Energy Density Functionals

Build a consistent microscopic framework for a unified description of bulk properties, excitations and reactions!
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Density Functionals
(self-consistent mean fields)

Configuration interaction
(Interacting Shell-Model)
**Nuclear Energy Density Functionals**: the many-body problem is mapped onto a one-body problem without explicitly involving inter-nucleon interactions!

**Self-consistent Kohn-Sham DFT**: includes correlations and therefore goes beyond the Hartree-Fock. It has the advantage of being a local scheme.

\[ v_s[\rho(r)] = v(r) + U[\rho(r)] + v_{xc}[\rho(r)] \]

- **external potential**
- **Hartree term**
- **exchange-correlation**

\[ v_{xc}[\rho(r)] = \frac{\delta E_{xc}[\rho(r)]}{\delta \rho(r)} \]

The practical usefulness of the Kohn-Sham scheme depends entirely on whether accurate approximations for \( E_{xc} \) can be found!

The exact density functional is approximated with **powers and gradients of ground-state nucleon densities and currents.**
Local densities and currents:

**T=0 density:**
\[ \rho_0(r) = \rho_0(r, r) = \sum \rho(r \sigma \tau; r \sigma \tau) \]

**T=1 density:**
\[ \rho_1(r) = \rho_1(r, r) = \sum \rho(r \sigma \tau; r \sigma \tau) \tau \]

**T=0 spin density:**
\[ s_0(r) = s_0(r, r) = \sum \rho(r \sigma \tau; r \sigma' \tau) \sigma_{\sigma' \sigma} \]

**T=1 spin density:**
\[ s_1(r) = s_1(r, r) = \sum \rho(r \sigma \tau; r \sigma' \tau) \sigma_{\sigma' \sigma} \tau \]

**Current:**
\[ j_T(r) = \frac{i}{2} (\nabla' - \nabla) \rho_T(r, r') \bigg|_{r=r'} \]

**Spin-current tensor:**
\[ J_T(r) = \frac{i}{2} (\nabla' - \nabla) \otimes s_T(r, r') \bigg|_{r=r'} \]

**Kinetic density:**
\[ \tau_T(r) = \nabla \cdot \nabla' \rho_T(r, r') \bigg|_{r=r'} \]

**Kinetic spin-density:**
\[ T_T(r) = \nabla \cdot \nabla' s_T(r, r') \bigg|_{r=r'} \]
Advantages of the Energy Density Functional approach to nuclear structure
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Important for extrapolations to regions far from stability!
Semi-empirical functionals

Infinite nuclear matter cannot determine the density functional on the level of accuracy that is needed for a quantitative description of structure phenomena in finite nuclei.

... start from a favorite microscopic nuclear matter EOS

... the parameters of the functional are fine-tuned to data of finite nuclei
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DD-PCI

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DD-PC1

... starts from microscopic nucleon self-energies in nuclear matter.

... parameters adjusted in self-consistent mean-field calculations of masses of 64 axially deformed nuclei in the mass regions $A \sim 150-180$ and $A \sim 230-250$. 
... calculated masses of finite nuclei are primarily sensitive to the three leading terms in the empirical mass formula:

\[ E_B = a_v A + a_s A^{2/3} + a_4 \frac{(N - Z)^2}{4A} + \ldots \]

... generate families of effective interactions characterized by different values of \(a_v\), \(a_s\) and \(a_4\), and determine which parametrization minimizes the deviation from the empirical binding energies of a large set of deformed nuclei.

**DD-PC1**

- Volume energy: \(a_v = -16.06\) MeV
- Surface energy: \(a_s = 17.498\) MeV
- Symmetry energy: \(\langle S_2 \rangle = 27.8\) MeV \((a_4 = 33\text{MeV})\)
Deformed nuclei

Binding energies used to adjust the parameters of the functional:

<table>
<thead>
<tr>
<th>$Z$</th>
<th>62</th>
<th>64</th>
<th>66</th>
<th>68</th>
<th>70</th>
<th>72</th>
<th>90</th>
<th>92</th>
<th>94</th>
<th>96</th>
<th>98</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_{min}$</td>
<td>92</td>
<td>92</td>
<td>92</td>
<td>92</td>
<td>92</td>
<td>72</td>
<td>140</td>
<td>138</td>
<td>138</td>
<td>142</td>
<td>144</td>
</tr>
<tr>
<td>$N_{max}$</td>
<td>96</td>
<td>98</td>
<td>102</td>
<td>104</td>
<td>108</td>
<td>110</td>
<td>144</td>
<td>148</td>
<td>150</td>
<td>152</td>
<td>152</td>
</tr>
</tbody>
</table>

$\alpha_v = -16.06 \text{ MeV}$
Systematic calculation of ground-state properties:

**Charge radii**

- **Nd** (a)
- **Sm** (b)
- **Gd** (c)
- **Dy** (d)
- **Er** (e)
- **Yb** (f)

**Quadrupole deformations**

- **Nd** (a)
- **Sm** (b)
- **Gd** (c)
- **Dy** (d)
- **Er** (e)
- **Yb** (f)
Excitation energies of collective modes:
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IVGDR
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IVGDR

\[ \begin{array}{cccc}
116 \text{Sn} & 118 \text{Sn} & 120 \text{Sn} & 124 \text{Sn} \\
(a) & (b) & (c) & (d) \\
\end{array} \]
Excitation energies of collective modes:

IVGDR

ISGMR

Monday, November 15, 2010
Excitation energies of collective modes:

**IVGDR**

(a) $^{116}\text{Sn}$  
(b) $^{118}\text{Sn}$  
(c) $^{120}\text{Sn}$  
(d) $^{124}\text{Sn}$

**ISGMR**

(a) $^{112}\text{Sn}$  
(b) $^{114}\text{Sn}$  
(c) $^{116}\text{Sn}$  
(d) $^{118}\text{Sn}$  
(e) $^{120}\text{Sn}$  
(f) $^{122}\text{Sn}$  
(g) $^{124}\text{Sn}$

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Nuclear Many-Body Correlations

**short-range**
(hard repulsive core of the NN-interaction)

**long-range**
nuclear resonance modes
(giant resonances)

**collective correlations**
large-amplitude soft modes:
(center of mass motion, rotation, low-energy quadrupole vibrations)
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...vary smoothly with nucleon number!
Can be included implicitly in an effective Energy Density Functional.

...sensitive to shell-effects and strong variations with nucleon number!
Cannot be included in a simple EDF framework.
Shape-coexistence in neutron-deficient Kr isotopes
Five-dimensional collective Hamiltonian

... nuclear excitations determined by quadrupole vibrational and rotational degrees of freedom

\[ H_{\text{coll}} = T_{\text{vib}}(\beta, \gamma) + T_{\text{rot}}(\beta, \gamma, \Omega) + V_{\text{coll}}(\beta, \gamma) \]

\[ T_{\text{vib}} = \frac{1}{2} B_{\beta\beta} \dot{\beta}^2 + \beta B_{\beta\gamma} \dot{\beta} \dot{\gamma} + \frac{1}{2} \beta^2 B_{\gamma\gamma} \dot{\gamma}^2 \]

\[ T_{\text{rot}} = \frac{1}{2} \sum_{k=1}^{3} I_k \omega_k^2 \]
Five-dimensional collective Hamiltonian

... nuclear excitations determined by quadrupole vibrational and rotational degrees of freedom

\[ H_{\text{coll}} = \mathcal{T}_{\text{vib}}(\beta, \gamma) + \mathcal{T}_{\text{rot}}(\beta, \gamma, \Omega) + \mathcal{V}_{\text{coll}}(\beta, \gamma) \]

\[ \mathcal{T}_{\text{vib}} = \frac{1}{2} B_{\beta\beta} \dot{\beta}^2 + \beta B_{\beta\gamma} \dot{\beta} \dot{\gamma} + \frac{1}{2} \beta^2 B_{\gamma\gamma} \dot{\gamma}^2 \]

\[ \mathcal{T}_{\text{rot}} = \frac{1}{2} \sum_{k=1}^{3} \mathcal{I}_k \omega_k^2 \]

The quasiparticle wave functions and energies generated from constrained self-consistent solutions of the RHB model, provide the microscopic input for the parameters of the collective Hamiltonian.
Rapidly-changing shapes in the N=28 isotones

Monday, November 15, 2010
$^{44}\text{S}$

$B(E2) = e^2 fm^4$

$\rho^2(E0) \times 10^3 = 23$

$\rho^2(E0) \times 10^3 = 8.7(7)$

DD-PC1

Exp.
EDF description of nuclear Quantum Phase Transitions
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Atomic nuclei → first- and second-order QPT occur between systems characterized by different ground-state shapes. Control parameter → number of nucleons.
EDF description of nuclear Quantum Phase Transitions

Atomic nuclei $\rightarrow$ first- and second-order QPT occur between systems characterized by different ground-state shapes. Control parameter $\rightarrow$ number of nucleons.
Fluctuations of quadrupole deformation parameters

- **Ba**
  - $\Delta \beta / \langle \beta \rangle$
  - $\Delta \gamma / \langle \gamma \rangle$

- **Xe**
  - $\Delta \beta / \langle \beta \rangle$
  - $\Delta \gamma / \langle \gamma \rangle$
Neutron-rich nuclei → predicted occurrence of a collective soft dipole mode (Pygmy Dipole Resonance)
Low-lying E1 strength in Ni isotopes

\[ {^{68}\text{Ni}} \]
Low-energy dipole response at finite temperature
Thermal unblocking of single-particle orbitals close to the Fermi level.

FTRRPA transition amplitudes at temperature $T = 2 \text{ MeV}$ for the dipole state at $E = 9.71 \text{ MeV}$ in $^{60}\text{Ni}$. Included are the contributions (in % in the second column) of the dominant configurations to the total sum of FTRRPA amplitudes: $\sum_{mi}(X_{mi}^2 - Y_{mi}^2)(n_i - n_m)$.

\[
\begin{array}{l|c}
\nu 2p_{3/2} & \rightarrow \nu 2d_{5/2} & 45.87 \\
\nu 1f_{5/2} & \rightarrow \nu 2d_{3/2} & 13.92 \\
\nu 2p_{3/2} & \rightarrow \nu 3s_{1/2} & 8.43 \\
\nu 1f_{7/2} & \rightarrow \nu 1g_{9/2} & 3.58 \\
\nu 2p_{1/2} & \rightarrow \nu 2d_{3/2} & 1.30 \\
\pi 2p_{3/2} & \rightarrow \pi 2d_{5/2} & 7.89 \\
\pi 2p_{3/2} & \rightarrow \pi 2d_{5/2} & 6.32 \\
\pi 1f_{5/2} & \rightarrow \pi 2d_{3/2} & 3.62 \\
\pi 1f_{7/2} & \rightarrow \pi 1g_{9/2} & 1.21 \\
\end{array}
\]

Same as in Table 1, but for the dipole states at 9.78 and 10.03 MeV in $^{62}\text{Ni}$.

\[
\begin{array}{l|c}
E = 9.78 \text{ MeV} & \\
\pi 2p_{3/2} & \rightarrow \pi 2d_{5/2} & 48.02 \\
\pi 1f_{5/2} & \rightarrow \pi 2d_{3/2} & 20.99 \\
\pi 2p_{3/2} & \rightarrow \pi 3s_{1/2} & 3.12 \\
\nu 2p_{3/2} & \rightarrow \nu 2d_{5/2} & 17.06 \\
\nu 1f_{5/2} & \rightarrow \nu 2d_{3/2} & 4.36 \\
\nu 1f_{7/2} & \rightarrow \nu 1g_{9/2} & 1.22 \\
\end{array}
\]

\[
\begin{array}{l|c}
E = 10.03 \text{ MeV} & \\
\nu 2p_{3/2} & \rightarrow \nu 2d_{5/2} & 26.55 \\
\nu 2p_{3/2} & \rightarrow \nu 3s_{1/2} & 3.59 \\
\pi 1f_{5/2} & \rightarrow \pi 2d_{3/2} & 63.60 \\
\pi 2p_{3/2} & \rightarrow \pi 2d_{5/2} & 2.55 \\
\end{array}
\]
unified microscopic description of the structure of stable and nuclei far from stability, and reliable extrapolations toward the drip lines.
Nuclear Energy Density Functional Framework

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- fully self-consistent (Q)RPA analysis of giant resonances, low-energy multipole response in weakly-bound nuclei, dynamics of exotic modes of excitation.
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✔ fully self-consistent (Q)RPA analysis of giant resonances, low-energy multipole response in weakly-bound nuclei, dynamics of exotic modes of excitation.

✔ when extended to take into account collective correlations, it describes deformations and shape-coexistence phenomena associated with shell evolution.