Fundamentals in density functional theory (YITP Workshop DFT 2022)
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Covariant Density Functional Theory with Localized Exchange Terms

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Phys. Rev. C 106, 034315 (2022) (Editor's Suggestion)

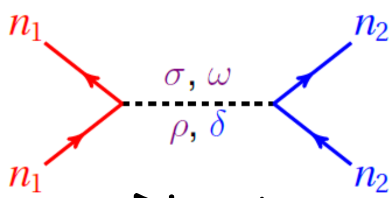
Contents

Covariant Density Functional Theory

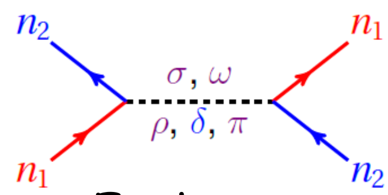
Covariant Density Functional Theory (CDFT)

Meng, Relativistic Density Functional for Nuclear Structure, World Scientific, 2016

- Meson-exchange: interact via exchange of mesons *Yukawa (1935)*



Direct
(Hartree)



Exchange
(Fock)

- Dirac equation

$$\begin{pmatrix} V_0 + S + M & \boldsymbol{\sigma}\cdot\boldsymbol{p} - \boldsymbol{\sigma}\cdot\boldsymbol{V} \\ \boldsymbol{\sigma}\cdot\boldsymbol{p} - \boldsymbol{\sigma}\cdot\boldsymbol{V} & V_0 - S - M \end{pmatrix} \begin{pmatrix} F_k \\ G_k \end{pmatrix} = \varepsilon_k \begin{pmatrix} F_k \\ G_k \end{pmatrix}$$

S: Scalar potential $\qquad$ $V^\mu = (V^0, \boldsymbol{V})$: Vector potential

Advantages of CDFT: Lorentz symmetry

P. Ring PST 150, 014035 (2012)

- Large spin-orbit potential
- Pseudospin symmetry
- Time-odd fields
- ……

Covariant Density Functional Theory

- Wide application of the covariant density functional theory (CDFT)

  - Ground state
    - ✓ Nuclear Mass

      Zhang et al., ADNDT 144, 101488 (2022)
    - ✓ Exotic Nuclei

      Meng and Ring, PRL 77, 3963 (1996)
  - Nuclear decay

    Niu et al., PLB 723, 172 (2013)

    Zhao et al., PRC 90, 054326 (2014)

    Lim et al., PRC 93, 014314 (2016)
  - Nuclear fission

    Lu, Zhao, and Zhou, PRC 85, 011301(R) (2012)

    Zhou, PS 91, 063008 (2016)

    Agbemava et al., PRC 95, 054324 (2017)

    Zhao et al., PRC 99, 054613 (2019)

    Ren et al., PRL 128, 172501 (2022)
  - Nuclear excitation

    König and Ring PRL 71, 3079 (1993)

    Afanasjev and Abusara PRC 82, 034329 (2010)

    Peng et al., PRC 78, 024313 (2008)

    Zhao et al., PRL 107, 122501 (2011)

    Nikšić et al., PRC 66, 064302 (2002)

    Paar et al., PRL 103, 032502 (2009)

    Liang et al., PRL 101, 122502(2008)

    Niu et al., PLB 681, 315 (2009)

    Nikšić et al., PRC 79, 034303 (2009)

    Li et al., PRC 79, 054301 (2009)

    Nikšić et al., PRC 73, 034308 (2006)

    Yao et al., PRC 81, 044311 (2010)
  - Nuclear reaction

    Ren, Zhao, and Meng, PLB 801, 135194 (2020)

    Ren, Zhao, and Meng, PRC 102, 044603 (2020)

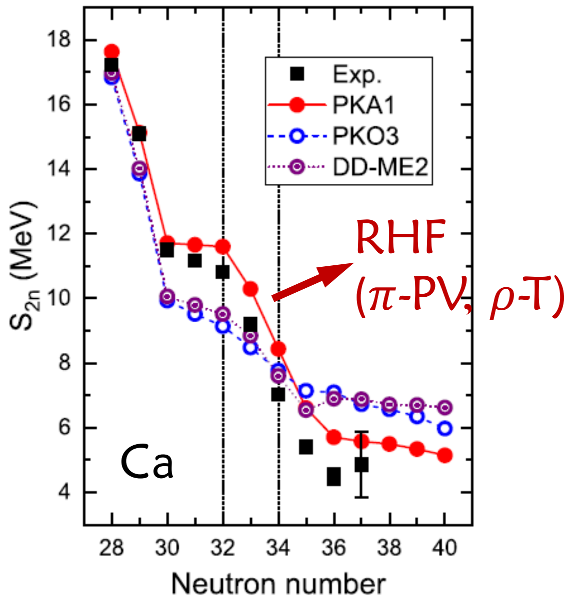
But the exchange terms are not taken into account explicitly

in most of the applications!

Importance of Exchange Terms

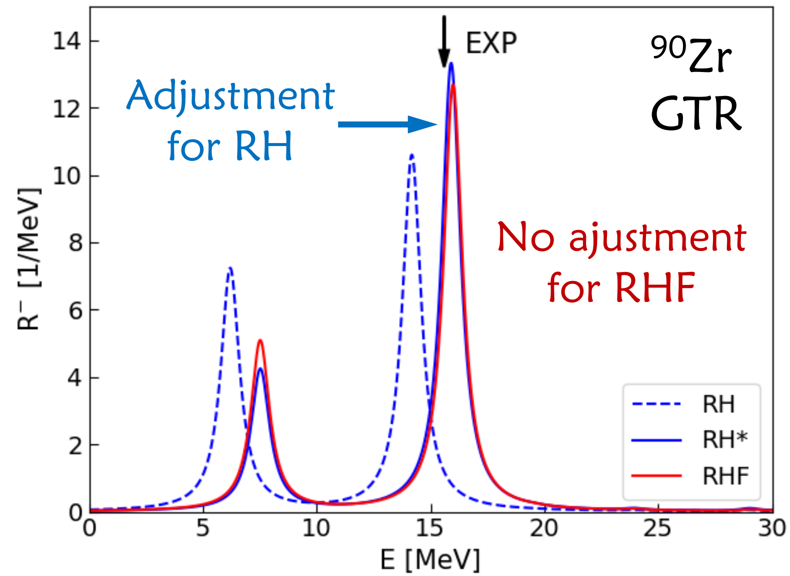
- Studies of the Relativistic Hartree-Fock (RHF) theory

Shell Structure



J. Liu et al., PLB 806, 135524 (2020)

Spin-Isospin Excitation



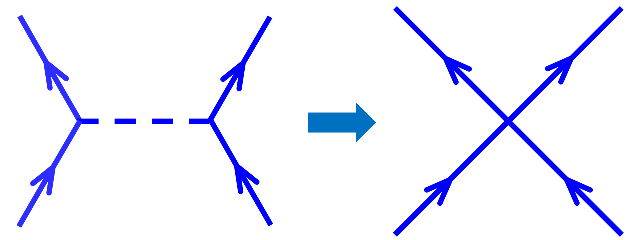
- The RHF equation contains nonlocal exchange potentials
  - It becomes complicated and is not DFT

Exchange Terms in Relativistic Point-Coupling Model

- Relativistic point-coupling model

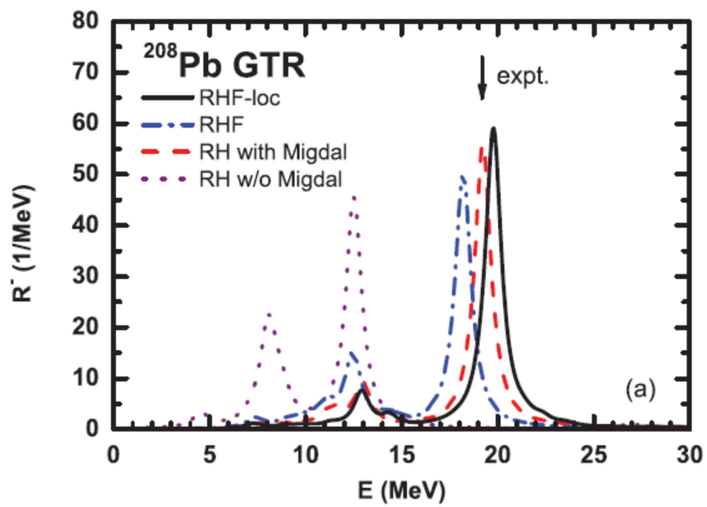
Manakos(1989), Nikolaus(1992), Bürvenich (2002), Nikšić (2008), Zhao (2010)

- Advantages
  - Avoid calculating the meson field
  - Easily extend to beyond mean-field calculations
  - Express the exchange terms as superpositions of direct terms *Sulaksono(2003)*



- Validity of localized exchange terms in RHF

It can reasonably describe the splittings of Dirac mass and spin-isospin excitations.



Liang et al., PRC 86, 021302(R) (2012)

Goal:

Develop a new covariant density functional with localized exchange terms

Contents

Lagrangian Density

☐ Lagrangian Density

$$\mathcal{L} = \mathcal{L}^{\rm free} + \mathcal{L}^{\rm 4f} + \mathcal{L}^{\rm der} + \mathcal{L}^{\rm em}$$

$$\begin{aligned}
\mathcal{L}^{\rm free} =& \bar{\psi}(i\gamma_\mu\partial^\mu - M)\psi \\
\mathcal{L}^{\rm 4f} =& -\frac{1}{2}\alpha_S(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_{tS}(\bar{\psi}\vec{\tau}\psi)(\bar{\psi}\vec{\tau}\psi) \\
& -\frac{1}{2}\alpha_V(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) - \frac{1}{2}\alpha_{tV}(\bar{\psi}\gamma_\mu\vec{\tau}\psi)(\bar{\psi}\gamma^\mu\vec{\tau}\psi) \\
& -\frac{1}{2}\alpha_T(\bar{\psi}\sigma_{\mu\nu}\psi)(\bar{\psi}\sigma^{\mu\nu}\psi) - \frac{1}{2}\alpha_{tT}(\bar{\psi}\sigma_{\mu\nu}\vec{\tau}\psi)(\bar{\psi}\sigma^{\mu\nu}\vec{\tau}\psi) \\
& -\frac{1}{2}\alpha_{PS}(\bar{\psi}\gamma_5\psi)(\bar{\psi}\gamma_5\psi) - \frac{1}{2}\alpha_{tPS}(\bar{\psi}\gamma_5\vec{\tau}\psi)(\bar{\psi}\gamma_5\vec{\tau}\psi) \\
& -\frac{1}{2}\alpha_{PV}(\bar{\psi}\gamma_5\gamma_\mu\psi)(\bar{\psi}\gamma_5\gamma^\mu\psi) - \frac{1}{2}\alpha_{tPV}(\bar{\psi}\gamma_5\gamma_\mu\vec{\tau}\psi)(\bar{\psi}\gamma_5\gamma^\mu\vec{\tau}\psi) \\
\mathcal{L}^{\rm der} =& -\frac{1}{2}\delta_S\partial_\mu(\bar{\psi}\psi)\partial^\mu(\bar{\psi}\psi) \\
\mathcal{L}^{\rm em} =& -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - e\frac{1-\tau_3}{2}\bar{\psi}\gamma_\mu\psi A^\mu
\end{aligned}$$

Scalar

Vector

Tensor

Pseudo-Scalar

Pseudo-Vector

☐ Hamiltonian

$$H = \int d\boldsymbol{x}\,\mathcal{H} = \int \boldsymbol{x}\left[\frac{\partial\mathcal{L}}{\partial\dot{\psi}}\dot{\psi} + \frac{\partial\mathcal{L}}{\partial\dot{A}_\mu}\dot{A}_\mu - \mathcal{L}\right]$$

☐ Slater determinant

$$|\Phi_0\rangle = \prod_{\alpha=1}^{A} c_\alpha^\dagger|-\rangle$$

Treatment of exchange terms

- Energy Functional $E = \langle \Phi_0 | H | \Phi_0 \rangle = E_{\mathrm{k}} + E_{\mathrm{4f}} + E_{\mathrm{der}} + E_{\mathrm{em}}$:

$$
\begin{aligned}
E_{\mathrm{4f}} &= E_{\mathrm{H}} + E_{\mathrm{F}} \\
&= \frac{1}{2} \int d\boldsymbol{r} \sum_{i;\alpha\beta} \alpha_i^{\mathrm{HF}} \left[\bar{\psi}_\alpha(\boldsymbol{r}) (\mathcal{O}\Gamma)_i \psi_\alpha(\boldsymbol{r}) \right] \left[\bar{\psi}_\beta(\boldsymbol{r}) (\mathcal{O}\Gamma)^i \psi_\beta(\boldsymbol{r}) \right] \\
&- \frac{1}{2} \int d\boldsymbol{r} \sum_{i;\alpha\beta} \alpha_i^{\mathrm{HF}} \left[\bar{\psi}_\alpha(\boldsymbol{r}) (\mathcal{O}\Gamma)_i \psi_\beta(\boldsymbol{r}) \right] \left[\bar{\psi}_\beta(\boldsymbol{r}) (\mathcal{O}\Gamma)^i \psi_\alpha(\boldsymbol{r}) \right]
\end{aligned}
$$

Direct term

Exchange term

- Fierz transformation

Sulaksono et al., Ann. Phys. 306, 36 (2003)
Greiner and Müller, Gauge Theory of Weak Interaction (2009)

$$
[\bar{\psi}_\alpha (\mathcal{O}\Gamma)_i \psi_\beta][\bar{\psi}_\beta (\mathcal{O}\Gamma)^i \psi_\alpha] = \sum_j \Lambda_{ij} [\bar{\psi}_\alpha (\mathcal{O}\Gamma)_j \psi_\alpha][\bar{\psi}_\beta (\mathcal{O}\Gamma)^j \psi_\beta]
$$

- $E_{4\mathrm{f}}$ can be re-expressed as

$$
E_{\mathrm{4f}} = \frac{1}{2} \int d\boldsymbol{r} \sum_{i;\alpha\beta} \alpha_i^{\mathrm{H}} \left[\bar{\psi}_\alpha(\boldsymbol{r}) (\mathcal{O}\Gamma)_i \psi_\alpha(\boldsymbol{r}) \right] \left[\bar{\psi}_\beta(\boldsymbol{r}) (\mathcal{O}\Gamma)^i \psi_\beta(\boldsymbol{r}) \right]
$$

where

$$
\alpha_i^{\mathrm{H}} = \sum_j C_{ij} \alpha_j^{\mathrm{HF}} = \sum_j (1 - \Lambda_{ji}) \alpha_j^{\mathrm{HF}}, \qquad i, j = S, tS, V, tV, T, tT, PS, tPS, PV, tPV
$$

Localized Relativistic Hartree-Fock-Bogoliubov Eq.

- Localized relativistic Hartree-Fock-Bogoliubov Equation

$$\begin{pmatrix} \hat{h}_D - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}_D^* + \lambda \end{pmatrix} \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix} = E_\alpha \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix}$$

- Single-particle hamiltonian $\hat{h}_D$:

$$\hat{h}_D = \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta[M + S + \gamma_\mu V^\mu + \sigma_{\mu\nu} T^{\mu\nu}]$$

$$S = \alpha_S \rho_S + \alpha_{tS} \tau_3 \rho_{tS} + \delta_S \Delta \rho_S \qquad \rho_S = \sum_{\alpha>0} \bar{V}_\alpha V_\alpha, \quad \rho_{tS} = \sum_{\alpha>0} \bar{V}_\alpha \vec{\tau} V_\alpha$$

$$V^\mu = \alpha_V j_V^\mu + \alpha_{tV} \tau_3 j_{tV}^\mu + e\frac{1-\tau_3}{2} A^\mu \qquad j_V^\mu = \sum_{\alpha>0} \bar{V}_\alpha \gamma^\mu V_\alpha, \quad j_{tV}^\mu = \sum_{\alpha>0} \bar{V}_\alpha \gamma^\mu \vec{\tau} V_\alpha$$

$$T^{\mu\nu} = \alpha_T j_T^{\mu\nu} + \alpha_{tV} \tau_3 j_{tT}^{\mu\nu} \qquad j_T^{\mu\nu} = \sum_{\alpha>0} \bar{V}_\alpha \sigma^{\mu\nu} V_\alpha, \quad j_{tT}^{\mu\nu} = \sum_{\alpha>0} \bar{V}_\alpha \sigma^{\mu\nu} \vec{\tau} V_\alpha$$

- Pairing Field Δ (Separable pairing force)

Tian, Ma, and Ring, PLB 676, 44 (2009)

$$\Delta_{ab} = \frac{1}{2} \sum_{cd} \langle ab | V^{pp} | cd \rangle \kappa_{cd}$$

$$V^{pp}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_1', \boldsymbol{r}_2') = -G\delta(\boldsymbol{R} - \boldsymbol{R}') P(\boldsymbol{r}) P(\boldsymbol{r}') \frac{1}{2}(1 - P^\sigma), \qquad P(\boldsymbol{r}) = \frac{1}{(4\pi a^2)^{3/2}} e^{-r^2/4a^2}$$

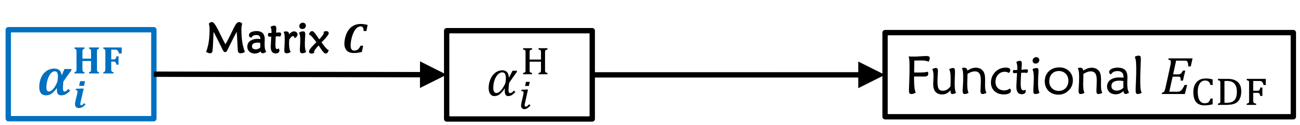
Contents

Determination of Coupling Constants

Effective Lagrangian Density

$$
\begin{aligned}
\mathcal{L} =& \bar{\psi}(i\gamma_\mu \partial^\mu - M)\psi \\
& - \frac{1}{2}\alpha_S(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) \\
& - \frac{1}{2}\alpha_{tS}(\bar{\psi}\vec{\tau}\psi)(\bar{\psi}\vec{\tau}\psi) \\
& - \frac{1}{2}\alpha_{tV}(\bar{\psi}\gamma_\mu\vec{\tau}\psi)(\bar{\psi}\gamma^\mu\vec{\tau}\psi) \\
& - \frac{1}{2}\alpha_T(\bar{\psi}\sigma_{\mu\nu}\psi)(\bar{\psi}\sigma^{\mu\nu}\psi) - \frac{1}{2}\delta_S\partial_\mu(\bar{\psi}\psi)\partial^\mu(\bar{\psi}\psi) \\
& - \frac{1}{2}\alpha_{tT}(\bar{\psi}\sigma_{\mu\nu}\vec{\tau}\psi)(\bar{\psi}\sigma^{\mu\nu}\vec{\tau}\psi) \\
& - \frac{1}{2}\alpha_{PS}(\bar{\psi}\gamma_5\psi)(\bar{\psi}\gamma_5\psi) - \frac{1}{2}\alpha_{tPS}(\bar{\psi}\gamma_5\vec{\tau}\psi)(\bar{\psi}\gamma_5\vec{\tau}\psi) \\
& - \frac{1}{2}\alpha_{PV}(\bar{\psi}\gamma_5\gamma_\mu\psi)(\bar{\psi}\gamma_5\gamma^\mu\psi) - \frac{1}{2}\alpha_{tPV}(\bar{\psi}\gamma_5\gamma_\mu\vec{\tau}\psi)(\bar{\psi}\gamma_5\gamma^\mu\vec{\tau}\psi) \\
& - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} - e\frac{1-\tau_3}{2}\bar{\psi}\gamma_\mu\psi A^\mu
\end{aligned}
$$

11 coupling constants:
Determined by fitting to bulk properties of nuclear matter and finite nuclei



Determination of Coupling Constants

Effective Lagrangian Density

$$
\begin{aligned}
\mathcal{L} =& \bar{\psi}(i\gamma_\mu \partial^\mu - M)\psi \\
&- \frac{1}{2}\alpha_S(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) \\
&- \frac{1}{2}\alpha_{tS}(\bar{\psi}\vec{\tau}\psi)(\bar{\psi}\vec{\tau}\psi) \\
&- \frac{1}{2}\alpha_{tV}(\bar{\psi}\gamma_\mu\vec{\tau}\psi)(\bar{\psi}\gamma^\mu\vec{\tau}\psi) \\
&- \frac{1}{2}\alpha_T(\bar{\psi}\sigma_{\mu\nu}\psi)(\bar{\psi}\sigma^{\mu\nu}\psi) - \frac{1}{2}\delta_S\partial_\mu(\bar{\psi}\psi)\partial^\mu(\bar{\psi}\psi) \\
&- \frac{1}{2}\alpha_{tT}(\bar{\psi}\sigma_{\mu\nu}\vec{\tau}\psi)(\bar{\psi}\sigma^{\mu\nu}\vec{\tau}\psi) \\
&- \frac{1}{2}\alpha_{PS}(\bar{\psi}\gamma_5\psi)(\bar{\psi}\gamma_5\psi) - \frac{1}{2}\alpha_{tPS}(\bar{\psi}\gamma_5\vec{\tau}\psi)(\bar{\psi}\gamma_5\vec{\tau}\psi) \\
&- \frac{1}{2}\alpha_{PV}(\bar{\psi}\gamma_5\gamma_\mu\psi)(\bar{\psi}\gamma_5\gamma^\mu\psi) - \frac{1}{2}\alpha_{tPV}(\bar{\psi}\gamma_5\gamma_\mu\vec{\tau}\psi)(\bar{\psi}\gamma_5\gamma^\mu\vec{\tau}\psi) \\
&- \frac{1}{4}F_{\mu\nu}F^{\mu\nu} - e\frac{1-\tau_3}{2}\bar{\psi}\gamma_\mu\psi A^\mu
\end{aligned}
$$

11 coupling constants:
Determined by fitting to bulk properties of nuclear matter and finite nuclei

α_i^{HF} → Matrix C → α_i^{H} → Functional E_{CDF}

5 Independent parameters

5 Constraints

Determination of Coupling Constants

Effective Lagrangian Density

Nuclear Matter: Empirical value and ab. initio calculations
Finite Nuclei: Experimental data of bulk properties

$$
\begin{aligned}
\mathcal{L} =& \bar{\psi}(i\gamma_\mu\partial^\mu - M)\psi \\
& - \frac{1}{2}\alpha_S(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) \\
& - \frac{1}{2}\alpha_{tS}(\bar{\psi}\vec{\tau}\psi)(\bar{\psi}\vec{\tau}\psi) \\
& - \frac{1}{2}\alpha_{tV}(\bar{\psi}\gamma_\mu\vec{\tau}\psi)(\bar{\psi}\gamma^\mu\vec{\tau}\psi) \\
& - \frac{1}{2}\alpha_T(\bar{\psi}\sigma_{\mu\nu}\psi)(\bar{\psi}\sigma^{\mu\nu}\psi) - \frac{1}{2}\delta_S\partial_\mu(\bar{\psi}\psi)\partial^\mu(\bar{\psi}\psi) \\
& - \frac{1}{2}\alpha_{tT}(\bar{\psi}\sigma_{\mu\nu}\vec{\tau}\psi)(\bar{\psi}\sigma^{\mu\nu}\vec{\tau}\psi) \\
& - \frac{1}{2}\alpha_{PS}(\bar{\psi}\gamma_5\psi)(\bar{\psi}\gamma_5\psi) - \frac{1}{2}\alpha_{tPS}(\bar{\psi}\gamma_5\vec{\tau}\psi)(\bar{\psi}\gamma_5\vec{\tau}\psi) \\
& - \frac{1}{2}\alpha_{PV}(\bar{\psi}\gamma_5\gamma_\mu\psi)(\bar{\psi}\gamma_5\gamma^\mu\psi) - \frac{1}{2}\alpha_{tPV}(\bar{\psi}\gamma_5\gamma_\mu\vec{\tau}\psi)(\bar{\psi}\gamma_5\gamma^\mu\vec{\tau}\psi) \\
& - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} - e\frac{1-\tau_3}{2}\bar{\psi}\gamma_\mu\psi A^\mu
\end{aligned}
$$

Step 1
Symmetric Nuclear Matter
Step 2
Splittings of Dirac Mass
Step 3
Symmetry Energy
Step 4
Finite Nuclei

Determined by Fierz Transformation

α_i^{HF} → **Matrix C** → α_i^{H} → Functional E_{CDF}

5 Independent parameters
5 Constraints

Determination of Coupling Constants

- **Effective Lagrangian Density**

Nuclear Matter: Empirical value and ab. initio calculations
Finite Nuclei: Experimental data of bulk properties

$$
\begin{aligned}
\mathcal{L} =& \bar{\psi}(i\gamma_\mu\partial^\mu - M)\psi \\
&- \frac{1}{2}\alpha_S(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) \\
&- \frac{1}{2}\alpha_{tS}(\bar{\psi}\vec{\tau}\psi)(\bar{\psi}\vec{\tau}\psi) \\
&- \frac{1}{2}\alpha_{tV}(\bar{\psi}\gamma_\mu\vec{\tau}\psi)(\bar{\psi}\gamma^\mu\vec{\tau}\psi) \\
&- \frac{1}{2}\alpha_T(\bar{\psi}\sigma_{\mu\nu}\psi)(\bar{\psi}\sigma^{\mu\nu}\psi) - \frac{1}{2}\delta_S\partial_\mu(\bar{\psi}\psi)\partial^\mu(\bar{\psi}\psi) \\
&- \frac{1}{2}\alpha_{tT}(\bar{\psi}\sigma_{\mu\nu}\vec{\tau}\psi)(\bar{\psi}\sigma^{\mu\nu}\vec{\tau}\psi) \\
&- \frac{1}{2}\alpha_{PS}(\bar{\psi}\gamma_5\psi)(\bar{\psi}\gamma_5\psi) - \frac{1}{2}\alpha_{tPS}(\bar{\psi}\gamma_5\vec{\tau}\psi)(\bar{\psi}\gamma_5\vec{\tau}\psi) \\
&- \frac{1}{2}\alpha_{PV}(\bar{\psi}\gamma_5\gamma_\mu\psi)(\bar{\psi}\gamma_5\gamma^\mu\psi) - \frac{1}{2}\alpha_{tPV}(\bar{\psi}\gamma_5\gamma_\mu\vec{\tau}\psi)(\bar{\psi}\gamma_5\gamma^\mu\vec{\tau}\psi) \\
&- \frac{1}{4}F_{\mu\nu}F^{\mu\nu} - e\frac{1-\tau_3}{2}\bar{\psi}\gamma_\mu\psi A^\mu
\end{aligned}
$$

Step 1
Symmetric Nuclear Matter
Step 2
Splittings of Dirac Mass
Step 3
Symmetry Energy
Step 4
Finite Nuclei

Determined by Fierz Transformation

Many-body correlations (in-medium effect)

- Density Dependent Coupling Constants

Satisfy: $f_i(1) = 1, \quad f_i''(0) = 0$

$$\alpha_i(\rho) = \alpha_i(\rho_{\text{sat.}})f(x), \quad f(x) = a_i\frac{1+b_i(x+d_i)^2}{1+c_i(x+d_i)^2} \qquad (x = \rho/\rho_{\text{sat.}}, i = S,\ V,\ tS,\ \text{and } tV)$$

Parameters of PCF-PK1

- Parameters of CDF PCF-PK1:

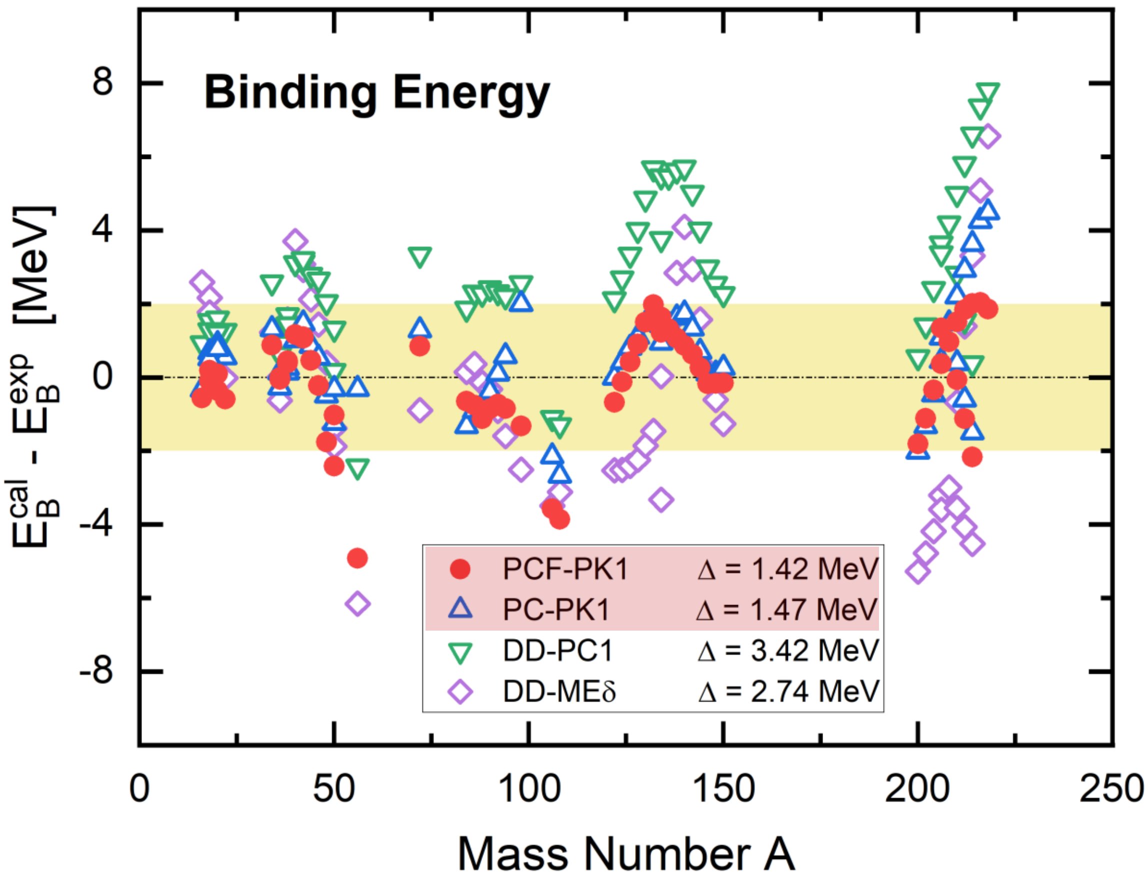
parameter	value	parameter	value
$\alpha_S(\rho_{\text{sat.}})$ [fm^2]	-6.315494	$\alpha_V(\rho_{\text{sat.}})$ [fm^2]	3.533254
a_S	1.425216	a_V	0.8075938
d_S	0.7498208	d_V	3.004506
$\alpha_{tS}(\rho_{\text{sat.}})$ [fm^2]	-1.980515	$\alpha_{tV}(\rho_{\text{sat.}})$ [fm^2]	2.975891
a_{tS}	2.328043	a_{tV}	2.546886
d_{tS}	0.7644323	d_{tV}	0.4547352
α_T [fm^2]	3.373807	δ_S [fm^4]	-0.6658080
G [MeV·fm^3]	657.5419		

- Compare to existed local covariant density functionals

		S	tS	V	tV	T	tT	PS	tPS	PV	tPV
Point-coupling	PCF-PK1	√	√	√	√	√	√	√	√	√	√
	PC-PK1	√		√	√						
	DD-PC1	√		√	√						
Meson-exchange		σ	δ	ω	ρ	π					
	DD-MEδ	√	√	√	√						

Binding Energy of Reference Nuclei

- Deviations of binding energies between theoretical and experimental values

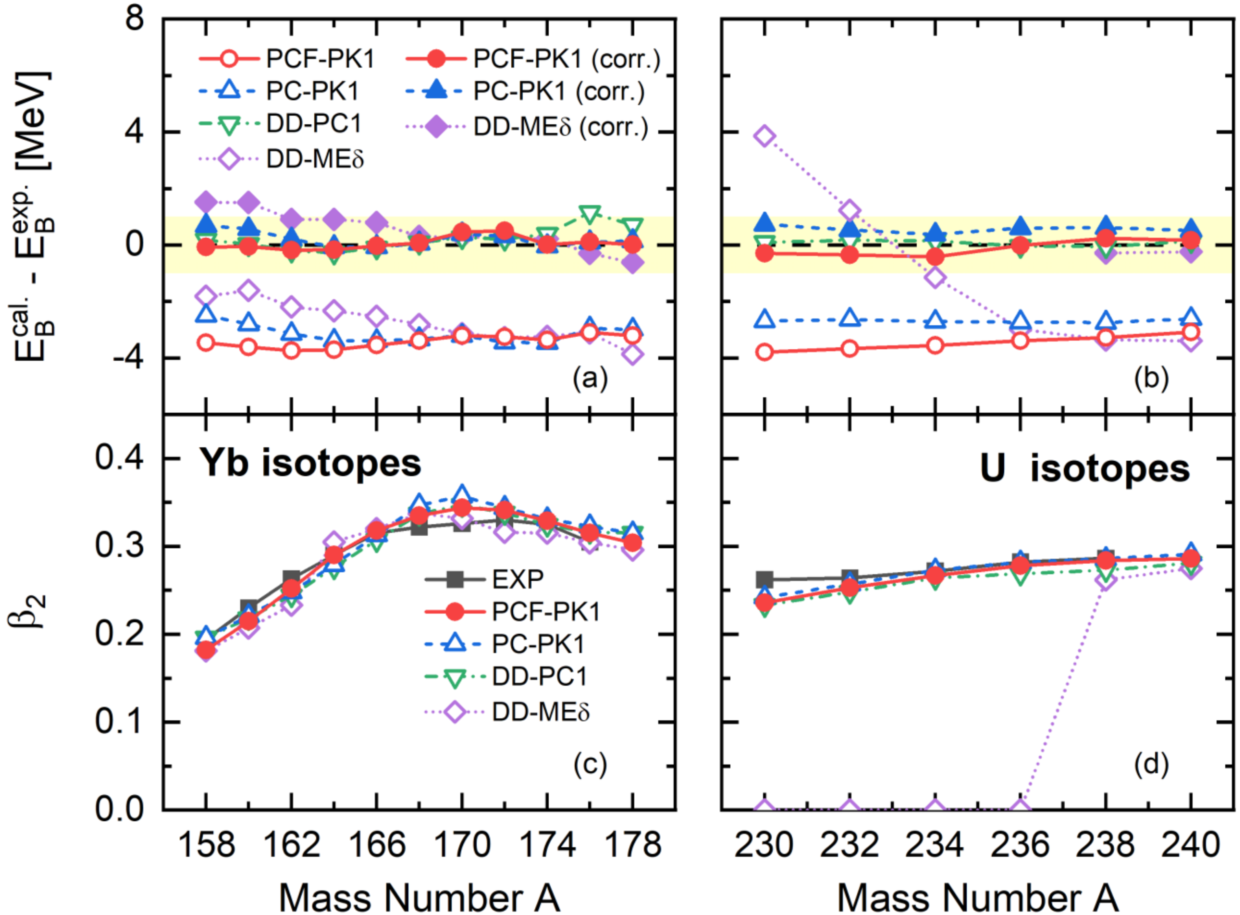


RMSD of binding energies for 60 reference nuclei calculated by PCF-PK1 is 1.42 MeV, which is comparable with one of the most successful functional PC-PK1.

Contents

Deformed Nuclei

- Binding Energy and deformation β_2 of Yb and U calculated by PCF-PK1



Exp. taken from Wang et al., CPC 41, 030003 (2017), Pritychenko et al., ADNDT 107, 1(2016)

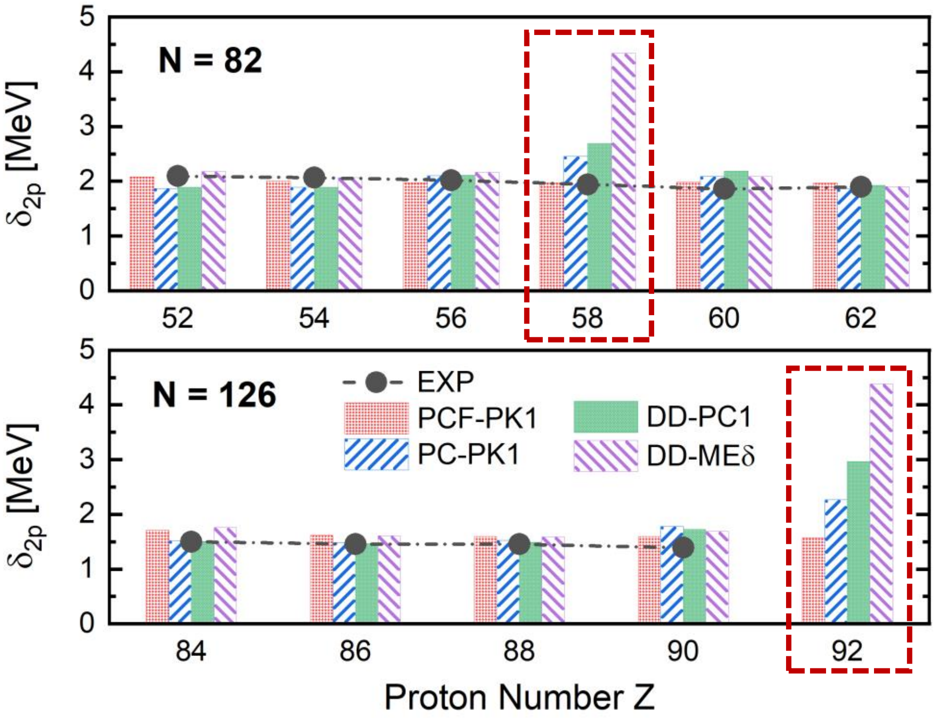
PCF-PK1 well describe the binding energy and deformation of Yb and U isotopes.

Spurious Shell

- Two-proton shell gap: Evaluate the size of shell gaps

$$\delta_{2p}(Z, N) = S_{2p}(Z, N) - S_{2p}(Z+2, N)$$

S_{2p}: Two-proton separation energy



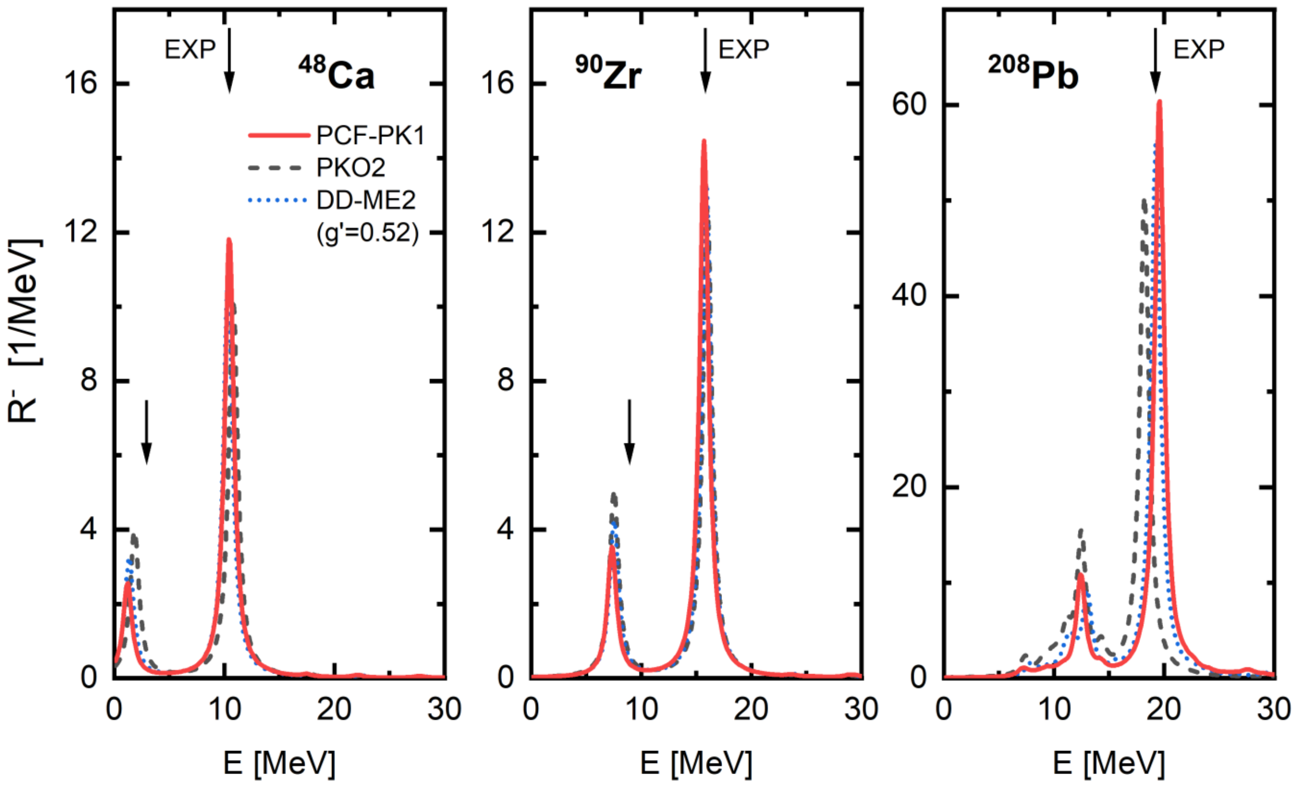
Exp from
Wang et al., CPC 41, 030003 (2017)

Z = 92 is not supported as a shell closure by recent experiment near N = 126.
Sun et al., PLB 771, 303 (2017)

PCF-PK1 improves the description of shell structures around Z=58 and Z=92.

Gamow-Teller Resonance

- Strength distribution of Gamow-Teller resonances for ^{48}Ca, ^{90}Zr, and ^{208}Pb



Exp from:

Anderson et al., PRC 31, 1161 (1985)

Bainum et al., PRL 44, 1751 (1980)

Wakasa et al., PRC 55, 2909 (1997)

Horen et al., PLB 95, 27 (1980)

Akimune et al., PRC 52, 604 (1995)

PCF-PK1 can self-consistently describe the GTR excitation energy without adjusting additional parameters.

Contents

Summary

- Based on relativistic point-coupling model, a new covariant density functional PCF-PK1 are developed with localized exchange terms. It can
  - Well describe the binding energy of finite nuclei, and has the same precision as existed functional PC-PK1
  - Eliminate the spurious shell closure at $Z = 58$ and $Z = 92$
  - Self-consistently describe the Gamow-Teller resonance

- For meson-exchange interaction, the exchange terms can be taken into account by the orbital-dependent relativistic density functional theory.

(In Preparation)

Thank you!