The isospin- and angular-momentum-projected DFT and beyond: formalism and applications

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- **MR DFT:** short presentation of main building blocks of our approach
  - mean-field (or nuclear DFT)
  - symmetry (rotational, isospin) breaking and restoration
    - unphysical (spontaneous) symmetry violation isospin projection
    - Coulomb rediagonalization (explicit symmetry violation)

- **Isospin impurities**

- **Superallowed beta decay** (sources of theoretical errors and limitations of the „static” MR DFT)

- **Extension:**
  - toward NO CORE shell model (CI) with basis cutoff dictated by the self-consistent p-h configurations
  - examples: $^{32}$Cl–$^{32}$S, $^{62}$Zn–$^{62}$Ga, $^{38}$Ca–$^{38}$K, $^{42}$Sc

- **Summary & perspectives.**
The nuclear effective theory is based on a simple and very intuitive assumption that low-energy nuclear theory is independent on high-energy dynamics.

\[ v_S(q^2) \approx v_S(0) + v_S^{(1)}(0)q^2 + v_S^{(2)}(0)q^4 \ldots , \]

\[ v_{\text{eff}}(r) \approx v_{\text{long}}(r) + ca^2 \delta_a(r) + d_1a^4 \nabla^2 \delta_a(r) + d_2a^4 \nabla \delta_a(r) \nabla + \ldots + g_1a^{n+2} \nabla^n \delta_a(r) + \ldots , \]

Skyrme interaction:

\[ \lim_{\alpha \to 0} \delta_a \]

\[ v(1, 2) = t_0(1 + x_0 \hat{P}_\sigma)\delta(r_{12}) + \frac{1}{2}t_1(1 + x_1 \hat{P}_\sigma) \left( \hat{k}'^2 \delta(r_{12}) + \delta(r_{12}) \hat{k}'^2 \right) + t_2(1 + x_2 \hat{P}_\sigma) \hat{k}' \delta(r_{12}) \hat{k} + \frac{1}{6}t_3(1 + x_3 \hat{P}_\sigma) \rho_0(\hat{R}) \delta(r_{12}) + iW_0(\sigma_1 + \sigma_2) \left( \hat{k}' \times \delta(r_{12}) \hat{k} \right) , \]

\[ r_{12} = r_1 - r_2 ; \ R = (r_1 + r_2)/2 ; \quad \hat{k} = \frac{1}{2i}(\nabla_1 - \nabla_2) \quad \hat{k}' = -\frac{1}{2i}(\nabla_1 - \nabla_2) \quad \text{relative momenta} \]

\[ \hat{P}_\sigma = \frac{1}{2}(1 + \sigma_1 \sigma_2) \quad \text{spin exchange} \]
Skyrme (hadronic) interaction conserves such symmetries like:

- **rotational (spherical) symmetry**
- **isospin symmetry:** $V_{nn}^{LS} = V_{pp}^{LS} = V_{np}^{LS}$ (in reality approximate)
- **parity**...

**Self-consistent solutions (Slater dets) break these symmetries (are deformed) spontaneously**

\[
\hat{R}(Q)|\varphi(Q_0)\rangle = |\varphi(Q')\rangle
\]

\[
\langle \varphi | \hat{H} | \varphi \rangle = \langle \varphi | \hat{R}^\dagger(Q) \hat{H} \hat{R}(Q) | \varphi \rangle
\]

advantages:
- built in correlations into single Slater determinant

disadvantages:
- symmetry must be restored to compare theory to data

Restoration $\rightarrow$ beyond mean-field $\rightarrow$ multi-reference density functional theory
There are two sources of the isospin symmetry breaking:
- **unphysical**, caused solely by the HF approximation
- **physical**, caused mostly by Coulomb interaction
  (also, but to much lesser extent, by the strong force isospin non-invariance)

Find self-consistent HF solution (including Coulomb) → deformed Slater determinant \(|HF\rangle\):

\[
|HF\rangle = \sum_{T \geq |T_z|} b_{T,T_z} |\alpha; T, T_z\rangle
\]

Apply the isospin projector:

\[
\hat{P}^T_{T_z T_z} = \frac{2T + 1}{2} \int_0^\pi d\beta \sin \beta d_{T_z T_z}^{T^*}(\beta) \hat{R}(\beta)
\]

in order to create good isospin „basis“:

\[
|\alpha; T, T_z\rangle = \frac{1}{b_{T,T_z}} \hat{P}_{T_z T_z}^T |HF\rangle
\]

Diagonalize total Hamiltonian in „good isospin basis“ \(|\alpha, T, T_z\rangle\) → takes physical isospin mixing

\[
\alpha_C^{AR} = 1 - |a_{T=T_z}^{n=1}|^2
\]


**Isospin-projection is non-singular:**


\[ \tilde{O}(\beta) = \begin{pmatrix} \cos \frac{\beta}{2} I_N & -\sin \frac{\beta}{2} O \\ \sin \frac{\beta}{2} O^\dagger & \cos \frac{\beta}{2} I_Z \end{pmatrix} \]

\[ \tilde{O}(\beta)^{-1} = \begin{pmatrix} \tilde{W} \frac{\cos \frac{\beta}{2}}{\cos^2 \frac{\beta}{2} I_N + \sin^2 \frac{\beta}{2} D^2} \tilde{W}^\dagger \\ V \frac{-\sin \frac{\beta}{2}}{\cos^2 \frac{\beta}{2} I_Z + \sin^2 \frac{\beta}{2} D^2} DV^\dagger \end{pmatrix} \]

SVD eigenvalues (diagonal matrix)

\[ O = WDV^\dagger \]

\[ \tilde{O}(\beta)^{-1} \sim \frac{1}{\cos \frac{\beta}{2}} \]

Singularity (if any) at \( \beta = \pi \)

is inherited by a transition density \( \tilde{\rho} \)

\[ \tilde{\rho} = \sum_{ij} \psi_i^* \tilde{O}_{ij}^{-1} \phi_j \]

Power \([\cos(\beta/2)]\) counting:

\[ \mathcal{H}(\beta) \sim \tilde{\rho}^\eta(\beta) \text{ Det} \tilde{O}(\beta) \]

\[ \int d\beta \sin \beta \; d_T^P T_z T_z (\beta) \; \tilde{\rho}^\eta(\beta) \; \text{Det} \tilde{O}(\beta) \propto \int d\beta \cos \xi \frac{\beta}{2} \]

in the worst case

i.e. for \( N=Z \) and \( k=1 \)

\[ \eta > 3 \] to get a singularity

|Det\( \tilde{O}(\beta) \)| = \( |\cos \frac{\beta}{2}|^{N-Z} \prod_{i=1}^{Z} (\cos^2 \frac{\beta}{2} + \sin^2 \frac{\beta}{2} D_i^2) \)

k is a multiplicity of zero singular values
Coupled AMP+IP projection is singular forcing us to use the Skyrme interaction SV (or density-independent interaction)
Isospin mixing & energy in the ground states of e-e N=Z nuclei:

HF tries to reduce the isospin mixing by: $\Delta \alpha_C \sim 30\%$

in order to minimize the total energy

There are no constraints on mixing coefficients

This is not a single Slater determinant

A. Corsi et al. PRC84, 041304 (2011)

E. Farnea et al. PLB551, 56 (2003)
Superallowed $0^+\to 0^+$ Fermi beta decays
(testing the Standard Model)

10 cases measured with accuracy $ft \sim 0.1\%$
3 cases measured with accuracy $ft \sim 0.3\%$

→ test of the CVC hypothesis
(Conserved Vector Current)

\[
\mathcal{F} t = ft (1 + \delta_R') [1 - (\delta_C - \delta_{NS})] = \frac{K}{2G_V^2 (1 + \Delta_R)}
\]

\[
\begin{array}{ccc}
1.5\% & 0.3\% & -1.5\% \\
\sim 2.4\%
\end{array}
\]

\[
\mathcal{F} t = 3072.2(8)
\]

\[
G_V (1+\Delta_R)^{1/2} (hc)^3 = 1.14961(15) \times 10^6 \text{ GeV}^2
\]

\[
\chi^2/\nu = 0.3
\]

\[
|V_{ud}| = 0.97418 \pm 0.00026
\]

→ test of unitarity of the CKM matrix

\[
|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.9997(6)
\]

\[
0.9490(4) \quad 0.0507(4) \quad <0.0001
\]

\[
\begin{pmatrix}
d' \\
s' \\
b'
\end{pmatrix} =
\begin{pmatrix}
V_{ud} & V_{us} & V_{ub} \\
V_{cd} & V_{cs} & V_{cb} \\
V_{td} & V_{ts} & V_{tb}
\end{pmatrix}
\begin{pmatrix}
d \\
s \\
b
\end{pmatrix}
\]

\[
\text{weak eigenstates} \quad \text{mass eigenstates}
\]

\[
\text{Cabibbo-Kobayashi-Maskawa}
\]

adopted from J.Hardy’s, ENAM’08 presentation
model dependence & model limitations

\[ \delta_c = \delta_{c1} + \delta_{c2} \]

\textbf{Liang & Giai & Meng}

\textbf{spherical RPA}
Coulomb exchange treated in the Slater approximation

\textbf{Hardy & Towner}

\textbf{mean field}
radial mismatch of the wave functions

\textbf{shell model configuration mixing}

\textbf{configuration mixing}

\textbf{Miller & Schwenk}
Mean-field can differentiate between $\nu \otimes \pi$ and $\overline{\nu} \otimes \overline{\pi}$ only through time-odd polarizations!

$T_z = -/+1$ (N-Z = -/+2)

$|<T_{+/-}|^2 = 2(1 - \delta_C)$

$J = 0^+, T = 1$

$T_z = 0$ (N-Z = 0)

How to calculate the superallowed Fermi beta decay using the DFT framework?
ground state in N-Z=+/-2 (e-e) nucleus

Project on good isospin (T=1) and angular momentum (I=0) (and perform Coulomb rediagonalization)

antialigned state in N=Z (o-o) nucleus

Project on good isospin (T=1) and angular momentum (I=0) (and perform Coulomb rediagonalization)

\[ |<T_{\approx 1}, T_z = +/-1, I=0| T_{\pm} |I=0, T_{\approx 1}, T_z = 0> |^2 = 2(1-\delta_C) \]
Tests of the weak-interaction flavor-mixing sector of the Standard Model of elementary particles

$|V_{ud}|$ & unitarity - world survey


Ft=3071.4(8)+0.85(85); $V_{ud}=0.97418(26)$

Ft=3070.4(9); $V_{ud}=0.97444(23)$ PRL

Ft=3073.6(12); $V_{ud}=0.97397(27)$ PRC
ISB corrections to the Fermi transitions in T=1/2 mirrors

W. Satuła, J. Dobaczewski, W. Nazarewicz, M. Rafalski

SM+WS results from:
N. Severijns, M. Tandecki, T. Phalet, and I. S. Towner,
**THEORETICAL UNCERTAINTIES**

- **Basis-size dependence:**
  ~5%

- **Configuration dependence:**

- **Functional dependence:**

  **SV:** $F_t = 3073.6(12)$
  $V_{ud} = 0.97397(27)$
  $|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.99935(67)$

  **SHZ2:** $F_t = 3075.0(12)$
  $V_{ud} = 0.97374(27)$
  $|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.99890(67)$

  $a_{sym} = 42.2 \text{MeV}!!!
MEAN-FIELD
compute "n" self-consistent Slater determinants corresponding to low-lying p-h excitations

\[ \phi_1 \phi_2 \phi_3 \ldots \phi_n \]

PROJECTION
non-orthogonal set of K- and T-mixed states

\[ \{|I>^{(1)}\}_{k_1} \{|I>^{(2)}\}_{k_2} \{|I>^{(3)}\}_{k_3} \ldots \{|I>^{(n)}\}_{k_n} \]

STATE MIXING
Hill-Wheeler equation: \( H\psi = E\psi \)
No-core configuration interaction (shell) model with basis cutoff dictated by the self-consistent p-h DFT states

\( ^{32}\text{Cl} \)

\[ \Delta E \text{ (MeV)} \]

\( I=0^+ \quad I=1^+ \quad I=2^+ \quad I=3^+ \)

- theory
- exp

$^{32}\text{S} \quad I=1^+$

$^{32}\text{Cl} \quad I=1^+$

$\delta_C \approx 6(2)\%$

Experiment: $\delta_C \approx 5.3(9)\%$

$\text{SM+WS calculations: } \delta_C \approx 4.6(5)\%$

No-core configuration-interaction formalism based on the isospin and angular momentum projected DFT

$^{62}\text{Zn, } I=0^+ \text{ states below } 5\text{MeV}$

- $^{62}\text{Zn, } I=0^+$ states below 5MeV

Excitation energy of $0^+$ states [MeV]

- EXP (old)
- SM (GXPF1)
- SM (MSDI3)
- EXP (new)
- SV$^{\text{mix}}$ (6 Slaters)

- W.S., J. Dobaczewski, M. Konieczka

- K.G. Leach et al.
  PRC88, 031306 (2013)

- HF

I=0$^+$ before mixing

$0^+$ ground state
Stability of NCCI calculation for $^{62}$Zn

g.s. + $\pi_1$ + $\nu_1$ + $\nu_2$ + $\pi_2$ + $\pi\pi_1$

Energy (MeV)

$\delta_c$ [%]

$E^{HF}$ (MeV)

~200 keV

normalized

$\nu_1$

$\pi_1$

$Z$

$X \sim Y$
A case of $A=38$ ($^{38}\text{Ca}\rightarrow^{38}\text{K}$)

Static approach gives: $\delta_C=8.9\%$

\[ \delta_C=1.5\% \]

\[ \delta_C=1.7\% \]

$I=0^+, T=1$

$^{38}\text{Ca}$

4 Slaters

$^{38}\text{K}$

3 Slaters
Mixing of states projected from the antialigned configurations:
We have to go BEYOND „STATIC” MR-EDF in order to address high-quality spectroscopic data available today.

First attempts are very encouraging at least concerning energy spectra!!!
$T=1, I=0^+$ isobaric analogue states from self-consistent 3D-isocranked HF: $h^\lambda = h - \lambda T$


$|n> + |p>$ separable solution

$TED_{th} - TED_{exp}$ [MeV]

$TED = B(T_z=1) + B(T_z=-1) - 2B(T_z=0)$

normalized: theory (red curve) shifted by 3.2MeV

separable solution
Regularization:

$$V^{2B}_{IMK} = \frac{2I+1}{8\pi^2} \int d\Omega \, D^{I^*}_{MK}(\Omega) \langle \Psi | \hat{V}^{2B}_{2I} | \Psi \rangle$$

$$\langle \Psi | \hat{V}^{2B}_{2B} | \Psi \rangle \rightarrow \langle \Psi | \hat{V}^{2B}_{2I} | \Psi \rangle$$

Regularized energies can be calculated by solving a set of linear equations.
Confidence level test based on the CVC hypothesis

T&H PRC82, 065501 (2010)

\[
\delta_C = 1 + \delta_{\text{NS}} - \frac{F_t}{\hat{F}_t(1+\delta_R)}
\]

Minimize RMS deviation between the calculated and experimental \(\delta_C\) with respect to \(F_t\).

\(\chi^2/n_d = 5.2\) for \(F_t = 3070.0\) s

75% contribution to the \(\chi^2\) comes from \(A = 62\)

From: W. Satuła, J. Dobaczewski, W. Nazarewicz, M. Rafalski