Non-empirical energy functionals from low-momentum interactions
I. Introduction to Energy Density Functional methods

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Lecture series

Outline

- Introduction to energy density functional methods
  - Basics of formalism
  - Empirical energy functionals: form, performances and limitations
  - Towards non-empirical energy functionals
- Low-momentum interactions from renormalization group methods
- The building of non-empirical energy functionals
Take-away message

Theoretical methods

- Ab-initio methods = $A$-body problem solved in terms of vacuum $H(\Lambda)$
- Ab-initio methods limited to $A \leq 16$ plus a few doubly-magic nuclei
- Approaches to heavier nuclei need to be benchmarked by ab-initio methods

Energy density functional method

- Two successive levels of implementation: single reference and multi reference
- Empirical energy functionals successful but lack predictive power
- Need to connect the energy functional to vacuum $H(\Lambda) = \text{non-empirical EDF}$
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1 Introduction
   - Basic facts about low-energy nuclear physics
   - Theoretical methods

2 Energy density functional methods
   - Sketch of the overall EDF formalism
   - Single-reference implementation: elements of formalism
   - Empirical energy functionals
   - Performances and limitations
   - Towards non-empirical energy functionals

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What is low-energy nuclear physics interested in?

In generic terms

- **Spectrum** of $H |\Psi_i^A\rangle = E_i^A |\Psi_i^A\rangle$ for all $A = N + Z$
- Observables for each state, e.g. $r^2 \equiv \langle \Psi_i^A | \sum_k A \hat{r}_k^2 |\Psi_i^A\rangle / A$
- **Decays** between $|\Psi_i\rangle$, i.e. nuclear, electromagnetic, electro-weak

Ground state

- Mass, deformation

Spectroscopy

- Excitations modes

Limits

- Drip-lines, halos

Reaction properties

- Fusion, transfer...

Heavy elements

- Fission, fusion, SHE

Astrophysics

- NS, SN, r-process
How does that translate to low-energy nuclear theory?

Goals for low-energy nuclear theory

- Model the unknown nuclear Hamiltonian $H$
- Solve $A$-body problem and describe properties of nuclei
- Understand states of nuclear matter in astrophysical environments
How does that translate to low-energy nuclear theory?

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Which theoretical method(s)?

Ab-initio methods

- Solve the N-body problem in terms of point-like nucleons $+ H(\Lambda)$

<table>
<thead>
<tr>
<th>Name</th>
<th>Short description</th>
<th>Variational</th>
<th>Scale as</th>
<th>Up to</th>
</tr>
</thead>
<tbody>
<tr>
<td>Few-body (Faddeev...)</td>
<td>$H \Psi = E \Psi$</td>
<td>Yes</td>
<td>$M^A$</td>
<td>$A = 2-4$</td>
</tr>
<tr>
<td>Green-Function</td>
<td>$\Psi(\tau) = e^{-(H-E)\tau} \Psi_T$, GFMC</td>
<td>Yes</td>
<td>$\frac{M!}{(M-A)!A!}$</td>
<td>$A &lt; 12$</td>
</tr>
<tr>
<td>No-core Shell Model</td>
<td>$H \Psi = E \Psi$</td>
<td>Yes</td>
<td>$4^A$</td>
<td>$A &lt; 16$</td>
</tr>
<tr>
<td>Coupled-Cluster (CC)</td>
<td>$</td>
<td>\Psi\rangle = e^S</td>
<td>\Psi_0\rangle$</td>
<td>No</td>
</tr>
</tbody>
</table>

M : configuration space size

- Limited reach over the mass table

From D. Lacroix
Which theoretical method(s)?

- No “one size fits all” theory for nuclei
- All theoretical approaches need to be linked

Low-momentum interactions
Introduction

1. Basic facts about low-energy nuclear physics
2. Theoretical methods

Energy density functional methods

2.1. Sketch of the overall EDF formalism
2.2. Single-reference implementation: elements of formalism
2.3. Empirical energy functionals
2.4. Performances and limitations
2.5. Towards non-empirical energy functionals

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Energy Density Functional method

Basic elements

- Approaches not based on a correlated wave-function
- Energy is postulated to be a functional of one-body density (matrices)
- Symmetry breaking is at the heart of the method
- Two formulations (i) Single-Reference (ii) Multi-Reference

Pros

- Use of full single-particle space
- Collective picture but fully quantal
- Universality of the EDF ($A \gtrsim 16$)
- Ground-state description
- Smoothly varying correlations

Difficulties

- No universal parametrization
- Empirical $\neq$ predictive power
- Spectroscopy
- Fluctuating correlations with $A$
- Limited accuracy ($\sigma_{2135}^{mass} \approx 700$ keV)

Low-momentum interactions
# Energy Density Functional method

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Energy Density Functional method

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- No universal parametrization
- Empirical ≠ predictive power
- Spectroscopy
- Fluctuating correlations with $A$
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Energy Density Functional method: single-reference implementation

One auxiliary vacuum $|\Phi\rangle$

$$E = \mathcal{E}[\rho, \kappa, \kappa^*]$$

\begin{align*}
\rho_{ij} &= \frac{\langle \Phi | a_j^\dagger a_i | \Phi \rangle}{\langle \Phi | \Phi \rangle} \\
\kappa_{ij} &= \frac{\langle \Phi | a_j a_i | \Phi \rangle}{\langle \Phi | \Phi \rangle} \\
\kappa_{ij}^* &= \frac{\langle \Phi | a_j^\dagger a_j^\dagger | \Phi \rangle}{\langle \Phi | \Phi \rangle}
\end{align*}

Correlations

- "Bulk" $\sim 800$ MeV
- "Static deformation" $\sim 20$ MeV

Broken symmetries

$N, Z, \tilde{P}, J^2, J_Z, \Pi, T^2$

Hartree-Fock-Bogoliubov

- Binding energies
- Shell structure
- Pairing gap
- Fission barriers
- Individual excitation
- Rotational excitation

Transition probabilities

- Selection rules lost

Low-momentum interactions
Energy Density Functional method: multi-reference implementation

Correlations
- "Collective fluctuations" \( \sim 4 \) MeV

\[ E = \sum_{AB} f_{AB} \mathcal{E}[\rho^{AB}, \kappa^{AB}, \kappa^{BA*}] \]

Set of auxiliary vacua \( \{|\Phi_A\rangle\} \)

\[ \rho_{ij}^{AB} = \frac{\langle \Phi_A|a_j^\dagger a_i|\Phi_B\rangle}{\langle \Phi_A|\Phi_B\rangle} \]

\[ \kappa_{ij}^{AB} = \frac{\langle \Phi_A|a_j^\dagger a_i|\Phi_B\rangle}{\langle \Phi_A|\Phi_B\rangle} \]

\[ \kappa_{ij}^{BA*} = \frac{\langle \Phi_A|a_i^\dagger a_j^\dagger|\Phi_B\rangle}{\langle \Phi_A|\Phi_B\rangle} \]

Symmetry restorations
- \( N, Z, \bar{P}, J^2, J_Z, \Pi, T^2 \)

Generator Coordinate Method
- \( \Delta_N, \Delta_Z, Q_{20}, Q_{30}, \cdots \)

Transition probabilities
- Selection rules restored

\[ \epsilon[\rho, \kappa, \kappa^*; |q|] \]

Harmonic limit
- QRPA
- Bohr Hamiltonian

Observables
- Same as SR
- Vibration excitations
- Rotational bands of transitional nuclei
- LACM and shape coexistence

Low-momentum interactions
Energy Density Functional method: some relevant questions

- $\mathcal{E}[\rho, \kappa, \kappa^*]$ built empirically so far
- Effective separation of scales for correlations
  - Bulk $\sim 800$ Mev $\propto A$
  - Collective def. $\leq 20$ Mev $= F(N_{val}, G_{deg})$
  - Collective fluct. $\leq 4$ MeV $= G(N_{val}, G_{deg})$
- Observables impacted by correlation
  - Symmetry breaking
  - Collective fluctuation

Non empirical?
- What form of vacuum $H$?
- Can we relate $\mathcal{E}[\rho, \kappa, \kappa^*]$ to $H$?
- Needed to go through $V_{eff}$?
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Elements of formalism

\[ \mathcal{E}[\rho, \kappa^*, \kappa] = \text{functional of one-body density matrices} \]

\[ \rho_{ji} \equiv \langle \Phi | b_{i}^{\dagger} b_{j} | \Phi \rangle ; \quad \kappa_{ji} \equiv \langle \Phi | b_{i} b_{j} | \Phi \rangle \]

defined in an arbitrary single-particle basis \( \{ b_{i}^{\dagger}; b_{i} \} \)
Single-reference EDF method

Elements of formalism

- $\mathcal{E}[\rho, \kappa^*, \kappa] =$ functional of one-body density matrices

- $|\Phi\rangle =$ auxiliary symmetry-breaking product state of reference

\[
|\Phi\rangle \equiv \prod_i \beta_i |0\rangle \\
\beta_i \equiv \sum_j U_{ji} b_j + V_{ji} b_j^+ \\
\text{and is a vacuum, i.e. } \beta_i |\Phi\rangle = 0 \ \forall i
\]

Low-momentum interactions
Single-reference EDF method

Elements of formalism

- $\mathcal{E}[\rho, \kappa^*, \kappa] = \text{functional of one-body density matrices}$
- $|\Phi\rangle = \text{auxiliary symmetry-breaking product state of reference}$
- Minimizing $\mathcal{E}[\rho, \kappa^*, \kappa]$ leads to Hartree-Fock-Bogoliubov-like equations

\[
\begin{pmatrix}
  h - \lambda & \Delta \\
  -\Delta^* & -h^* + \lambda
\end{pmatrix}
\begin{pmatrix}
  U_i \\
  V_i
\end{pmatrix}
= E_i
\begin{pmatrix}
  U_i \\
  V_i
\end{pmatrix}
\]

- Effective potentials and vertices are defined through

\[
h_{ij} \equiv \frac{\delta \mathcal{E}}{\delta \rho_{ji}} \equiv t_{ij} + \sum_{kl} \overline{v}_{ikjl}^p \rho_{lk} \quad ; \quad \Delta_{ij} \equiv \frac{\delta \mathcal{E}}{\delta \kappa_{ij}^*} \equiv \frac{1}{2} \sum_{kl} \overline{v}_{ijkl}^{pp} \kappa_{kl}
\]

- $\overline{v}^{ph} / \overline{v}^{pp} = \text{Consistent many-body expansion in terms of NN/NNN}$
- Quasiparticle w.f. $(U_i, V_i)$, energy $E_i$, densities...
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Empirical parameterizations of $\mathcal{E}[\rho, \kappa, \kappa^*]$; e.g. Skyrme or Gogny

Local Skyrme EDF for even-even nuclei ground-state

- Density matrices expressed in position $\otimes$ spin $\otimes$ isospin s.p. basis

  \[
  \rho_{\bar{r}\sigma q \bar{r}' \sigma' q} \equiv \langle \Phi | c^\dagger (\bar{r}' \sigma' q) c(\bar{r} \sigma q) | \Phi \rangle
  \]

  \[
  \kappa_{\bar{r}\sigma q \bar{r}' \sigma' q} \equiv \langle \Phi | c(\bar{r}' \sigma' q) c(\bar{r} \sigma q) | \Phi \rangle
  \]

- Local densities

  \[
  \rho_q(\bar{r}) \equiv \sum_\sigma \rho_{\bar{r}\sigma q \bar{r} \sigma q}
  \]

  Matter

  \[
  \tau_q(\bar{r}) \equiv \sum_\sigma \nabla \cdot \nabla' \rho_{\bar{r}\sigma q \bar{r}' \sigma q} \bigg|_{\bar{r}=\bar{r}'}
  \]

  Kinetic

  \[
  J_{q,\mu\nu}(\bar{r}) \equiv \frac{i}{2} \sum_{\sigma\sigma'} (\nabla' - \nabla)_\mu \rho_{\bar{r}\sigma q \bar{r}' \sigma' q}^\sigma' \sigma \bigg|_{\bar{r}=\bar{r}'}
  \]

  Spin-current tensor

  \[
  J_{q,\kappa}(\bar{r}) \equiv \sum_{\mu,\nu=x} \epsilon_{\kappa\mu\nu} J_{q,\mu\nu}(\bar{r})
  \]

  Spin-orbit

  \[
  \tilde{\rho}_q(\bar{r}) \equiv \sum_\sigma \kappa_{\bar{r}\sigma q \bar{r} \sigma q}^\sigma \sigma_z \bar{\sigma}
  \]

  Pair

- Build scalar EDF from such densities, e.g. at 2$\text{nd}$ order in $\sigma_\nu$ and $\nabla$

Low-momentum interactions
Empirical parameterizations of $\mathcal{E}[\rho, \kappa, \kappa^*]$; e.g. Skyrme or Gogny

**Local Skyrme EDF for even-even nuclei ground-state**

- Universal form ($A \gtrsim 16$) but no universal parametrization

$$
\mathcal{E}[\rho, \kappa, \kappa^*] = \sum_{qq'} \int d\vec{r} \left[ C^{\rho \rho}_{qq'} \rho_q(\vec{r}) \rho_{q'}(\vec{r}) + C^{\rho \Delta \rho}_{qq'} \rho_q(\vec{r}) \Delta \rho_{q'}(\vec{r}) + C^{\rho \tau}_{qq'} \rho_q(\vec{r}) \tau_{q'}(\vec{r}) \\
+ C^{\rho \nabla \cdot J}_{qq'} \rho_q(\vec{r}) \vec{v} \cdot \vec{J}_{q'}(\vec{r}) + C^{JJ_c}_{qq'} \sum_{\mu, \nu = x}^z J_{q, \mu \nu}(\vec{r}) J_{q', \mu \nu}(\vec{r}) \\
+ C^{JJ_t}_{qq'} \sum_{\mu, \nu = x}^z \left[ J_{q, \mu \nu}(\vec{r}) J_{q', \nu \mu}(\vec{r}) + J_{q, \mu \nu}(\vec{r}) J_{q', \nu \mu}(\vec{r}) \right] \right] \\
+ \sum_q \int d\vec{r} C^{\rho \bar{\rho}}_{qq} |\bar{\rho}_q(\vec{r})|^2 + \text{additional terms involving gradients}
$$

- Density-dependent couplings, i.e. $C^{ff'}_{qq'}$ may depend on $\vec{r}$ as well
- Fitted on INM OES and selection of finite nuclei data
- Usually derived from the density-dependent Skyrme+DDD "interaction"
Empirical parameterizations of $\mathcal{E}[\rho, \kappa, \kappa^*]$; e.g. Skyrme or Gogny

Local Skyrme EDF for even-even nuclei ground-state

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\[
\mathcal{E}[\rho, \kappa, \kappa^*] = \sum_{qq'} \int d\vec{r} \left[ C_{qq'}^{\rho\rho} \rho_q(\vec{r}) \rho_{q'}(\vec{r}) + C_{qq'}^{\rho\Delta\rho} \rho_q(\vec{r}) \Delta \rho_{q'}(\vec{r}) + C_{qq'}^{\rho\tau} \rho_q(\vec{r}) \tau_{q'}(\vec{r}) \right. \\
+ \left. C_{qq'}^{\rho \nabla J} \rho_q(\vec{r}) \nabla \cdot \vec{J}_{q'}(\vec{r}) + C_{qq'}^{JJ_c} \sum_{\mu, \nu = x}^z J_{q,\mu\nu}(\vec{r}) J_{q',\mu\nu}(\vec{r}) \right. \\
+ \left. C_{qq'}^{JJ_t} \sum_{\mu, \nu = x}^z \left[ J_{q,\mu\mu}(\vec{r}) J_{q',\nu\nu}(\vec{r}) + J_{q,\mu\nu}(\vec{r}) J_{q',\nu\mu}(\vec{r}) \right] \right]
\]

\[+ \sum_q \int d\vec{r} \, C_{qq}^{\tilde{\rho}\tilde{\rho}} |\tilde{\rho}_q(\vec{r})|^2 + \text{additional terms involving gradients}\]

- Density-dependent couplings, i.e. $C_{qq'}^{ff'}$ may depend on $\vec{r}$ as well
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- Usually derived from the density-dependent Skyrme+DDD "interaction"
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Local Skyrme EDF for even-even nuclei ground-state

- Universal form ($A \gtrsim 16$) but no universal parametrization

$$E[\rho, \kappa, \kappa^*] = \sum_{qq'} \int d\vec{r} \left[ C_{qq'}^{\rho_\rho} \rho_q(\vec{r}) \rho_{q'}(\vec{r}) + C_{qq'}^{\rho_\Delta} \rho_q(\vec{r}) \Delta \rho_{q'}(\vec{r}) + C_{qq'}^{\rho_\tau} \rho_q(\vec{r}) \tau_{q'}(\vec{r}) \right. $$

$$+ C_{qq'}^{\rho_\nabla J} \rho_q(\vec{r}) \nabla \cdot \vec{J}_{q'}(\vec{r}) + C_{qq'}^{JJ_c} \sum_{\mu, \nu = x} J_q,\mu \nu(\vec{r}) J_{q'},\mu \nu(\vec{r}) \bigg]$$

$$+ C_{qq'}^{JJ_t} \sum_{\mu, \nu = x} \left[ J_q,\mu \mu(\vec{r}) J_{q'},\nu \nu(\vec{r}) + J_q,\mu \nu(\vec{r}) J_{q'},\nu \mu(\vec{r}) \right] \bigg]$$

$$+ \sum_q \int d\vec{r} C_{qq}^{\tilde{\rho} \tilde{\rho}} |\tilde{\rho}_q(\vec{r})|^2 + \text{additional terms involving gradients}$$

- Density-dependent couplings, i.e. $C_{qq'}^{eff}$ may depend on $\vec{r}$ as well
- Fitted on INM OES and selection of finite nuclei data
- Usually derived from the density-dependent Skyrme+DDD "interaction"
Empirical parameterizations of $\mathcal{E}[\rho, \kappa, \kappa^*]$; e.g. Skyrme or Gogny

Density-dependent Skyrme "force" for the particle-hole part

- Schematic effective vertex, i.e. a convenient intermediate to generate $\mathcal{E}^{\rho\rho 1+\alpha}$

$$
\begin{align*}
\nu_{\text{cent}} &= \ t_0 \ (1 + x_0 P_\sigma) \ \delta(\vec{r}) \\
&+ \ \frac{1}{2} \ t_1 \ (1 + x_1 P_\sigma) \ [\delta(\vec{r}) \ \vec{k}'^2 + \vec{k}'^2 \ \delta(\vec{r})] \\
&+ \ \ t_2 \ (1 + x_2 P_\sigma) \ \vec{k}' \cdot \delta(\vec{r}) \ \vec{k} \\
&+ \ \frac{1}{6} \ t_3 \ (1 + x_3 P_\sigma) \ \rho_0^\alpha(\vec{r}) \ \delta(\vec{r})
\end{align*}
$$

$$
\begin{align*}
\nu_{\text{ls}} &= \ i W_0 \ (\vec{\sigma}_1 + \vec{\sigma}_2) \ \vec{k}' \wedge \delta(\vec{r}) \ \vec{k} \\
\nu_{\text{tens}} &= \ \frac{t_e}{2} \ \left\{ \left[ 3 (\vec{\sigma}_1 \cdot \vec{k}') (\vec{\sigma}_2 \cdot \vec{k}') - (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \ \vec{k}'^2 \right] \ \delta(\vec{r}) \\
&+ \ \delta(\vec{r}) \ \left[ 3 (\vec{\sigma}_1 \cdot \vec{k}) (\vec{\sigma}_2 \cdot \vec{k}) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \ \vec{k}^2 \right] \right\} \\
&+ \ \ t_o \ \left\{ 3 (\vec{\sigma}_1 \cdot \vec{k}') \ \delta(\vec{r}) (\vec{\sigma}_2 \cdot \vec{k}) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \ \vec{k}' \cdot \delta(\vec{r}) \ \vec{k} \right\}
\end{align*}
$$

- Only $C_{\rho\rho}^\rho_{\alpha\alpha'}$ depends on the density
Empirical parameterizations of $\mathcal{E}[\rho, \kappa, \kappa^*]$; e.g. Skyrme or Gogny

### Density-dependent Skyrme "force" for the particle-hole part

- Schematic effective vertex, i.e. a convenient intermediate to generate $\mathcal{E}^{\rho\rho^{1+\alpha}}$

### Density-dependent delta "interaction" for the particle-particle part

- Schematic effective vertex, i.e. a convenient intermediate to generate $\mathcal{E}^{\kappa\kappa}$

\[
\tilde{v}_{\text{cent}} = \frac{1}{2} \tilde{t}_0 \left( 1 - \eta \frac{\rho_0(\vec{r})}{\rho_{\text{sat}}} \right) (1 - P_{\sigma}) \delta(\vec{r})
\]

- $C_{qq}^{\tilde{\rho}\tilde{\rho}}(\vec{r})$ is constant over the "Volume" ($\eta = 0$) or "Surface"-peaked ($\eta = 1$)

- Pairing correlations
  - Are characterized by the dependence of the EDF on $\kappa/\tilde{\rho}$
  - Are responsible for the superfluid nature of (most of the) nuclei
  - Impact low-energy properties of finite nuclei and neutron stars
  - Reflect (mostly) the strong NN attraction in the $^1S_0$ channel

Low-momentum interactions
Empirical parameterizations of $\mathcal{E}[\rho, \kappa, \kappa^*]$; e.g. Skyrme or Gogny

### Density-dependent Skyrme "force" for the particle-hole part
- Schematic effective vertex, i.e. a convenient intermediate to generate $\mathcal{E}^{\rho_1+\alpha}$

### Density-dependent delta "interaction" for the particle-particle part
- Schematic effective vertex, i.e. a convenient intermediate to generate $\mathcal{E}^{\kappa\kappa}$

### Energy density functional $\mathcal{E}[\rho, \kappa, \kappa^*]$
- **Does NOT mimic a Hartree-Fock approximation in terms of NN+NNN**
- **Mocks up correlations BEYOND Hartree-Fock (see Lecture 3)**
  - Through rich (enough?) functional form
  - Through fitting of parameters
- **Not all correlations are easily resummed into $\mathcal{E}[\rho, \kappa, \kappa^*]$ itself**
  - Symmetry breaking captures important correlations
  - Need for explicit configuration mixing = Multi-reference EDF method
Single-particle field $h^q$

$h^q$ from the Skyrme EDF

$$h_{ij}^q \equiv \frac{\delta E}{\delta \rho_{ji}^q} = \int d\tilde{r} \, \varphi_i^+(\tilde{r}) \, h^q(\tilde{r}) \, \varphi_j(\tilde{r})$$

where the local field takes the form

$$h_q(\tilde{r}) \equiv -\nabla \cdot B_q(\tilde{r}) \nabla + U_q(\tilde{r}) - \frac{i}{2} \sum_{\mu,\nu=x}^z \left[ W_{q,\mu\nu}(\tilde{r}) \nabla_\mu + \nabla_\mu W_{q,\mu\nu}(\tilde{r}) \right] \sigma_\nu$$

with multiplicative potentials defined as

$$U_q(\tilde{r}) \equiv \frac{\delta E}{\delta \rho^q(\tilde{r})}$$

$$B_q(\tilde{r}) \equiv \frac{\delta E}{\delta \tau^q(\tilde{r})}$$

$$W_{q,\mu\nu}(\tilde{r}) \equiv \frac{\delta E}{\delta J_{q,\mu\nu}(\tilde{r})}$$

Low-momentum interactions
Single-particle field $h^q$

$h^q$ drives the correlated (!) s.p. motion

- $h^q$ provides the "shell structure"
  \[
  h^q(\vec{r'}) \varphi_i(\vec{r'}) \equiv \epsilon_i \varphi_i(\vec{r'})
  \]

  Separation energies
  - $\epsilon_p \approx \mathcal{E}_p^{N+1} - \mathcal{E}_0^N \approx E_p^{N+1} - E_0^N$
  - $\epsilon_h \approx \mathcal{E}_0^N - \mathcal{E}_h^{N-1} \approx E_0^N - E_h^{N-1}$

  Excitation energies
  - $\epsilon_p - \epsilon_h \approx \mathcal{E}_{ph}^N - \mathcal{E}_0^N \approx E_{ph}^N - E_0^N$

- Keep in mind missing correlations
  - Symmetry breaking
    - Pairing via breaking of $N$
    - Quadrupole via breaking of $J^2$
  - Configuration mixing
    - Symmetry restorations
    - Dynamical part-vib coupling

Low-momentum interactions
Pairing field $\Delta^q$

$\Delta^q_{ij} \equiv \frac{\delta \mathcal{E}}{\delta \kappa^q_{ij}} = \int d\vec{r} \left[ \varphi_i^\dagger(\vec{r} q) \Delta_q(\vec{r}) \varphi_j^*(\vec{r} q) - \varphi_j^\dagger(\vec{r} q) \Delta_q(\vec{r}) \varphi_i^*(\vec{r} q) \right]$ where the local field takes the form

$\Delta_q(\vec{r}) = -\tilde{U}_q(\vec{r}) i \sigma_y + \cdots$

with multiplicative potentials defined as

$\tilde{U}_q(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta \tilde{\rho}_q^*(\vec{r})}$

\[ ... \]

- UV divergence of local pairing EDF must be regularized/renormalized
Pairing field $\Delta^q$

$\Delta^q$ drives pair scattering

- Correlates nucleon pairs in time-reversal states
- Results in smoothed-out single-particle occupations (canonical basis)

\[
\rho_{ii} = v_i^2 = \frac{1}{2} \left[ 1 - \frac{\epsilon_i - \epsilon_F}{\sqrt{(\epsilon_i - \epsilon_F)^2 + \Delta_{ii}^2}} \right]
\]
Hartree-Fock-Bogoliubov scheme

Hartree-Fock-Bogoliubov eigenvalue problem

- Modified $v_i^2$ feedback onto $h^q$ which feedbacks onto pair scattering...

![Diagram of the Hartree-Fock-Bogoliubov scheme]

- Quasi-particle energy $E_i \approx \sqrt{(\epsilon_i - \epsilon_F)^2 + \Delta_{ii}^2} \geq \Delta_F$

Low-momentum interactions
Hartree-Fock-Bogoliubov scheme

Hartree-Fock-Bogoliubov eigenvalue problem

- Pairing changes the nature of elementary excitations $|\Phi_{ij}\rangle = \beta_i^\dagger \beta_j^\dagger |\Phi\rangle$

$$\mathcal{E}_{ij}^{\langle N \rangle} - \mathcal{E}_0^{\langle N \rangle} = E_i + E_j \xrightarrow{\Delta=0} |\epsilon_p - \epsilon_F| + |\epsilon_h - \epsilon_F| = \epsilon_p - \epsilon_h$$

- Spectrum $E_i$ versus $|\epsilon_i - \epsilon_F|$ with
  - $\Delta = 0$: SP
  - $\Delta = 0$: QP
  - $\Delta \neq 0$

- Gap opens at low energy + mix of hole- and particle-like excitations

Low-momentum interactions
Outline

1. Introduction
   - Basic facts about low-energy nuclear physics
   - Theoretical methods

2. Energy density functional methods
   - Sketch of the overall EDF formalism
   - Single-reference implementation: elements of formalism
   - Empirical energy functionals
   - Performances and limitations
   - Towards non-empirical energy functionals

3. Bibliography
Performance of empirical EDFs (spherical HFB calculations)

Performance of existing EDFs
- Tremendous over known nuclei
- Especially for bulk properties
- Role of symmetry breaking

"Asymptotic freedom"
- Into "the next major shell"
- For most observables
- Signals poor predictive power

Spectroscopy
- The real challenge for the future...

Binding energy in Sn, Dy and Pb isotopes

[DFTM pairing
--- Sn-SLY4  --- Sn-SKP
-. Dy-SLY4  --- Dy-SKP
--- Pb-SLY4  --- Pb-SKP

Exp-Sn  Exp-Dy  Exp-Pb

[J. Sadoudi, T. D., unpublished]

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Charge radius in Sn, Dy and Pb isotopes

![Graph showing charge radius vs. mass number A for Sn, Dy, and Pb isotopes with different EDFs and experimental data.](image)
Performance of empirical EDFs (spherical HFB calculations)

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**Binding energy in Sn isotopes**

- [J. Sadoudi, T. D., unpublished]
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Pairing gaps in Sn isotopes

Spectroscopy
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Spectroscopy

- The real challenge for the future...

Two-neutron sep. energy in Sn isotopes

Sn isotopes DFTV pairing

- SLY4
- rho160
- T26
- T6

Exp

[J. Sadoudi, T. D., unpublished]
Performance of empirical EDFs

Performance of existing EDFs

- Tremendous successes for known nuclei
- "Asymptotic freedom" as one enters "the next major shell"

Crucial undergoing works

- **Enrich the analytical structure of empirical functionals**
  - Tensor terms, e.g. [T. Lesinski et al., PRC76, 014312]
  - Higher-order derivatives [B. G. Carlsson et al., PRC78, 044326]
  - $\rho_n - \rho_p$ dependence to $C_{qq}^{\tilde{\rho}\tilde{\rho}}(\vec{r})$, e.g. [J. Margueron et al., PRC77, 054309]

- Improve fitting protocols = data, algorithm and post-analysis
Performance of empirical EDFs

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One can also propose a complementary approach...
- Data not always constrain unambiguously non-trivial characteristics of EDF
- Interesting not to rely entirely on trial-and-error and fitting data
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Constructing non-empirical EDFs for nuclei

Long term objective
Build non-empirical EDF in place of existing models
Constructing non-empirical EDFs for nuclei

Long term objective
Build non-empirical EDF in place of existing models

Empirical
Empirical
Non-empirical
Low-$k$ NN+NNN
QCD / $\chi$-EFT

Finite nuclei and extended nuclear matter

Low-momentum interactions
Long term project and collaboration

Design *non-empirical* Energy Density Functionals

- Bridge with *ab-initio* many-body techniques
- Calculate properties of heavy/complex nuclei from NN+NNN
- Controlled calculations with theoretical error bars

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3 Bibliography
Selected bibliography

P. Ring, P. Schuck,
*The nuclear many-body problem*, 1980, Springer-Verlag, Berlin

M. Bender, P.-H. Heenen, P.-G. Reinhard,
Rev. Mod. Phys. 75 (2003) 121