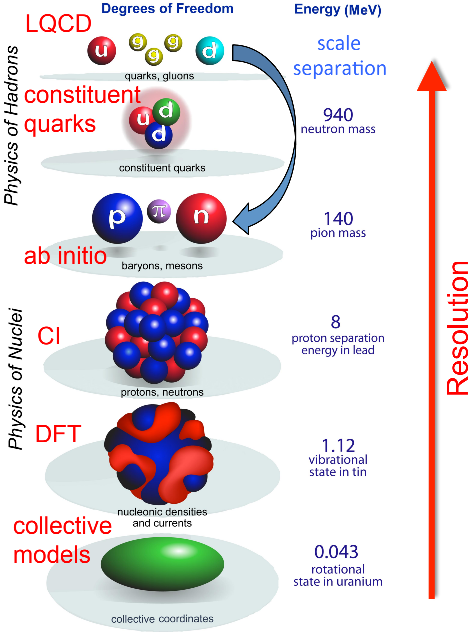
Nuclear DFT and effective actions (EFT)

Hierarchy of nuclear degrees of freedom



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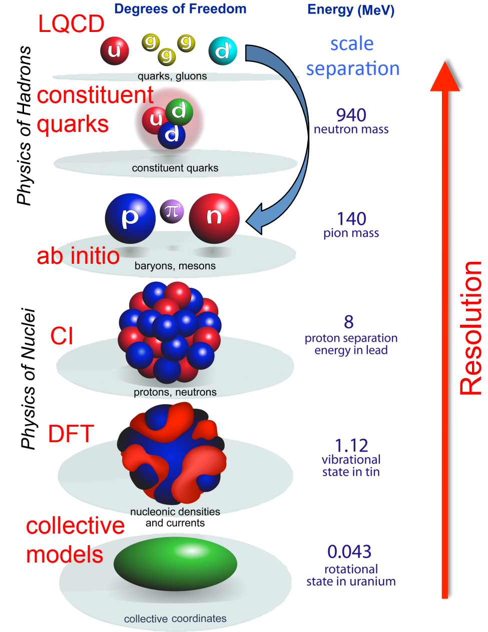

Multiple phenomenologies

- Constituent quarks
- Meson exchange models
- Cluster models
- Collective models
- Nuclei as Fermi liquids
- Nuclear pairing

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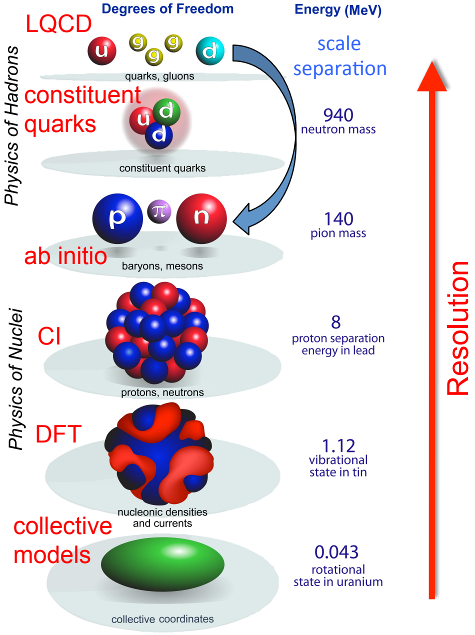

Reductive *and* Emergent

⟹ EFT (see 2017 Saclay workshop)

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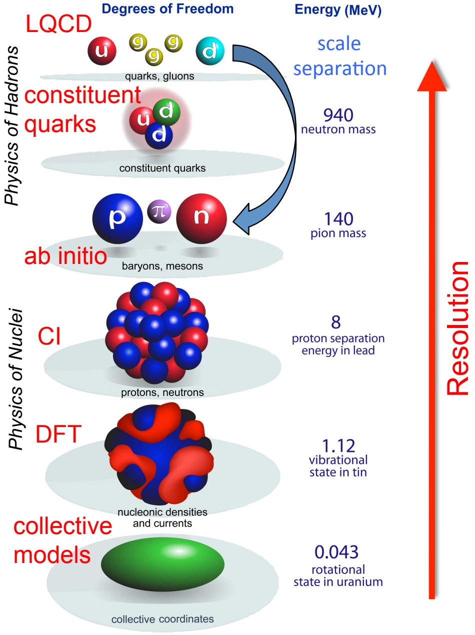
"Behind every successful emergent phenomenology there is an EFT (or EFTs) waiting to be uncovered"

Hierarchy of nuclear degrees of freedom



Reductive *and* Emergent

$\Longrightarrow$ EFT (see 2017 Saclay workshop)

- Chiral quark model
- Chiral EFT: nucleons, [Δ's,] pions; [within HO basis]
- Pionless EFT: nucleons only (low-energy few-body) or nucleons and clusters (halo)
- EFT for deformed nuclei: systematic collective dofs (Papenbrock et al.)
- EFT at the Fermi surface (Landau-Migdal theory; superfluidity): quasi-nucleons

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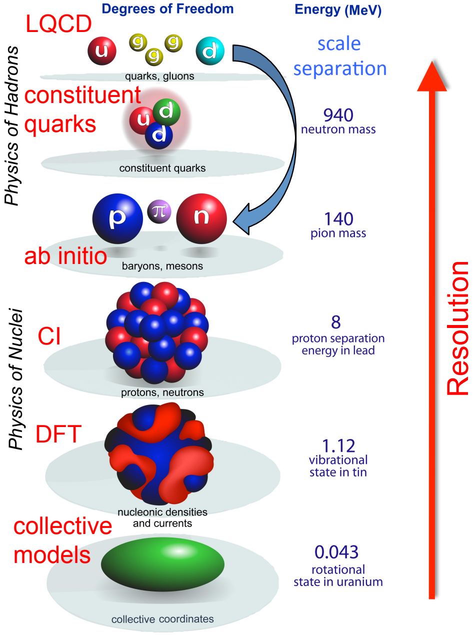

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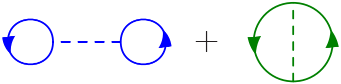
Where does EDF/DFT fit in?

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 (or SR $\to$ MR)]
3. Evaluate observables (masses, radii, β-decay, fission . . .)

Often interpreted as Kohn-Sham density functional theory

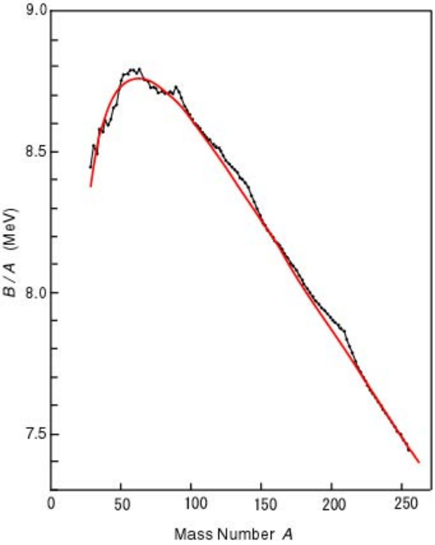
Motivations for doing better than empirical EDFs

- 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)
- …

Emergent features of nuclear energy density functionals

- Precise liquid drop systematics
- Shell structure
- Superfluidity
- Low-lying collectivity (RPA)

- Naturalness of parameter values reflect underlying chiral physics
- But SVD analyses reflect hierarchy of physics



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- Precise liquid drop systematics
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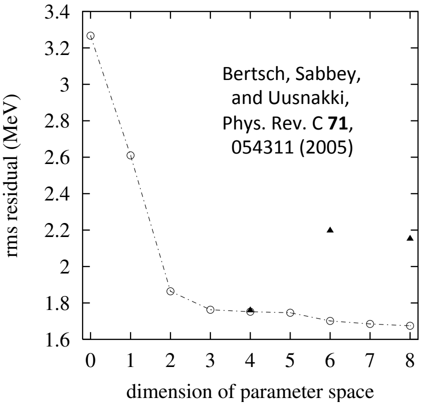
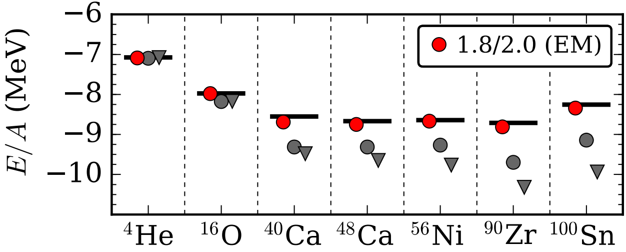
- Naturalness of parameter values reflect underlying chiral physics
- But SVD analyses reflect hierarchy of physics
  - Multiple studies show relatively few *important* parameters and they reflect emergent properties
  - Bulgac et al., "A Minimal Nuclear Energy Density Functional"



See also Toivanen et al., PRC (2008)

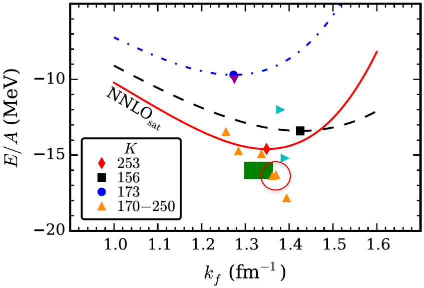
Fine-tuned potentials based on chiral EFT [from G. Hagen]

Accurate BEs from light → heavy → infinite matter from a chiral interaction



1.8/2.0 (EM) from K. Hebeler *et al* PRC (2011)
The other chiral NN + 3NFs are from Binder et al, PLB (2014)

- Accurate binding energies up to mass 100 from a chiral NN + 3NF
- Fit to nucleon-nucleon scattering and BEs and radii of A=3,4 nuclei
- Reproduces saturation point in nuclear matter within uncertainties
- Deficiencies: Radii are less accurate



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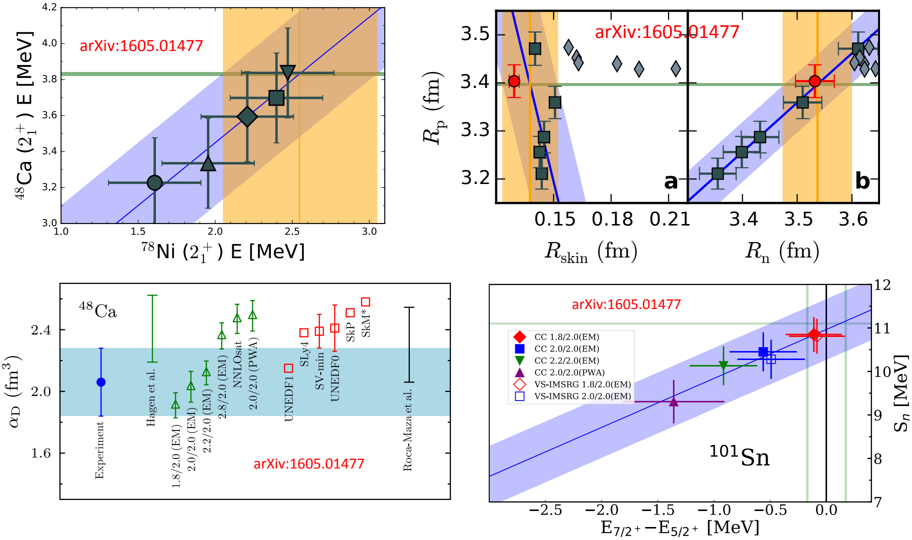

What is the take-away message from phenomenological success?

General questions for phenomenological EDFs

- Are density dependencies too simplistic? How do you know?
- How should we organize possible terms in the EDF?
- Where is pion physics resolved? Does near-unitarity matter?
- 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 guided by EFT

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

1. Long-distance chiral physics from Weinberg PC 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 and test
   - [See also J. Dobaczewski arXiv:1507.00697 for ab initio $\rightarrow$ EDF]
4. RG evolution of effective action functional [Jens Braun et al.]
   - See H. Liang et al. [arXiv:1710.00650] for recent implementation

Can we develop bottom-up EFT for DFT using a QFT formulation?

[See expansion about unitary limit in talks at this workshop!]

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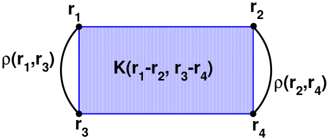
Density matrix expansion (DME) revisited [Negele/Vautherin]

- Dominant chiral EFT MBPT contributions can be put into form

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



- Earlier work: momentum space with non-local interactions

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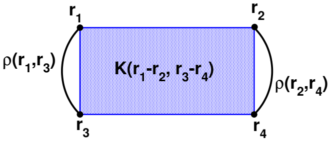

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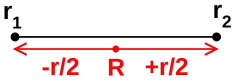
- DME: Expand ρ in local operators w/factorized non-locality

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\epsilon_\alpha \leq \epsilon_F} \phi^\dagger_\alpha(\mathbf{r}_1)\phi_\alpha(\mathbf{r}_2) = \sum_n \Pi_n(\mathbf{r})\langle \mathcal{O}_n(\mathbf{R})\rangle$$



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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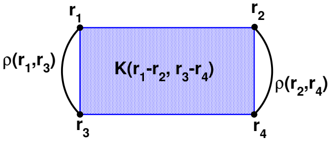

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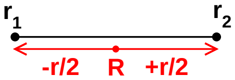

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- Original NV DME expands about nuclear matter (k-space + NNN)

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

DME vs. Operator Product Expansion (OPE)

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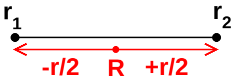

- Cf. OPE for unitary gas contact properties [E. Braaten arXiv:1008.2922]

$$O_A(\mathbf{R} + \frac{1}{2}\mathbf{r})O_B(\mathbf{R} - \frac{1}{2}\mathbf{r}) = \sum_C f_{A,B}^C(\mathbf{r})O_C(\mathbf{R})$$

$$\Longrightarrow \quad \psi_\sigma^\dagger(\mathbf{R} + \frac{1}{2}\mathbf{r})\psi_\sigma(\mathbf{R} - \frac{1}{2}\mathbf{r}) = \psi_\sigma^\dagger\psi_\sigma(\mathbf{R}) + \frac{1}{2}\mathbf{r}\cdot[\psi_\sigma^\dagger\boldsymbol{\nabla}\psi_\sigma(\mathbf{R}) - \boldsymbol{\nabla}\psi_\sigma^\dagger\psi_\sigma(\mathbf{R})]$$

$$- \frac{r}{8\pi}g_0^2(\Lambda)\psi_1^\dagger\psi_2^\dagger\psi_2\psi_1(\mathbf{R}) + \cdots$$

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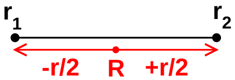

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- OPE is short-distance expansion including interactions; DME is resummed (with "freedom") but non-interacting ρ (HF only)

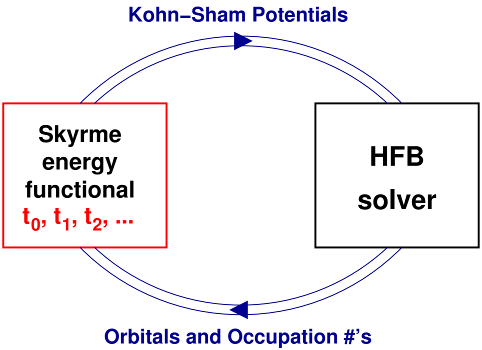
$$\sum_\alpha \phi_\alpha^\dagger(\mathbf{r}_1)\phi_\alpha(\mathbf{r}_2) = e^{\mathbf{r}\cdot(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)/2}\sum_\alpha \phi_\alpha^\dagger(\mathbf{R}_1)\phi_\alpha(\mathbf{R}_2)\Big|_{\mathbf{R}_1=\mathbf{R}_2=\mathbf{R}}$$

- Is there anything to learn here? E.g., about going beyond HF?

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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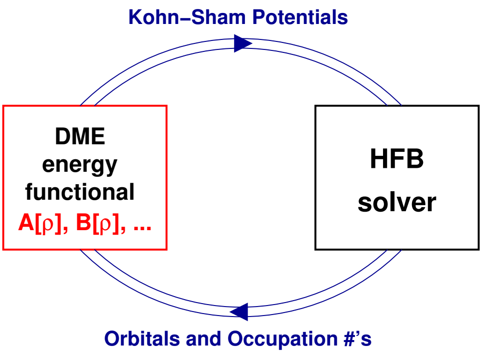

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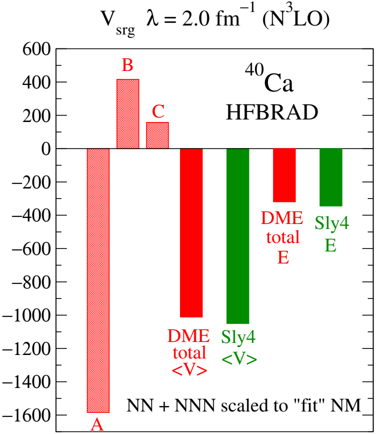
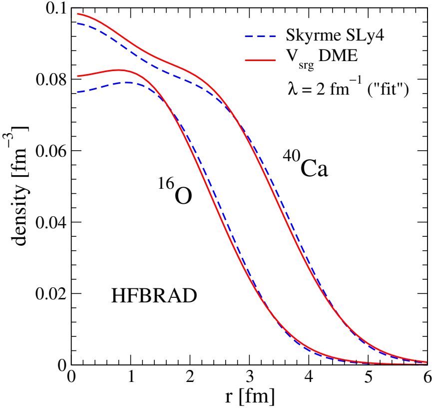
Full ab-initio: Is Negele-Vautherin DME good enough?

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

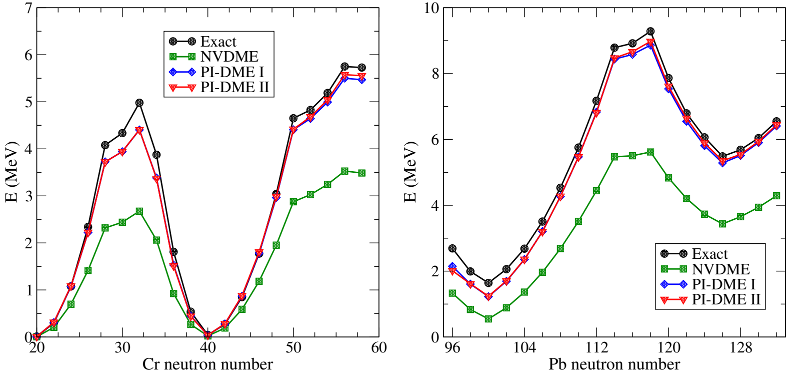




- Do densities look like nuclei from Skyrme EDF's? Yes!
- Are the error bars competitive? No! 1 MeV/A off in ^{40}Ca
  $\Longrightarrow$ rethink application of DME

Improved DME for pion exchange tests

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



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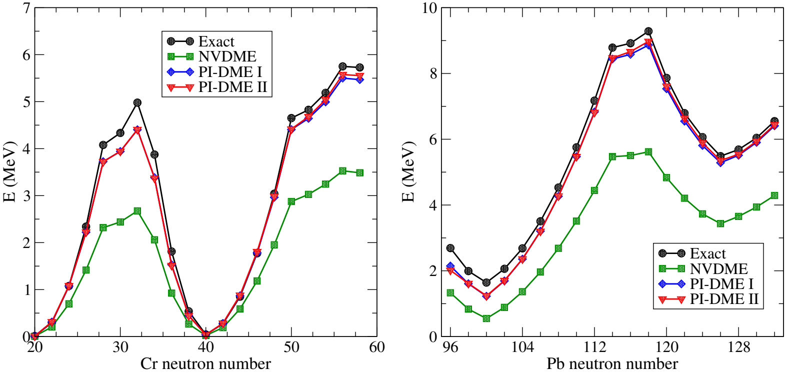

- Can we see pions? Revised gameplan: [Stoitsov et al., Bogner et al.]
  - Add NN/NNN pion exchange through N^2LO at HF level
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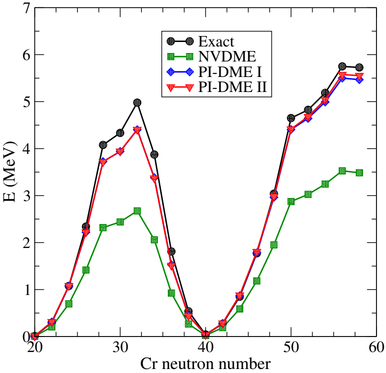

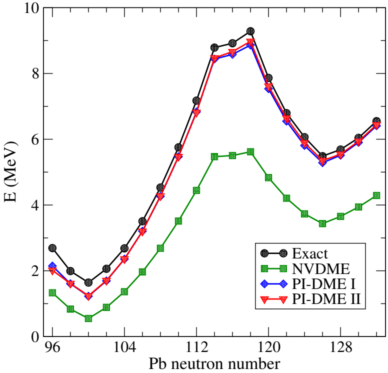

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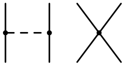
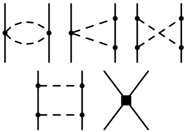
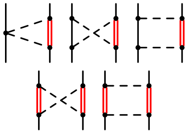
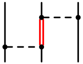
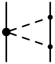
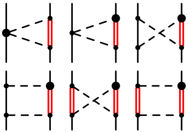
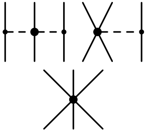
- New developments: use local *regulated* NN + NNN [Alex Dyhdalo, OSU]

Long-range parts of chiral expansion with and without Δs

	NN force		$3N$ force	
	Δ-less EFT	Δ contributions	Δ-less EFT	Δ contributions
LO		—	—	—
NLO			—	
N^2LO				—

See A. Dyhdalo, S. K. Bogner and R. J. Furnstahl, “Applying the Density Matrix Expansion with Coordinate-Space Chiral Interactions,” Phys. Rev. C **95**, 054314 (2017) for details.

Implementation by R. Navarro Pérez and N. Schunck (LLNL)

Microscopically constrained EDF

Implementing Chiral Interactions in DFT

- Hartree-Fock fields from Chiral interactions

Skyrme + Gaussian Hartree + DME Fock

UNEDF2 like and refitted to masses and radii

Chrial and fixed for a given order, LECs and regulator

- Start with a ‘conservative’ regulator, r_c = 2.0 fm
- Refit skyrme parameters
- Move to a ‘less conservative’ regulator
- Rinse and repeat

Study the effect of the regulator and rise of finite size effects

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Microscopically constrained EDF

Density Matrix Expansion

- Non-local densities when working with finite range potentials

$$V_H^{NN} \sim \int dR\, dr \langle r | V^{NN} | r \rangle \rho_1 (R + \frac{r}{2}) \rho_2 (R - \frac{r}{2})$$

$$V_F^{NN} \sim \int dR\, dr \langle r | V^{NN} | r \rangle \rho_1 (R - \frac{r}{2}, R + \frac{r}{2}) \rho_2 (R + \frac{r}{2}, R - \frac{r}{2}) P_{12}$$

- Density Matrix Expansion

$$\rho (R + \frac{r}{2}, R - \frac{r}{2}) \approx \Pi_0^{\rho} (k_F r) \rho (R)$$

$$+ \frac{r^2}{6} \Pi_2^{\rho} (kF\, r) [\frac{1}{4} \Delta \rho (R) - \tau (R) + \frac{3}{5} k_F^2 \rho (R)]$$

Density dependent couplings enter in the Fock Energy

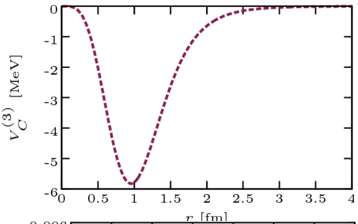
Implementation by R. Navarro Pérez and N. Schunck (LLNL)

Microscopically constrained EDF

Finite Range Chiral Potentials

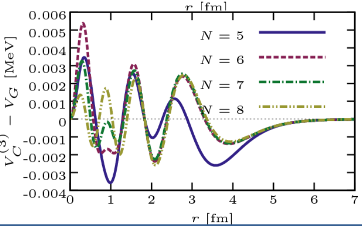
- Chiral potentials are regulated

$$V_c(r) \propto \left[1 - e^{-r^2/r_c^2}\right]^n \frac{e^{-2x}}{r^6}(\dots)$$



- Expand as a sum of Gaussians

$$V_G(r) = \sum_{i=1}^{N-1} V_i\left(e^{-\mu_i r^2} - e^{-\mu_N r^2}\right)$$



Allows to use the already implemented Gogny machinery

Implementation by R. Navarro Pérez and N. Schunck (LLNL)

Microscopically constrained EDF

Density Dependent Couplings

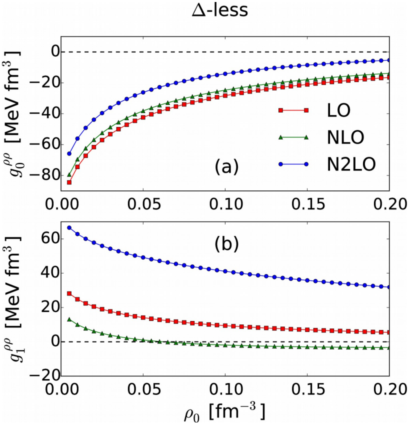
- Expensive numerical integrals

$$g_t^{\rho\rho}(\rho) \propto \int dr\, r^2 \left\{ \left[\Pi_0^{\rho}(k_F r) \right]^2 + \ldots \right\} \left[V_c(r) + 3 W_c(r) + \ldots \right]$$

- Interpolating function

$$g_t^{\rho\rho}(\rho) = g_0 + \sum_{i=1}^{M} a_i \left[\tan^{-1}\left(b_i \rho^{c_i} \right) \right]^i$$

- The same for 3N forces



Derivatives with respect of ρ are available

Implementation by R. Navarro Pérez and N. Schunck (LLNL)

Microscopically constrained EDF

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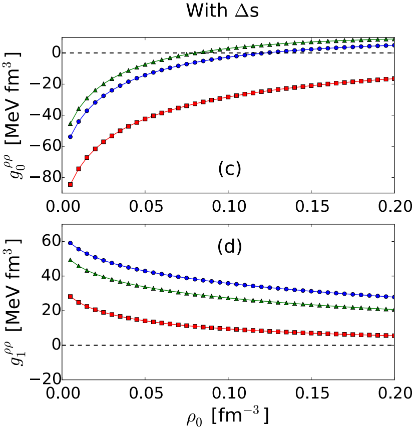

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Implementation by R. Navarro Pérez and N. Schunck (LLNL)

Microscopically constrained EDF

Infinite Nuclear Matter Properties

- Used to constrain the Skyrme phenomenological parameters
- Energy density in nuclear matter

$$W(\rho_0) = [C_0^{\rho\rho} + g_0^{\rho\rho}(\rho_0) + \rho_0 h_0^{\rho\rho}(\rho_0)]\rho_0 + [C_0^{\rho\tau} + g_0^{\rho\tau}(\rho_0) + \rho_0 h_0^{\rho\tau}(\rho_0)]\tau_0 + W_{FR}(\rho_0)$$

- Taylor expansion around saturation density

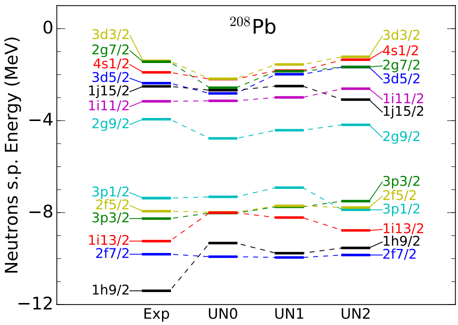
$$W(\rho_0) = \frac{E^{NM}}{A} + \frac{P^{NM}}{\rho_c^2}(\rho_0 - \rho_c) + \frac{K^{NM}}{18\rho_c^2}(\rho_0 - \rho_c)^2 + \cdots$$

- Calculate derivatives of W(ρ_0) and solve for $C_0^{\rho\rho}, C_0^{\rho\tau}, C_1^{\rho\rho}, C_1^{\rho\tau}, \ldots$

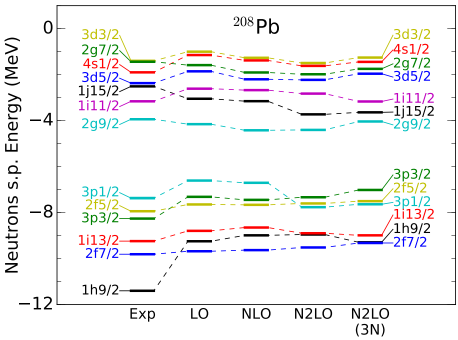
Use NMP as inputs to obtain Skyrme couplings

Preliminary results: Single-particle levels

UNEDF EDFs

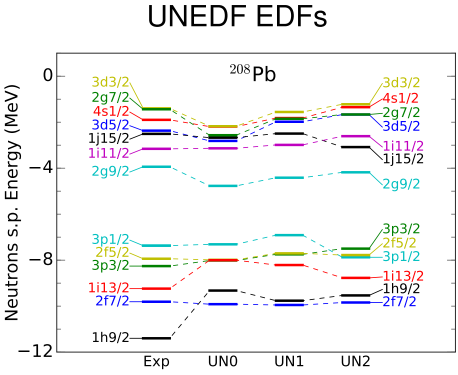


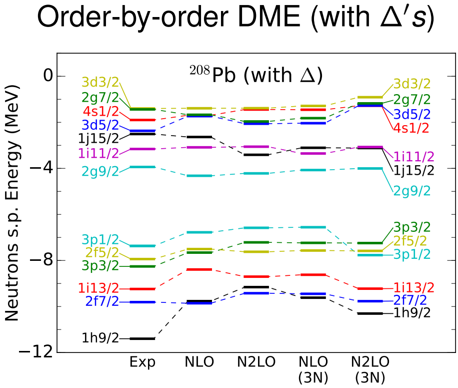
Order-by-order DME (no $\Delta's$)



Can we conclude anything from this? Are fine details important?

Preliminary results: Single-particle levels





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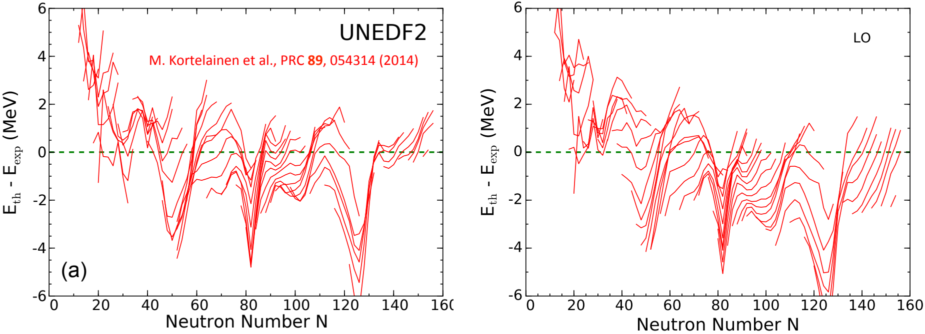
Preliminary results: Mass residuals (single reference)

NOTE: Residuals for interactions with 3NF not complete yet



What can conclude from these? Is MR necessary to judge DME?

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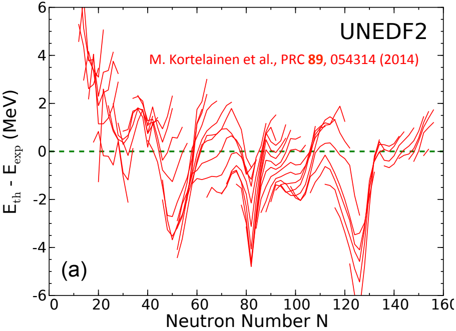

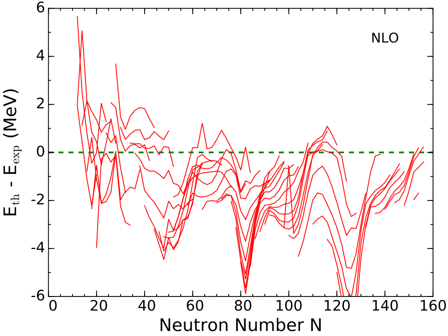

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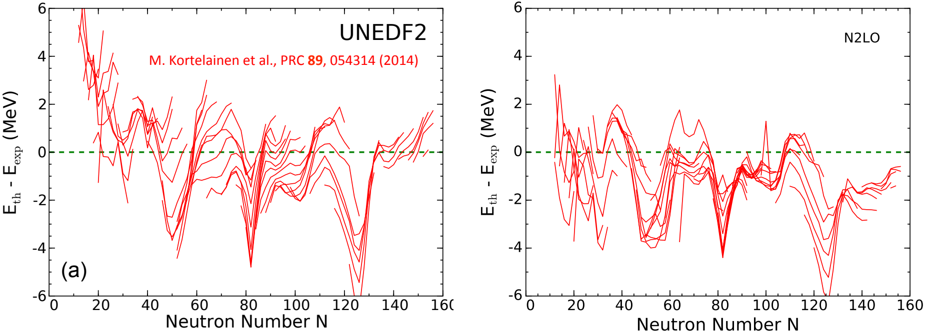

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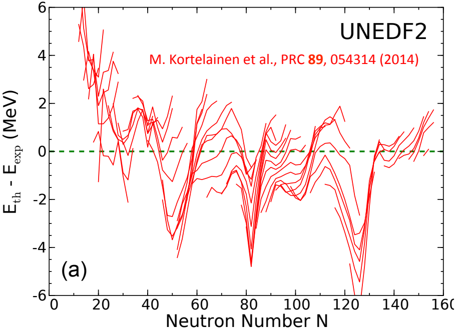

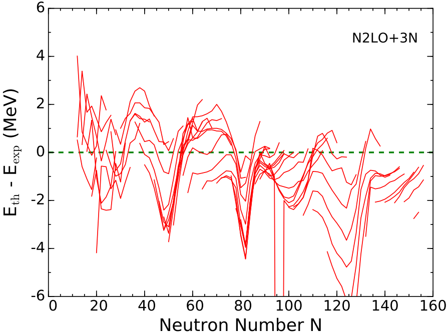

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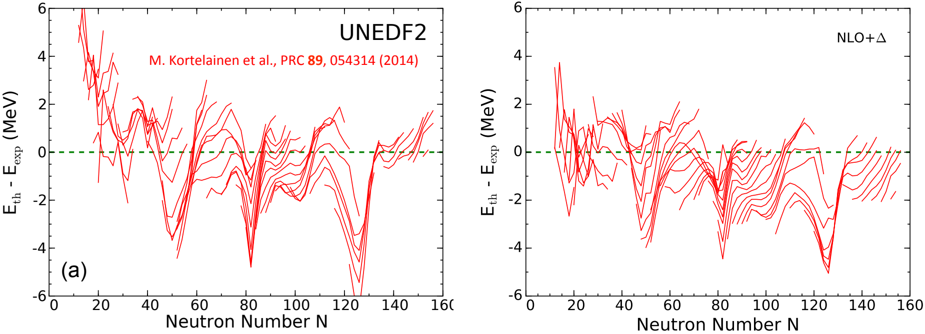

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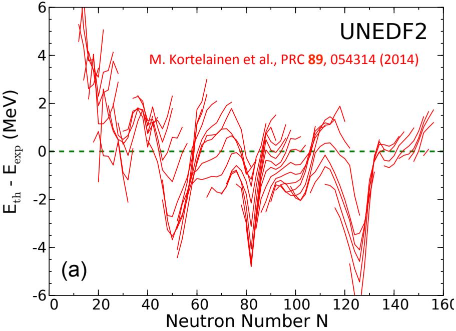

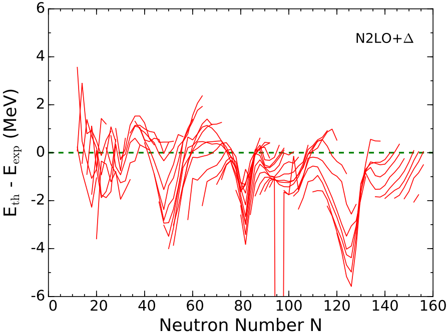

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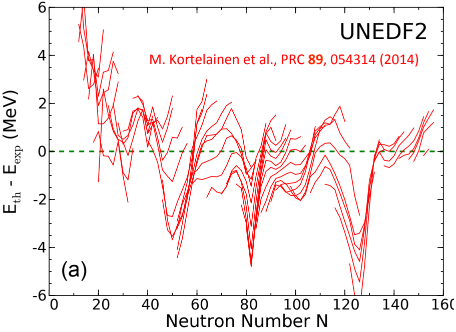
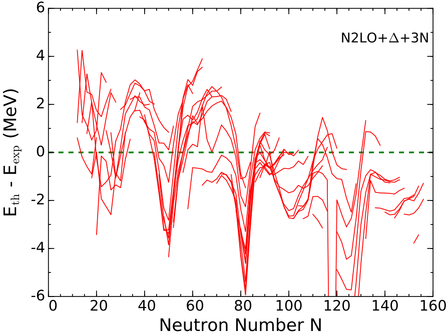




What can conclude from these? Is MR necessary to judge DME?

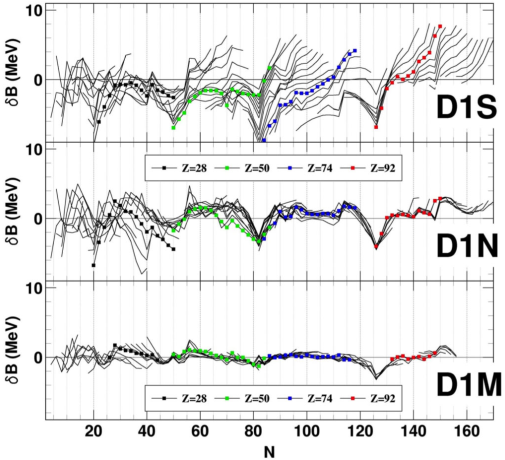
Cf. effect on Gogny HFB mass residuals of (some) BMF

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

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

- $\approx$ 14 parameters
- quadrupole correlations included self-consistently
- D1M: $\delta B_{rms} = 0.8\,\mathrm{MeV}$ for 2353 masses
- $\sigma \approx 0.65\,\mathrm{MeV}$ for 2064 β-decay energies
- radii, giant resonances and fission properties
- does not include particle-vibration coupling

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



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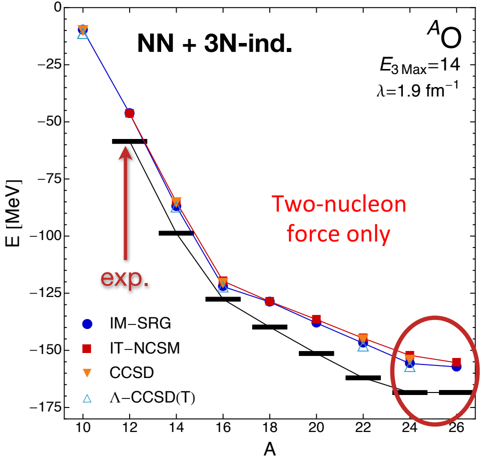

[Old calculations from Hergert et al., Cipollone et al. (2013). Now also SCGF and AFDMC!]

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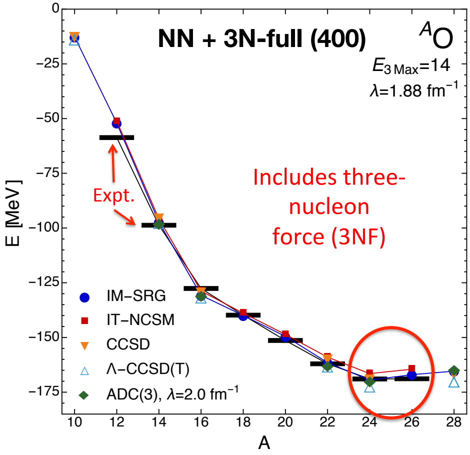

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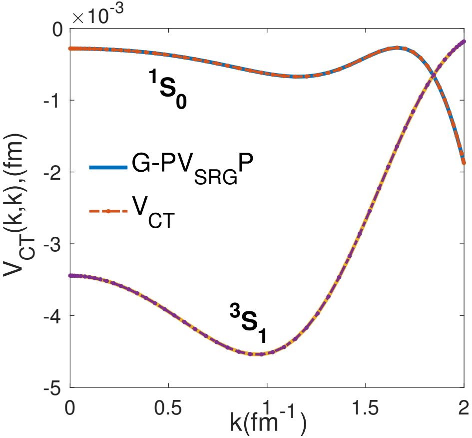
DME: going forward

- Clearly we need to include beyond-mean-field physics to address EDF needs!
- Test systematics along isotope chains. E.g., role of 2π 3NF
- Beyond HF in DME $\Longrightarrow$ are higher orders resolved?
  - Cf. local counterterms for T-matrix contributions above cutoff Λ (here: $\Lambda \to k_{\mathrm{F}}$)
  - Y. Zhang (OSU): Higher-order G-matrix well represented by gradient terms up to ∇^4 near $k_{\mathrm{F\,sat}}$



Outline

Viewpoint: nuclear reduction and emergence

Progress report on new DME implementation

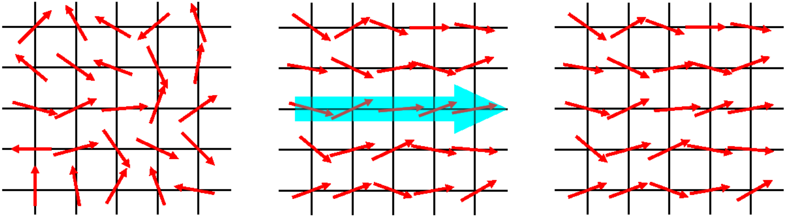
Nuclear DFT and effective actions (EFT)

Many 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)? What about collective surface vibrations?
- Can we implement such an EFT without losing the favorable computational scaling of current nuclear EDFs?

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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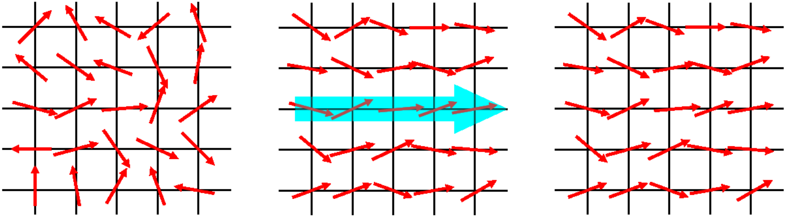


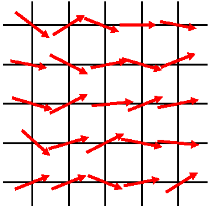
  - if $F[H]$ calculated perturbatively, $M[H = 0] = 0$ to all orders
  - Legendre transform Helmholtz free energy $F(H)$:

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

  - 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 $\Gamma[M]$



source magnet

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

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

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

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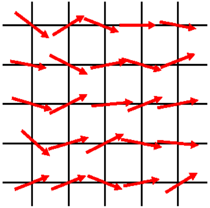

source	magnet

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

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

- *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 $\rho_{\rm gs}(\mathbf{x})$!

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),

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

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

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

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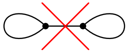
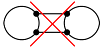
- $\Gamma[\rho]$: expectation value of $\widehat{H}$ in ground state generated by $J[\rho]$

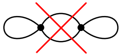
$$\frac{1}{\beta}\Gamma[\rho] = E_0(J) - \int J\,\rho = \langle \widehat{H} + J\,\widehat{\rho}\rangle_J - \int J\,\rho = \langle \widehat{H} \rangle_J \xrightarrow{J \to 0} E_0$$

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

But there are different effective action formulations

- 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
  - See nucl-th/0208058 for dilute EFT in large $N \Longrightarrow$ 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
  - Cf. self-consistent Green's functions or RG-evolved effective action

- Source coupled to local composite operator, e.g., $J(x)\phi^2(x)$
  - 2PPI (two-particle-point-irreducible) effective action 
  - Kohn-Sham DFT from order-by-order inversion method
  - Careful: new divergences arise (e.g., pairing)

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:

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

- Find $\Gamma[\rho,\phi]$ from $W[J_0, j_0]$ by inversion $(\Delta = \Delta_0 + \Delta_1 + \cdots)$
- 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., $\frac{1}{2}\zeta j^2$)

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:

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

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

In general: adding more sources improves variational probing *and* KS Green's function gets closer to full Green's function (see old refs)

What would a condensed matter theorist do?

From Altland and Simons "Condensed Matter Field Theory":

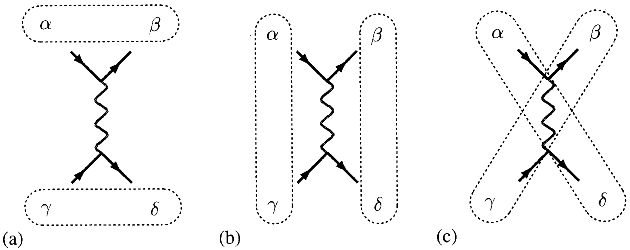

Figure 6.1 On the different channels of decoupling an interaction by Hubbard–Stratonovich transformation. (a) Decoupling in the "density" channel; (b) decoupling in the "pairing" or "Cooper" channel; and (c) decoupling in the "exchange" channel.

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

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

- Or exploit freedom in saddlepoint evaluation [see Negele and Orland]

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:

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

  - 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

- See Zinn-Justin, Path Integrals in Quantum Mechanics
  - In general, introduce collective coordinates; if possible, switch
  - If not feasible, apply Faddeev-Popov's method (cf. quantizing non-abelian gauge theories)

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  - If not feasible, apply Faddeev-Popov's method (cf. quantizing non-abelian gauge theories)
- Another 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?

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  - Can the procedure be adapted to DFT?
- Status report
  - Past progress: negligible
  - Current plan: revisiting for model problems; cautiously optimistic
  - Help would be welcome!

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)? What about surface vibrations?
- Can we implement such an EFT without losing favorable computational scaling?