Ab Initio Density Functional Theory for Nuclei

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July, 2008
Outline

Overview: UNEDF project and Ab Initio DFT

Current Status and Possible Problems

Outlook and Additional Issues for Nuclear DFT

Extras
Outline

Overview: UNEDF project and Ab Initio DFT

Current Status and Possible Problems

Outlook and Additional Issues for Nuclear DFT

Extras
SciDAC 2 Project: Building a Universal Nuclear Energy Density Functional

- Understand nuclear properties “for element formation, for properties of stars, and for present and future energy and defense applications”

- Scope is all nuclei, with particular interest in reliable calculations of unstable nuclei and in reactions
  \[ \rightarrow \text{DFT is method of choice} \]

- Order of magnitude improvement over present capabilities
  \[ \rightarrow \text{precision calculations of masses, . . .} \]

- Connected to the best microscopic physics

- Maximum predictive power with well-quantified uncertainties

[See http://www.scidacreview.org/0704/html/unedf.html by Bertsch, Dean, and Nazarewicz]
SciDAC 2 Project: **Building a Universal Nuclear Energy Density Functional**

- Collaboration of physicists, applied mathematicians, and computer scientists
- Funding in US but international collaborators also
Paths to a Nuclear Energy Functional (EDF)

- Empirical energy functional (Skyrme or RMF)
- Emulate Coulomb DFT: LDA based on precision calculation of uniform system $E[\rho] = \int d\mathbf{r} \mathcal{E}(\rho(\mathbf{r}))$ plus constrained gradient corrections ($\nabla \rho$ factors)

- SLDA (Bulgac et al.)
- Fayans and collaborators (e.g., nucl-th/0009034)
  \[ \mathcal{E}_v = \frac{2}{3} \varepsilon_F \rho_0 \left[ a_+^{\nu} \frac{1-h_1^\nu x_+^{1/3}}{1-h_2^\nu x_+^{1/3}} x_+^2 + a_-^{\nu} \frac{1-h_1^\nu x_+^{1/3}}{1-h_2^\nu x_+^{1/3}} x_-^2 \right] \]
  where $x_\pm = (\rho_n \pm \rho_p)/2\rho_0$

- RG approach (J. Braun, from Polonyi and Schwenk, nucl-th/0403011)
- EDF from perturbative chiral interactions + DME (Kaiser et al.)
- Constructive Kohn-Sham DFT with RG-softened $V_\chi^{EFT}$'s
Two-Neutron Separation Energies

The graph shows the separation energy for two neutrons as a function of the neutron number and proton number. The lines indicate the N = Z and N = 2Z conditions. The color coding represents the two-neutron separation energy in MeV.
Quadrupole Deformations and $B(E2)$
Fission: Energy Surface from DFT
HFB Mass Formula: $\Delta m \sim 1–2 \text{ MeV}$

Deviation from experiment

- Current empirical functionals hit wall at $\sim 1–2 \text{ MeV}$ (!)
- Accuracy of an ab initio functional fit to few-body data?
New-generation energy density functionals

Jacek Dobaczewski
University of Warsaw & University of Jyväskylä

In collaboration with:
Gillis Carlsson, Markus Kortelainen,
Kazuhito Mizuyama, Jussi Toivanen

UNEDF Annual Workshop, Pack Forest (WA)
June 23-26, 2008
Nuclear Energy Density Functional

We consider the EDF in the form,

$$\mathcal{E} = \int d^3 r \mathcal{H}(r),$$

where the energy density $\mathcal{H}(r)$ can be represented as a sum of the kinetic energy and of the potential-energy isoscalar ($t = 0$) and isovector ($t = 1$) terms,

$$\mathcal{H}(r) = \frac{\hbar^2}{2m} \tau_0 + \mathcal{H}_0(r) + \mathcal{H}_1(r),$$

which for the time-reversal and spherical symmetries imposed read:

$$\mathcal{H}_t(r) = C_t^\rho \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^{\Delta \rho} \rho_t \Delta \rho_t + \frac{1}{2} C_t^J J_t^2 + C_t^{\nabla J} \rho_t \nabla \cdot J_t.$$

Following the parametrization used for the Skyrme forces, we assume the dependence of the coupling parameters $C_t^\rho$ on the isoscalar density $\rho_0$ as:

$$C_t^\rho = C_{t0}^\rho + C_{tD}^\rho \rho_0^\alpha.$$

The standard EDF depends linearly on 12 coupling constants,

$$C_{i0}^\rho, \ C_{iD}^\rho, \ C_i^\tau, \ C_i^{\Delta \rho}, \ C_i^J, \ \text{and} \ C_i^{\nabla J},$$

for $t = 0$ and 1.
How well can we describe masses with 12 coupling constants?

Bertsch, Sabbey, and Uusnakki
How well can we describe single-particle energies with 12 coupling constants?

How to extend the nuclear energy density functional beyond the current standard form?

Quest for the spectroscopic-quality functional

I. Density dependence of all the coupling constants

\[ C^m_t(\rho_0, \rho_1) = C^m_t \left[ 1 + \alpha^m_t \left( 1 - \left( \frac{\rho_0}{\rho_{\text{sat}}} \right)^\gamma^m_t \right) + \beta^m_t \left( \frac{\rho_1}{\rho_{\text{sat}}} \right)^2 n^m_t \right] \]

II. Derivatives of higher order up to N^3LO:

\[ \rho^{mn}_{ILkJ'J} = (\tilde{\nu}^m_I) (\tilde{k}^n_L \rho_k)_{J'J} \quad \text{for} \quad k = 0, 1 \quad \text{and} \quad m+n \leq 6 \]

III. Products of more than two densities, for example:

\[ \rho^2 \tau^2, \quad \rho \tau \Delta \rho, \ldots \]
Issues with Empirical EDF’s

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

⇒ Turn to microscopic many-body theory for guidance
(although *not* for higher precision description!)
Comparing Dilute and Skyrme Functionals

- Skyrme energy density functional (for $N = Z$)

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

- Dilute $\rho \tau J$ energy density functional for $\nu = 4$ ($V_{\text{external}} = 0$)

$$E[\rho, \tau, J] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8} C_0 \rho^2 + \frac{1}{16} (3C_2 + 5C'_2) \rho \tau + \frac{1}{64} (9C_2 - 5C'_2)(\nabla \rho)^2 
- \frac{3}{4} C''_2 \rho \nabla \cdot J + \frac{c_1}{2M} C_0^2 \rho^{7/3} + \frac{c_2}{2M} C_0^3 \rho^{8/3} + \frac{1}{16} D_0 \rho^3 + \cdots \right\}$$

- 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? Are proposed extensions enough?
  
  - Isn’t this a “perturbative” expansion?
Major UNEDF Research Areas

- **Ab initio structure** — Nuclear wf’s from microscopic NN···N
  - NCSM/NCFC, CC, GFMC/AFMC
  - AV18/ILx, chiral EFT $\rightarrow V_{\text{low } k}$

- **Ab initio energy functionals** — DFT from microscopic N···N
  - Cold atoms — superfluid LDA+ as prototype for nuclear DFT
  - $\chi$EFT $\rightarrow V_{\text{low } k} \rightarrow \text{MBPT} \rightarrow \text{DME}$

- **DFT applications** — Technology to calculate observables
  - Skyrme HFB+ for all nuclei (solvers)
  - Fitting the functional to data (e.g., correlation analysis)

- **DFT extensions** — Long-range correlations, excited states
  - LACM, GCM, TDDFT, QRPA, CI

- **Reactions** — Low-energy reactions, fission, . . .
Overview: UNEDF project and Ab Initio DFT

Current Status and Possible Problems

Outlook and Additional Issues for Nuclear DFT

Extras
UNEDF Interconnections for Ab Initio Functionals

Ab Initio WF Methods
CC: UT/ORNL (Dean, Hagen, Papenbrock)
NCFC: ISU (Maris, Vary)
LLNL (Navratil)

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

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

Interactions
Chiral EFT
Bonn/Julich
(Epelbaum, Nogga)
Salamanca/Idaho
(Entem, Machleidt)
Vlowk/SRG
OSU, MSU
TRIUMF (Schwenk)

Participant color key:
UNEDF
International collaborator
Outside UNEDF
Ab Initio WF Methods
CC: UT/ORNL (Dean, Hagen, Papenbrock)
NCFC: ISU (Maris, Vary)
LLNL (Navratil)

Wider range of nuclei
Full 3NF
Ab Initio densities
External potentials

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

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

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

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

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

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

Participant color key:
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Interactions
Chiral EFT
Bonn/Julich
(Epelbaum, Nogga)
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Vlowk/SRG
OSU, MSU
TRIUMF (Schwenk)

N3LO 3NF
Explicit Delta’s
New 3NF fits
SRG 3NF evolution

UNEDF Interconnections for Ab Initio Functionals
Microscopic Nuclear Structure Methods

- **Wave function methods** (GFMC/AFMC, NCSM/FCI, CC, …)
  - many-body wave functions (in approximate form!)
  - $\Psi(x_1, \cdots, x_A) \Rightarrow$ everything (if operators known)
  - limited to $A < 100$ (??)

- **Green’s functions** (see W. Dickhoff and D. Van Neck text)
  - response of ground state to removing/adding particles
  - single-particle Green’s function $\Rightarrow$ expectation value of one-body operators, Hamiltonian
  - energy, densities, single-particle excitations, …

- **DFT** (see C. Fiolhais et al., *A Primer in Density Functional Theory*)
  - response of energy to perturbations of the density $J(x)\psi^\dagger\psi$
  - natural framework is effective actions for composite operators $\Gamma[\rho] = \Gamma_0[\rho] + \Gamma_{\text{int}}[\rho]$ (e.g., for EFT/DFT) but also consider quantum chemistry MBPT+ approach (Bartlett et al.)
  - energy functional $\Rightarrow$ plug in candidate density, get out trial energy, minimize (variational?)
  - energy and densities (TDFT $\Rightarrow$ excitations)
Orbital Dependent DFT (OEP, OPM, ...) [J. Drut]

- Construct expansion for $\Gamma_{\text{int}}[\rho, \tau, J, \ldots]$; densities are sums over orbitals solving from Kohn-Sham S-eqn with $J_0(r), \ldots$
- Self-consistency from $J(r) = 0 \implies J_0(r) = \frac{\delta \Gamma_{\text{int}}[\rho, \ldots]}{\delta \rho(r)}$
  - i.e., Kohn-Sham potential is functional derivative of interacting energy functional (or $E_{\text{xc}}$) wrt densities
- How do we calculate this functional derivative?
- Approximations with explicit $\rho(r)$ dependence: LDA, DME, ...
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- How do we calculate this functional derivative?
- Approximations with explicit $\rho(r)$ dependence: LDA, DME, …
- Orbital-dependent DFT $\implies$ full derivative via chain rule:

$$J_0(r) = \frac{\delta \Gamma_{\text{int}}[\phi_\alpha, \epsilon_\alpha]}{\delta \rho(r)} = \int dr' \frac{\delta J_0(r')}{\delta \rho(r)} \sum_\alpha \left\{ \int dr'' \left[ \frac{\delta \phi_\alpha^+(r'')}{\delta J_0(r')} \frac{\delta \Gamma_{\text{int}}}{\delta \phi_\alpha(r'')} + \text{c.c.} \right] \\
+ \frac{\delta \epsilon_\alpha}{\delta J_0(r')} \frac{\partial \Gamma_{\text{int}}}{\partial \epsilon_\alpha} \right\}$$

- Solve the OPM equation for $J_0$ using $\chi_s(r, r') = \delta \rho(r)/\delta J_0(r')$

$$\int d^3r' \chi_s(r, r') J_0(r') = \Lambda_{xc}(r)$$

- $\Lambda_{xc}(r)$ is functional of the orbitals $\phi_\alpha$, eigenvalues $\epsilon_\alpha$, and $G_{KS}^0$
Microscopic EDF’s from the DME

- Dominant MBPT contributions to bulk properties take the form
  \[ \langle V \rangle \sim \text{Tr}_1 \text{Tr}_2 \int d\mathbf{R} \, dr_{12} \, dr_{34} \, \rho(\mathbf{r}_1, \mathbf{r}_3) \, K(\mathbf{r}_{12}, \mathbf{r}_{34}) \, \rho(\mathbf{r}_2, \mathbf{r}_4) + \text{NNN} \ldots \]

  \begin{align*}
  \bullet & \text{ density matrices and s.p. propagators} \\
  \bullet & \text{ finite range and non-local resummed vertices } K \\
  \end{align*}

- DME \implies \text{ expand DM in local operators w/factorized non-locality}

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

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

  Maps \( \langle V \rangle \) into a extended Skyrme-like EDF!

- Original DME \implies \text{calculate } \Pi_n \text{ from expanding about infinite NM}

- Optimized DME \implies \text{Fit } \Pi_n, \text{ constrain by symmetries and sum rules}

- density dependencies, isovector, time-odd,... missing in Skyrme
Density Matrix Expansion Revisited [Negele/Vautherin]

- DME: Write one-particle density matrix in Kohn-Sham basis

\[ \rho(r_1, r_2) = \sum_{\epsilon_\alpha \leq \epsilon_F} \psi^\dagger_\alpha(r_1) \psi_\alpha(r_2) \]

- \( \rho(r_1, r_2) \) falls off with \(|r_1 - r_2|\) \(\implies\) expand in \(r\) (and resum)

- Fall off is well approximated by nuclear matter
  \(\implies\) expand so that first term exact in uniform system
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- \(\rho(r_1, r_2)\) falls off with \(|r_1 - r_2|\) \(\implies\) expand in \(r\) (and resum)
- Fall off is well approximated by nuclear matter \(\implies\) expand so that first term exact in uniform system
- Change to \(R = \frac{1}{2}(r_1 + r_2)\) and \(r = r_1 - r_2\) and resum in \(r\)

$$\rho(R + r/2, R - r/2) = e^{r \cdot (\nabla_1 - \nabla_2)/2} \rho(r_1, r_2)|_{r=0}$$

$$\implies \frac{3j_1(rk_F)}{rk_F} \rho(R) + \frac{35j_3(rk_F)}{2rk_F^3} \left( \frac{1}{4} \nabla^2 \rho(R) - \tau(R) + \frac{3}{5} k_F^2 \rho(R) + \cdots \right)$$

- In terms of local densities \(\rho(R), \tau(R), \ldots \implies\) DFT with these
- Extend to \(k\) space, NNN [Bogner, rjf, Platter]
Physics of the DME  [Negele et al.]

- Local rather than global properties of density matrix
- Not a short-distance expansion; keeps long-range effects
  - Expanding the difference between exact and nuclear matter results in powers of $s$ (nuclear matter $k_F$)

- Exact neutron density matrix squared in $^{208}$Pb compared with DME

- Improvements . . . [B. Gebremariam, S. Bogner, T. Duguet]
DME for Low-momentum Interactions (HF/NN only)

- Test with HO model; cf. schematic $V$’s (1970’s)
- $\Lambda$–independent errors $\approx +5\text{ MeV (NLO)}, \approx -10\text{ MeV (N}^3\text{LO)}$

HO Model: $\langle V \rangle_{\text{DME}} - \langle V \rangle_{\text{exact}} [\text{MeV}]

\[ \begin{align*}
\Lambda [\text{fm}^{-1}] & \quad \langle V \rangle_{\text{DME}} - \langle V \rangle_{\text{exact}} [\text{MeV}] \\
1.5 & \quad -40 \\
2 & \quad -20 \\
2.5 & \quad 0 \\
3 & \quad 20 \\
3.5 & \quad 40 \\
4 & \quad \text{Negele-Vautherin G-matrix} \\
& \quad \text{Brink-Boeker (Sprung et. al.)} \\
& \quad V_{\text{low } k} (\text{NLO}) \\
& \quad V_{\text{low } k} (\text{N}^3\text{LO}) \\
\end{align*} \]

\[ V_{\text{low } k} \Lambda = 2.0 \text{ fm}^{-1} (\text{N}^3\text{LO}) \]
Adaptation to Skyrme HFB Implementations

\[ E_{\text{Skyrme}} = \frac{\tau}{2M} + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^{2+\alpha} + \frac{1}{16} (3t_1 + 5t_2) \rho \tau + \frac{1}{64} (9t_1 - 5t_2) |\nabla \rho|^2 + \cdots \]

\[ \implies E_{\text{DME}} = \frac{\tau}{2M} + A[\rho] + B[\rho] \tau + C[\rho] |\nabla \rho|^2 + \cdots \]

Kohn–Sham Potentials

Skyrme energy functional \( t_0, t_1, t_2, \ldots \)

HFB solver

Orbitals and Occupation #'s

\[ J_0(r) = \frac{\delta E_{\text{int}}[\rho]}{\delta \rho(r)} \iff \left[-\frac{\nabla^2}{2m} - J_0(x)\right] \psi_\alpha = \varepsilon_\alpha \psi_\alpha \implies \rho(x) = \sum_\alpha n_\alpha |\psi_\alpha(x)|^2 \]
Adaptation to Skyrme HFB Implementations

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

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

Kohn–Sham Potentials

DME energy functional
\[ A[\rho], B[\rho], \ldots \]

HFB solver

Orbitals and Occupation #’s

\[ J_0(r) = \frac{\delta E_{\text{int}}[\rho]}{\delta \rho(r)} \iff \left[ -\frac{\nabla^2}{2m} - J_0(x) \right] \psi_\alpha = \varepsilon_\alpha \psi_\alpha \Rightarrow \rho(x) = \sum_\alpha n_\alpha |\psi_\alpha(x)|^2 \]
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\[ \implies \mathcal{E}_{\text{DME}} = \frac{\tau}{2M} + A[\rho] + B[\rho] \tau + C[\rho] |\nabla \rho|^2 + \cdots \]

Kohn–Sham Potentials

Orbital dependent functional
Solve OPM

HFB solver

\[ J_0(r) = \frac{\delta E_{\text{int}}[\rho]}{\delta \rho(r)} \iff [-\nabla^2 - J_0(x)] \psi_\alpha = \varepsilon_\alpha \psi_\alpha \implies \rho(x) = \sum_\alpha n_\alpha |\psi_\alpha(x)|^2 \]
Validation of HFBRAD_DME Implementation

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

$$V_{\text{srg}} \lambda = 2.0 \text{ fm}^{-1} (N^3 \text{LO})$$

- Do densities look like nuclei from Skyrme EDF’s? (Yes)
New low-momentum NNN fits and Nuclear Matter

Smooth cutoff $V_{\text{low } k}$ from N$^3$LO(500)

N$^2$LO 3NF fit to $A = 3, 4$

B.E. and $^4\text{He}$ radii

self-bound w/ saturation

Loop expansion (perturbative) about HF becomes sensible

$\Lambda = 1.8 \text{ fm}^{-1}$
$\Lambda = 2.0 \text{ fm}^{-1}$
$\Lambda = 2.2 \text{ fm}^{-1}$
$\Lambda = 2.8 \text{ fm}^{-1}$

Hartree-Fock
New low-momentum NNN fits and Nuclear Matter

Λ-dependence => theoretical error bands (lower limit)

Assess the impact of large uncertainties in the $c_i$'s appearing in 2- and 3-body TPEP

Vary the order of the underlying EFT

Sensitivity to many-body approximations

**Diagram:**

- **Energy/nucleon [MeV] vs. $k_F$ [fm$^{-1}$]**
  - $V_{\text{low } k}$ NN from N$^3$LO (500 MeV)
  - 3NF fit to $E_3^H$ and $r_4^{\text{He}}$
  - $2.0 < \Lambda_{3\text{NF}} < 2.5$ fm$^{-1}$
  - 2nd order
  - Colors represent different $\Lambda$ values: $\Lambda = 1.8$ fm$^{-1}$ (green), $\Lambda = 2.0$ fm$^{-1}$ (red), $\Lambda = 2.2$ fm$^{-1}$ (purple), $\Lambda = 2.8$ fm$^{-1}$ (blue)
New low-momentum NNN fits and Nuclear Matter

Excellent saturation w/out fine-tuning to nuclear matter

1) \( V_{\text{NNN}} \Rightarrow V_{2N}(r) \)
2) HF propagators
3) Beyond 2-hole lines?
4) Angle-averaging
5) Particle-hole channel
6) …

But…

Ladder sum \( \gg \) 2nd-order

Coupled-cluster calculations of nuclear matter, \( ^{16}\text{O} \) and \( ^{40}\text{Ca} \) would be a huge help!

To do: asymmetric matter
Guidance from NM for fixing EFT couplings

Different $\Lambda$-dependence for the 2 ways of fitting the 3NF lec’s

Supports suggestion of Navratil et al. to use $^4$He radii to constrain fits of 3NF couplings ($c_E$ and $c_D$)

Large uncertainties in extracting $c_3$, $c_4$ from $\pi N$ and $NN$ => use NM to constrain (sensitivity at the 2-3 MeV level)
Sample Observations From HFBRAD\_DME

- Untuned new 3NF fits to $V_{\text{low } k}$ and SRG [$N^3\text{LO (500 MeV)}$]
- best nuclear matter $\implies ^{40}\text{Ca}$ underbound by $\approx 1 \text{ MeV/A}$

$$V_{\text{low } k} \Lambda = 2.0 \text{ fm}^{-1} \ (N^3\text{LO})$$

$$V_{\text{SRG}} \lambda = 2.0 \text{ fm}^{-1} \ (N^3\text{LO})$$

- $B$ large $\implies M_{0}^*$ low compared to Sly4. Problem?
- Does power counting support gradient expansion?
DFT Validation Against *Ab Initio* Calculations

**“Coester Lines”**
- Compare systematics, e.g., by varying 3NF coupling in Hamiltonian

**External Potentials**
- DFT from response of energy to perturbation of densities
  ➞ Apply external fields

**Graph 1:**
- Binding Energy [MeV]
- Parameters:
  - $N_{\text{CC}}$ = 2
  - $V_{\text{SRG}}[\lambda = 1.9 \text{ fm}^{-1}]$
  - $+ 3\text{NF contact only}$

**Graph 2:**
- $(E_{\text{tot}} - U_{\text{ext}})/A$ [MeV]
- Parameters:
  - $^{12}\text{C NCFC}$
  - $^8\text{He NCFC (no coul.)}$
  - $h\Omega$ of harmonic trap
  - $5 \text{ MeV}$

**Near future:** Full 3NF, more external fields, other nuclei . . .
DFT Validation Against Ab Initio Calculations

“Coester Lines”

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

External Potentials

- DFT from response of energy to perturbation of densities

⇒ Apply external fields

Near future: Full 3NF, more external fields, other nuclei . . .
Possible Reasons for the Poor Agreement

1) DME averages out too much information

- COM P-dependence (spatial non-locality)
- energy-dependence

Errors of 1 MeV/nucleon in infinite NM
Possible Reasons for the Poor Agreement

2) Gradient expansion breaks down when saturation not good

e.g., N3LO NM looks reasonable at lower densities despite poor saturation

Ab-initio results for O16 and Ca40 pretty decent, but DME is poor

Gradients no longer “small” since DME = expansion about NM?

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<th>O16</th>
<th>Ca40</th>
<th>Ca48</th>
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<td>3.35</td>
</tr>
</tbody>
</table>
Possible Reasons for the Poor Agreement

3) Errors in the Hartree contribution $\Rightarrow$ feedback via self-consistency

Exact $\rho(R + r/2)\rho(R - r/2)$

DME

Treat Hartree exactly a-la Coulomb? [Negele and Vautherin, Sprung et al.]
Possible Reasons for the Poor Agreement

4) Inadequacy of many-body approximations (I.e., LO Brueckner)

\[ \kappa = \langle \chi | \chi \rangle \]  
\[ |\chi(r)\rangle = \text{defect w.f.} \]

\[ \frac{\delta E(3\text{hole} - \text{lines})}{E(2\text{hole} - \text{lines})} \sim \kappa \]

3-hole-line correction could contribute at the few MeV level, even at low \( \Lambda \)

Coupled-cluster NM calculation to assess H.O.T. would help!

5) Approximate treatment of 3NF

\[ V_{3N} \rightarrow \text{Tr}_3 \left[ V_{3N} A_{123} \right] \sim \text{Tr}_3 \left[ V_{3N} \right] \]

6) Implementation errors in HFBRAD (rearrangement terms, etc.)
Long-Range Chiral EFT  ➔  Enhanced Skyrme

- Add long-range ($\pi$-exchange) contributions in the density matrix expansion (DME)
  - NN/NNN through N$^2$LO derived [SKB,BG]
- Refit the Skyrme parameters
- Test for sensitivities and improved observables (isotope chains)
- Spin-orbit couplings from $2\pi$ 3NF particularly interesting
- Can we “see” the pion in medium to heavy nuclei?

<table>
<thead>
<tr>
<th>Order</th>
<th>2N forces</th>
<th>3N forces</th>
<th>4N forces</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO</td>
<td>$Q^0$</td>
<td>X</td>
<td>H</td>
</tr>
<tr>
<td>NLO</td>
<td>$Q^2$</td>
<td>X</td>
<td>K</td>
</tr>
<tr>
<td>N$^2$LO</td>
<td>$Q^3$</td>
<td>K</td>
<td>X</td>
</tr>
<tr>
<td>N$^3$LO</td>
<td>$Q^4$</td>
<td>+</td>
<td>...</td>
</tr>
</tbody>
</table>
Scalar Part of Negele-Vautherin DME (NVDME)

- Compare exact and DME for angle-averaged quantities:

\[ F_{s,\text{exch}}(R, r) = \int d\Omega_r \rho_q(r_1, r_2)\rho_q(r_2, r_1) \]

- Scalar NVDME for exchange is pretty good but there is room for improvement, especially at the surface

- What about the vector part (in spin space) \( s_q \)?
Improved DME for $\int d\Omega_r \mathbf{s}_n(r_1, r_2) \cdot \mathbf{s}_n(r_2, r_1)$ [B.G. et al.]
Improved DME for $\int d\Omega_r \mathbf{s}_n(r_1, r_2) \cdot \mathbf{s}_n(r_2, r_1)$ [B.G. et al.]
Consider Hartree-Fock with One-Pion Exchange

- NV used a different approach from the scalar expansion:

\[ s_q(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2)^{\text{NVDME}} \rightarrow i \frac{j_0(rk_F)}{2} \mathbf{r} \times \mathbf{J}_q(\mathbf{R}) \]

- Look at \( \int d\mathbf{r} \, d\mathbf{R} \, V_{1\pi}(r) \mathbf{s}_n(\mathbf{r}_1, \mathbf{r}_2) \cdot \mathbf{s}_n(\mathbf{r}_2, \mathbf{r}_1) \):
Consider Hartree-Fock with One-Pion Exchange

- NV used a different approach from the scalar expansion:

\[ s_q(R + r/2, R - r/2) \xrightarrow{\text{NVDME}} \frac{i}{2} j_0(rk_F) \mathbf{r} \times \mathbf{J}_q(R) \]

- Look at \( \int dr \, dR \, V_{1\pi}(r) \mathbf{s}_n(r_1, r_2) \cdot \mathbf{s}_n(r_2, r_1) \):

- BG et al.: use phase-space averaging for finite nuclei
Overview: UNEDF project and Ab Initio DFT

Current Status and Possible Problems

Outlook and Additional Issues for Nuclear DFT

Extras
(Some) Important Issues for Nuclear DFT

- DFT for self-bound systems
  - Does DFT even exist? (HK theorem for intrinsic states?)
  - Effective actions: symmetry breaking and zero modes
- Game plans proposed:
  - J. Engel: find intrinsic functional (one-d boson system)
  - B. Giraud et al.: use harmonic oscillator trap
  - J. Braun et al.: deal with soliton zero modes using Fadeev-Popov method [e.g., Calzetta/Hu cond-mat/0508240]
- Organization about mean field: need convergent expansion
  - Need freedom to choose background field to fix density
  - Can DFT deal with nuclear short-range correlations?
  - Claim: need low-momentum interactions ($\chi_{\text{EFT}} \rightarrow V_{\text{low } k}$)
- Effectiveness of approximations (e.g., DME)
- What about single-particle spectra?
  - Connect to Green’s function formulation?
  - Bartlett claims good reproduction for Coulomb systems
- How to best deal with long-range correlations? pairing?
- Alternative functionals (e.g., T. Papenbrock)
Outline

Overview: UNEDF project and Ab Initio DFT

Current Status and Possible Problems

Outlook and Additional Issues for Nuclear DFT

Extras
Content of Extras

- Misconceptions
- DFT from perturbative chiral interactions + DME (Kaiser et al.)
- DFT from RG (Jens Braun)
- Non-empirical pairing functional for nuclei
- Power counting in functionals
- BBG and G-matrix
Misconceptions vs. Correct Interpretations

- DFT is a Hartree-(Fock) approximation to an effective interaction
  - DFT can accomodate *all* correlations in principle, but in practice they may be included perturbatively (which can fail for some $V$’s)
- Nuclear matter is strongly nonperturbative in the potential
  - “perturbativeness” is highly resolution dependent
- (Fill in the blank) is responsible for nuclear saturation
  - another resolution-dependent inference
- Evolving low-momentum interactions loses important information
  - long-range physics is preserved
  - relevant short-range physics encoded in potential
- Low-momentum NN potentials are just like G-matrices
  - important distinction: conventional G-matrix still has high-momentum, off-diagonal matrix elements
DFT from Perturbative Chiral Interactions + DME

- N. Kaiser et al. in ongoing series of papers (nucl-th/0212049, 0312058, 0312059, 0406038, 0407116, 0509040, 0601100, ...)

- Fourier transform of expanded density matrix defines a momentum-space medium insertion, leading to EDF:

- Three-body forces from explicit $\Delta$, e.g.,

- Perturbative expansion for energy tuned to nuclear matter

- Many analytic results $\Longrightarrow$ qualitative insight, checks for quantitative calculations with low-momentum interactions
Density Functional RG for Nuclei

Density Functional: \( \Gamma_\lambda[\rho] = \ln \int \mathcal{D}\psi\,\mathcal{D}\psi' e^{-S_\lambda[\psi^\dagger,\psi]} + \int \frac{\delta\Gamma_\lambda}{\delta \rho} \cdot (\psi^\dagger \psi) \)

\[ S_\lambda[\psi^\dagger, \psi] = \int \psi^\dagger \left[ \partial_t - \frac{1}{2m} \Delta + (1 - \lambda) U_\lambda \right] \psi + \frac{1}{2} \int \psi^\dagger \psi \lambda V_{\text{low } k} \psi^\dagger \psi + (\lambda V_{3N} \text{ will be included later}) \]

- Density basis expansion scales favorably to heavy nuclei
- Allows for a calculation of ground-state energy and density from nuclear forces
- In production: results for \(^{16}\text{O}\)

Example: RG flow of the ground-state density for 1d model ("smeared-out" \( \delta \)-function interaction)
Observables Sensitive to 3N Interactions?

- Study systematics along isotopic chains
- Example: kink in radius shift \( \langle r^2 \rangle (A) - \langle r^2 \rangle (208) \)

- Associated phenomenologically with behavior of spin-orbit
  - isoscalar to isovector ratio fixed in original Skyrme
- Clues from chiral EFT contributions?
  - Kaiser et al.: ratio of isoscalar to isovector spin-orbit
Non-Empirical Pairing Functional for Nuclei
T. Duguet (Saclay); T. Lesinski, K. Bennaceur, J. Meyer (Lyon)

- New spherical code BSLHFB
  - spherical Bessel function basis
  - finite-range / non-local pairing interactions in EDF
  - operator representation: sum of separable terms (rank 2 for $V_{\text{low } k}$)

- Pairing at lowest order in NN (nuclear + Coulomb)
  - use $V_{\text{low } k}$ at $\Lambda \approx 2 \text{ fm}^{-1}$ as NN pairing interaction
  - Use SLY5 Skyrme for ph EDF with fixed $m_0^*/m = 0.7$

- Studied $m^*(k, k_F)$ for cutoffs $\Lambda$ (K. Hebeler, T.D., A. Schwenkenk)
  - consistent ph/pp scales needed
  - $V_{\text{low } k}$ ok with $m_{\text{Skryme}}(k_F)$
Pairing Gaps from $V_{\text{low } k} + \text{Coulomb Near Data!}$

Current limitations
- Three-body force missing
- No density/spin/isospin fluctuations (Milan: +40%!?)
- Phenom. ph functional and momentum-independent $m_0^*$

Upgrade plans
- Other observables (Lesinski), deformed nuclei (Rotival)
- Incorporate NNN (Lesinski)
- Check fluctuations
- Construct ph part (BG, VR)
Power Counting in Skyrme and RMF Functionals?

- Old NDA analysis: [Friar et al., rjf et al.]
  \[ c \left( \psi \psi^\dagger \right)^l \left[ \frac{\nabla}{\Lambda} \right]^n \left( f_\pi^2 \Lambda \right)^2 \]
  \[ \rho \leftrightarrow \psi \psi^\dagger \]
  \[ \tau \leftrightarrow \nabla \psi \psi^\dagger \cdot \nabla \psi \]
  \[ J \leftrightarrow \psi \psi^\dagger \nabla \psi \]

- Density expansion?
  \[ \frac{1}{7} \leq \frac{\rho_0}{f_\pi^2 \Lambda} \leq \frac{1}{4} \]
  for \( 1000 \geq \Lambda \geq 500 \)

\[ k_F = 1.35 \text{ fm}^{-1} \]

\[ e_0 \]

\[ \text{natural (\( \Lambda=600 \text{ MeV} \))} \]

\[ \text{Skyrme \( \rho^n \)} \]

\[ \text{RMFT-II \( \rho^n \) net} \]

\[ \text{RMFT-I \( \rho^n \) net} \]
Bethe-Brueckner-Goldstone Power Counting

Strong short-range repulsion $\implies$ Sum $V$ ladders $\implies$ $G$

$V_{\text{low } k}$ momentum dependence + phase space $\implies$ perturbative
Bethe-Brueckner-Goldstone Power Counting

Strong short-range repulsion
\[ \implies \text{Sum } V \text{ ladders } \implies G \]

\[ V_{\text{low } k} \text{ momentum dependence + phase space } \implies \text{perturbative} \]

\( \Lambda: |\mathbf{P}/2 \pm \mathbf{k}| > k_F \text{ and } |\mathbf{k}| < \Lambda \)

\( F: |\mathbf{P}/2 \pm \mathbf{k}| < k_F \)

\begin{align*}
\text{N}^3\text{LO} [600 \text{ MeV}] \\
\lambda = 2.0 \text{ fm}^{-1} \\
\Lambda = 2.0 \text{ fm}^{-1} 
\end{align*}
Compare Potential and G Matrix: AV18

1S0 bare potential

1S0 SRG potential

1S0 bare G Matrix, E=-207.4

1S0 SRG G Matrix, E=-207.4
Compare Potential and G Matrix: AV18

1S0 bare potential

1S0 SRG potential

1S0 bare G Matrix, E=23.0

1S0 SRG G Matrix, E=23.0
Compare Potential and G Matrix: AV18

3S1 bare potential

3S1 SRG potential

3S1 bare G Matrix, E=-207.4

3S1 SRG G Matrix, E=-207.4
Compare Potential and G Matrix: AV18
Compare Potential and G Matrix: N\(^3\)LO (500 MeV)
Compare Potential and G Matrix: $N^3$LO (500 MeV)
Compare Potential and G Matrix: $N^3$LO (500 MeV)
Compare Potential and G Matrix: $N^3$LO (500 MeV)
Hole-Line Expansion Revisited (Bethe, Day, ...)

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

  ![Fourth-order diagrams](image)

  ![Third-order diagram](image)

- "Conventional" $G$ matrix still couples low-$k$ and high-$k$
  - add a hole line $\Rightarrow$ ratio $\approx \sum_{n \leq k_F} \langle bn | (1/e)G | bn \rangle \approx \kappa \approx 0.15$
  - no new hole line $\Rightarrow$ ratio $\approx -\chi(r = 0) \approx -1 \Rightarrow$ sum all orders

- Low-momentum potentials decouple low-$k$ and high-$k$
  - add a hole line $\Rightarrow$ still suppressed
  - no new hole line $\Rightarrow$ also suppressed (limited phase space)
  - freedom to choose single-particle $U$ $\Rightarrow$ use for Kohn-Sham

Result: functional density (DFT) should work
Comparison to ab-initio calculations

Start from *the same* Hamiltonian and compare ab initio solution to the Microscopic DFT calculation based on the DME functional.

CC or FCI calculations of nuclei and nuclei in external fields \([\text{energies, densities, density matrices,}...\])

How important is non-locality and how accurate is the DME?

Are systematics reproduced by DME as we vary parameters (e.g., 3NF couplings, RG cutoff \(\Lambda\), order of input EFT, ...) in \(H\)?

Is the many-body treatment of nuclear matter sufficient?

Early indications are that non-trivial extensions of the DME are needed [see B. Gebremariam and J. Drut later]
Comparison to ab-initio calculations

CC and DFT calculations of $^{16}\text{O}$ (w/3N contact of varying strength)

Quantitative and qualitative disagreement btw. coupled-cluster and DFT calculation. What is going on?