

**INT PROGRAM INT-13-3**

**Quantitative Large Amplitude Shape Dynamics:** 

**fission and heavy ion fusion**

*September 23 - November 15, 2013*

# New generation of relativistic approach for nuclear structure

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EDF – CDFT – RMF – RHF – RBHF



# **Outline**

- $\Box$ Introduction
- $\Box$ CDFT at the Hartree level (success)
- $\Box$ CDFT at the Hartree-Fock level (new learning)
- $\Box$ Full Dirac Brueckner-Hartree-Fock (expection)
- $\Box$ DBHF calculation for <sup>16</sup>O, <sup>40</sup>Ca, <sup>48</sup>Ca and <sup>56</sup>Ni
- $\Box$ Summary & Perspectives



#### **Nuclear Energy Density Functional**

**Nuclear Energy Density Functionals:** the many-body problem is mapped onto a one-body problem without explicitly involving inter-nucleon interactions!

#### **Kohn-Sham Density Functional Theory**

For any interacting system, there exists a **local single-particle potential**  $h(r)$ **,** such that the exact groundstate density of the interacting system can be reproduced by **non-interacting particles** moving in this local potential.

$$
E[\hat{\rho}] = \langle \Psi | H | \Psi \rangle \qquad \hat{h} = \frac{\delta E}{\delta \hat{\rho}}
$$

The practical usefulness of the Kohn-Sham scheme depends entirely on whether **Accurate Energy Density Functional can be found!** 

#### 2013-10-10



 $\bullet$  Nuclear energy density functional has been introduced by effective Hamiltonians

$$
E = \langle \Psi | H | \Psi \rangle \approx \langle \Phi | \hat{H}_{eff}(\hat{\rho}) | \Phi \rangle = E[\hat{\rho}]
$$

- $\bullet$ More degrees of freedom: spin, isospin, relativistic, pairing
- $\bullet$ • Nuclei are self-bound systems;  $\rho(r)$  here denotes the intrinsic density.
- $\bullet$ Density functional is probably not exact, but a very good approximation.
- $\bullet$  The functional are adjusted to characteristic properties of nuclear matter and/or finite nuclei and (in future) to ab-initio results.

#### Nuclear functional usually used:

- non-relativistic zero range forces (Skyrme)
- $\triangleright$  non-relativistic finite range forces of Gaussian shape (Gogny)
- $\triangleright$  relativistic (covariant) density functional theory (RMF)



# $(\overline{\psi} \circ \Gamma \psi), 0 \in \{1, \overrightarrow{\tau}\}, \Gamma \in \{1, \gamma_{\mu}, \gamma_{5}, \gamma_{5} \gamma_{\mu}, \sigma_{\mu \nu}\}\$

**Lagrangian density:** For the nucleon Dirac spinor field  $\psi$ , there are ten building blocks characterized by their transformation characteristics in isospin and Minkowski space.

$$
L = \overline{\psi}(i\gamma_{\mu}\partial^{\mu} - m)\psi
$$
  
\n
$$
-\frac{1}{2}\alpha_{s}(\overline{\psi}\psi)(\overline{\psi}\psi) - \frac{1}{2}\alpha_{v}(\overline{\psi}\gamma_{\mu}\psi)(\overline{\psi}\gamma^{\mu}\psi) - \frac{1}{2}\alpha_{\text{TV}}(\overline{\psi}\overline{\tau}\gamma_{\mu}\psi)(\overline{\psi}\overline{\tau}\gamma^{\mu}\psi)
$$
  
\n
$$
-\frac{1}{3}\beta_{s}(\overline{\psi}\psi)^{3} - \frac{1}{4}\gamma_{s}(\overline{\psi}\psi)^{4} - \frac{1}{4}\gamma_{v}[(\overline{\psi}\gamma_{\mu}\psi)(\overline{\psi}\gamma^{\mu}\psi)]^{2}
$$
  
\n
$$
-\frac{1}{2}\delta_{s}\partial_{v}(\overline{\psi}\psi)\partial^{\nu}(\overline{\psi}\psi) - \frac{1}{2}\delta_{v}\partial_{v}(\overline{\psi}\gamma_{\mu}\psi)\partial^{\nu}(\overline{\psi}\gamma^{\mu}\psi) - \frac{1}{2}\delta_{\text{TV}}\partial_{v}(\overline{\psi}\overline{\tau}\gamma_{\mu}\psi)\partial^{\nu}(\overline{\psi}\overline{\tau}\gamma_{\mu}\psi)
$$
  
\n
$$
-e\frac{1-\tau_{3}}{2}\overline{\psi}\gamma^{\mu}\psi A_{\mu} - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}
$$
 Higher order terms  
\nLocalized form of Fock terms



## Parameterizations PC-PK1

#### **Zhao, Li, Yao, Meng, PRC 82, 054319 (2010)**





Fitting to 60 binding energies, 17 charge radii, and empirical pairing gaps of 60 selected spherical nuclei.

2013-10-10



Deformed nuclei



**Zhao, Li, Yao, Meng, PRC 82, 054319 (2010)**



## Fission barrier in actinides

The structure of <sup>240</sup>Pu and its double-humped fission barrier: a standard benchmark for self-consistent mean-field models



- $\checkmark$  The deformation of the ground state and the excited energy of the fission isomer are reproduced well;
- much closer to the available data. Li, Niksic, Vretenar, Ring, Meng, Phys.Rev.C81, 064321 (2010)  $\checkmark$  The inclusion of triaxial shapes lowers the inner barrier by  $\approx$  2 MeV,



## $240$ Pu: 3D PES (β<sub>20</sub>, β<sub>22</sub>, β<sub>30</sub>) in MD constraint CDFT

β2, β3, …: Geng, Meng, Toki, 2007, Chinese Phys. Lett. 24-1865 β2, γ, …: Meng, Peng, Zhang, Zhou, 2006, PRC 73-037303



- • Axial & reflection symmetric shapes for ground state & isomer, the latter is stiffer
- •Triaxial shape around the inner barrier
- • Triaxial & octupole shape around the outer barrier; this is also true for other actinide nuclei

Lu, Zhao, Zhou, PRC85 (2012) 011301R  $\beta_{\lambda\mu}$  with even  $\mu$  are included automatically





### Simultaneous quadrupole and octupole shape phase transitions in Thorium



Z. P. Li, B. Y. Song, J. M. Yao, D. Vretenar, J. Meng **Simultaneous quadrupole and octupole shape phase transitions in Thorium** arXiv:1304.3766 [nucl-th] Physics Letters B *In Press, Available online 21 September 2013*



**Data for 2149 nuclei from Audi et al. NPA2003**



**Zhao, Song, Sun. Geissel, Meng, Phys. Rev. C 86, 064324 (2012) Crucial test for covariant density functional theory with new and accurate mass measurements from Sn to Pa**

#### **Long-term plan**

11**Improve the mass description based on CDFT to σ <sup>~</sup>0.5 MeV.**



### Extending the nuclear chart by continuum: from oxygen to lead



Xiaoying Qu, Ying Chen, Shuangquan Zhang, Pengwei Zhao, Ik Jae Shin, Yeunhwan Lim, Youngman Kim, Jie Meng **[arXiv:1309.3987] Extending the nuclear chart by continuum: from oxygen to titanium**







## **Very successful in nuclear physics**

Ring PPNP1996, Vretenar Phys.Rep.2005, Meng PPNP2006

- Spin-orbit splitting
- Pseudo-spin symmetry
- $\triangleright$  Nuclear saturation properties
- $\triangleright$  Exotic nuclei

……

Excellent reproduction of nuclear properties



Meng, Peng, Zhang, Zhao, Front. Phys.2013





## **The relativistic Hartree-Fock theory**

Bouyssy PRC 1987 Bernardos PRC 1993 Marcos JPG 2004 Bürvenich PRC 2002

#### In addition of the RMF advantages

- $\triangleright$  Pion contribution included
- $\triangleright$  Nuclear effective mass
- $\triangleright$  Fully self-consistent description for spin-isospin excitation

**15**

 $\blacktriangleright$ ……

Long PLB2006, Long PRC2007, Liang PRL2008, Liang PRC2009

15



 $\triangleright$  Single particle Hamiltonian: Kinetic energy: Local potentials:

Non-local Potentials:

$$
h^{\text{kin}}(\mathbf{r}, \mathbf{r}') = [\alpha \cdot \mathbf{p} + \beta M] \delta(\mathbf{r}, \mathbf{r}'),
$$
  
\n
$$
h^{\text{D}}(\mathbf{r}, \mathbf{r}') = [\Sigma_T(\mathbf{r})\gamma_5 + \Sigma_0(\mathbf{r}) + \beta \Sigma_S(\mathbf{r})] \delta(\mathbf{r}, \mathbf{r}'),
$$
  
\n
$$
h^{\text{E}}(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} Y_G(\mathbf{r}, \mathbf{r}') & Y_F(\mathbf{r}, \mathbf{r}') \\ X_G(\mathbf{r}, \mathbf{r}') & X_F(\mathbf{r}, \mathbf{r}') \end{pmatrix}
$$

Pairing Force: Gogny D1S

$$
V(\mathbf{r},\mathbf{r}') = \sum_{i=1,2} e^{((r-r')/\mu_i)^2} (W_i + B_i P^{\sigma} - H_i P^{\tau} - M_i P^{\sigma} P^{\tau})
$$

▶ Dirac Woods-Saxon Basis: solve the integro-differential RHFB equation



## Charge-exchange excitation modes

#### RH + RPA

- $\Diamond$  No contribution from isoscalar mesons ( <sup>σ</sup>,<sup>ω</sup>), because exchange terms are missing.
- $\Diamond$   $\pi$ -meson is dominant in this resonance.
- $\Leftrightarrow$  zero-range pionic counter-term g' has to be refitted to reproduce the data.

#### RHF + RPA

- $\Diamond$  Isoscalar mesons  $(\sigma,\omega)$  play an essential role via the exchange terms.
- $\Diamond$  While,  $\pi$ -meson plays a minor role.  $\diamond$  g' = 1/3 is kept for self-consistency.



![](_page_17_Picture_0.jpeg)

### Lcalized form of Fock terms

![](_page_17_Figure_2.jpeg)

The fine structure of spin-dipole excitations in O-16 is reproduced quite well in <sup>a</sup> fully self-consistent RPA calculation based on the RHF theory

#### **Liang, Giai, Meng PRL 101, 122502 (2008) Liang, Zhao, Meng Phys. Rev. C 85, 064302 (2012)**

![](_page_17_Figure_5.jpeg)

- **A localized form of Fock terms** is proposed with considerable simplicity as compared to the conventional Fock terms.
- • Based on this localized RHF theory, the spindipole excitation in Zr-90 is well reproduced with a RPA calculation.

2013-10-10 **Liang, Zhao, Ring, Roca-Maza, Meng Phys. Rev. C 86, 021302 (2012)**

•

![](_page_18_Picture_0.jpeg)

#### New generation CDFT: *ab initio* calculation

![](_page_19_Picture_0.jpeg)

## *ab initio-***---- "from the beginning"**

- $\blacktriangleright$ without additional assumptions
- $\blacktriangleright$ without additional parameters

## *ab initio* **in nuclear physics**

- $\blacktriangleright$ with realistic nucleon-nucleon interaction
- $\blacktriangleright$ with some few-body methods and many-body methods, such as Monte Carlo method, shell model and energy density functional theory

![](_page_19_Figure_8.jpeg)

![](_page_20_Picture_0.jpeg)

## ab initio calculation in nuclear physics

## *ab initio* **calculation for light nuclei**

![](_page_20_Figure_3.jpeg)

Pieper, Wiringa, et al

Expt.

### *ab initio* **calculation for heavier nuclei**

- > Coupled Channel method Hagen PRL2009
- $\triangleright$  BHF theory

Hjorth-Jensen Phys.Rep.1995 With HJ potential Dawson Ann.Phys.1962 With Reid potential Machleidt NPA1975

![](_page_20_Picture_88.jpeg)

With Bonn potentials Muether PRC1990 16<sub>O</sub> in BHF method in Bonn potential

![](_page_21_Picture_0.jpeg)

## *ab initio* CDFT calculation for nucleus

## **Relativistic Brueckner Hartree-Fock: nuclear matter**

 $\triangleright$  Nuclear matter Anastasio PRep 1978 Brockmann PLB 1984 ter Haar PRep. 1987 Defining an effective medium dependent meson-exchange interaction based upon the nuclear matter G matrix Brockmann PRC1990 Brockmann PRL 1992 Fritz PRL 1993

#### *ab initio* **calculation CDFT attempt for finite nucleus: extracted interaction from the** *ab initio* **calculation for nuclear matter**

> Density-dependent relativistic mean field theory Brockmann PRL1992 > Density-dependent relativistic Hartree-Fock theory Fritz PRL1993

![](_page_22_Picture_0.jpeg)

#### **Relativistic Brueckner Hartree-Fock calculation for finite nucleus**

- *ab initio* **CDFT / Full Relativistic Brueckner Hartree-Fock calculation for finite nucleus with expansion in Harmonics Oscillator (HO) basis**
- $\blacktriangleright$ **Effective NN interaction: Brueckner G-matrix in HO basis**
- **Solve relativistic Hartree-Fock (RHF) equation in HO basis with the G-matrix in HO basis**

![](_page_23_Picture_0.jpeg)

T-Matrix and G-Matrix

![](_page_23_Figure_2.jpeg)

#### **Bethe-Goldstone Equation**

![](_page_23_Figure_4.jpeg)

$$
G = V + V \frac{Q}{E - H_0} G
$$

- $\triangleright$  *E* is the starting energy
- *Q* is the Pauli operator
- *G*-matrix is for many-body problem

![](_page_23_Figure_10.jpeg)

![](_page_24_Picture_0.jpeg)

Bethe-Goldstone equation

**Bethe-Goldstone equation in basis space**

$$
\langle nm|G(\omega)|n'm'\rangle = \langle nm|V|n'm'\rangle + \sum_{\varepsilon_i,\varepsilon_j>\varepsilon_F} \frac{\langle nm|V|ij\rangle\langle ij|G(\omega)|n'm'\rangle}{\omega - (\varepsilon_i + \varepsilon_j)}
$$

where  $\mathcal{E}_F$  is the Fermi energy,  $\omega = \mathcal{E}_m + \mathcal{E}_n$  is the starting energy and  $\;l,J$  are intermediate states.  $\mathcal{L} = \mathcal{E}_m + \mathcal{E}_n$  is the starting energy and  $(i, j)$ 

#### **Bethe-Goldstone equation in plane wave basis**

$$
G_{ll'}^{\alpha}(kk'K\omega) = V_{ll'}^{\alpha}(kk') + \sum_{ll'} \frac{d^3q}{(2\pi)^3} V_{ll'}^{\alpha}(kq) \frac{Q(q,K)}{\omega - H_0} G_{ll'}^{\alpha}(qk'K\omega)
$$

where  $\alpha$  is a shorthand notation for  $J, S, L$  and  $T$ .

**Matrix inversion method**

$$
G = \left(1 - \frac{V}{\omega - H_0}\right)^{-1} V
$$

![](_page_25_Figure_0.jpeg)

![](_page_26_Picture_0.jpeg)

Relativistic Brueckner Hartree-Fock theory

**Relativistic Brueckner Hartree-Fock (RBHF) equation**

$$
\sum_{n'} (\alpha \cdot p + \beta M + \beta \Gamma^{BHF})_{nn'} \psi_{n'} = \varepsilon_n \psi_n
$$

where  $\Gamma^{BHF}_{nn'}$  is related with the density matrix  $\rho_{nn'}$ 

$$
\Gamma_{nn'}^{BHF}=G_{nnnn'm'}\rho_{mm'}-G_{nnmm'n'}\rho_{mm'}
$$

#### **RHF equation in HO basis**

$$
\begin{pmatrix} A_{nn'}^{BHF} & B_{n\overline{n'}}^{BHF} \\ B_{n'n}^{BHF} & C_{\overline{n}\overline{n'}}^{BHF} \end{pmatrix} \begin{pmatrix} f_n^{(a)} \\ g_n^{(a)} \end{pmatrix} = \mathcal{E}_a \begin{pmatrix} f_n^{(a)} \\ g_n^{(a)} \end{pmatrix}
$$

where

$$
A_{nn'}^{BHF} = (\alpha \cdot p + \beta M)_{nn'} + \sum_{b} \sum_{m,m'} f_m^{(b)} f_m^{(b)} (G_{nmn'm'} - G_{nmm'n'})
$$
  
\n
$$
B_{n\overline{n'}}^{BHF} = (\alpha \cdot p + \beta M)_{n\overline{n'}} + \sum_{b} \sum_{m,m'} f_m^{(b)} g_{m'}^{(b)} (G_{nm\overline{n'}m'} - G_{nm\overline{m'}n'})
$$
  
\n
$$
C_{\tilde{n}\overline{n'}}^{BHF} = (\alpha \cdot p + \beta M)_{\tilde{n}\overline{n'}} + \sum_{20\overline{\beta_3}} \sum_{m,m'} g_{m'}^{(b)} g_{m'}^{(b)} (G_{\tilde{n}\overline{m}\overline{n'}m'} - G_{\tilde{n}\overline{m}\overline{m'}n'}).
$$

![](_page_27_Picture_0.jpeg)

Numerical check: RHF equation in HO &RHO basis

## **Example**

 $\triangleright$  Object: <sup>16</sup>O

> Interaction: Bouyssy C Bouyssy PRC1987

 Basis: Harmonics Oscillator (HO) (*N=*12) Relativistic Harmonics Oscillator (RHO) (*N<sub>F</sub>*=12, *N<sub>D</sub>*=8)

## **The properties of** <sup>16</sup> O

![](_page_27_Picture_79.jpeg)

The properties of 16O with different methods with Bouyssy interaction

[1] Bouyssy PRC1987

Hu, Meng, Ring, *to be published.*

![](_page_28_Picture_0.jpeg)

## Convergence of RBHF theory

## **Example**

- $\triangleright$  Object: <sup>16</sup>O
- > Interaction: Bonn A Machleidt ANP1987
- Basis: Harmonics Oscillator (HO)

![](_page_28_Figure_7.jpeg)

![](_page_29_Picture_0.jpeg)

![](_page_29_Picture_32.jpeg)

[1] Audi NPA2003, [2] Muether PRC1990, [3]Long PLB2006

### **Energy components of 16O in RBHF theory**

![](_page_29_Picture_33.jpeg)

Hu, Meng, Ring, *to be published.*

![](_page_30_Picture_0.jpeg)

#### **Single proton energies for 16O in RBHF theory**

![](_page_30_Picture_51.jpeg)

![](_page_30_Figure_4.jpeg)

![](_page_31_Picture_1.jpeg)

**The scalar and vector potentials in RMF and RBHF theories**

![](_page_31_Figure_3.jpeg)

**Spin-orbit force in RMF theory**

$$
U_{s.o.} \propto (U_{V} - U_{s}) \vec{L} \cdot \vec{S}
$$

DDRH and DDRHF based on RBHF

PEKING UNIVERSITY **The Lagrangian of Density-dependent RH (DDRH) theory** 

北京大学

Brockmann PRL1992

 $(\rho)$ 

 $\rho$  )  $\sigma$ 

 $\rho) \omega$ 

 $S$   $\bar{\phantom{a}}$   $\delta$   $\sigma B$ 

**DDRH\***

 $\sigma$ 

 $\omega$ 

 $U_s = g$ 

 $=$ 

 $U_{\scriptscriptstyle V}$  = g

Ξ

 $V$   $\bar{\phantom{a}}$   $\delta$   $\omega B$ 

 $(\rho)$ 

$$
L = \overline{\psi}_N (i\gamma_\mu \partial^\mu - M_N - g_{\sigma N}(\rho)\sigma - g_{\omega N}(\rho)\gamma_\mu \omega^\mu - e\gamma_\mu \frac{1 - \tau^3}{2} A^\mu) \psi_N
$$
  
+ 
$$
\frac{1}{2} \partial_\mu \sigma \partial^\mu \sigma - \frac{1}{2} m_\sigma^2 \sigma^2 - \frac{1}{4} \Omega_{\mu\nu} \Omega^{\mu\nu} + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu
$$

**The Lagrangian of Density-dependent RHF (DDRHF) theory** 

Fritz PRL1993

$$
L = \overline{\psi}_N (i\gamma_\mu \partial^\mu - M_N - g_{\sigma N}(\rho) \sigma - g_{\omega N}(\rho) \gamma_\mu \omega^\mu - \frac{f_{\pi N}}{m_\pi}(\rho) \tau^a \gamma_5 \gamma_\mu \partial^\mu \pi^a - e \gamma_\mu \frac{1 - \tau^3}{2} A^\mu) \psi_N
$$
  
+ 
$$
\frac{1}{2} \partial_\mu \sigma \partial^\mu \sigma - \frac{1}{2} m_\sigma^2 \sigma^2 - \frac{1}{4} \Omega_{\mu\nu} \Omega^{\mu\nu} + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu
$$
  
+ 
$$
\frac{1}{2} \partial_\mu \pi^a \partial^\mu \pi^a - \frac{1}{2} m_\pi^2 \pi^{a2}
$$
  
U<sub>V</sub> =  $g_{\sigma B}(\rho) \sigma$   

$$
U_V = g_{\omega B}(\rho) \omega
$$

![](_page_33_Picture_0.jpeg)

#### **Properties of 16O**

![](_page_33_Figure_3.jpeg)

[1] Audi NPA2003

\* DD couplings extracted from RBHF theory at nuclear matter

Hu, Meng, Ring, *to be published.* Also have not a set of  $\frac{34}{4}$ 

![](_page_34_Picture_0.jpeg)

DDRH and DDRHF based on RBHF

#### **Single particle levels in 16O**

![](_page_34_Figure_3.jpeg)

Hu, Meng, Ring, *to be published.*

DDRH and DDRHF based on RBHF

![](_page_35_Picture_1.jpeg)

![](_page_35_Figure_2.jpeg)

![](_page_36_Picture_0.jpeg)

#### **Relation between binding energy and radii of 16 O**

![](_page_36_Figure_3.jpeg)

![](_page_37_Picture_0.jpeg)

#### **Relation between binding energy and radii**

![](_page_37_Figure_2.jpeg)

![](_page_38_Picture_0.jpeg)

### **Ground state properties in RBHF theory**

![](_page_38_Picture_46.jpeg)

#### **Deviations of binding energy between data and RBHF calculation**

![](_page_38_Picture_47.jpeg)

 $\triangleright$ The binding energy is reproduced within10% in RBHF

 $\triangleright$  The spin-orbit splitting is small

Hu, Meng, Ring, *to be published.*

![](_page_39_Picture_0.jpeg)

# Summary and Perspectives

- New generation of CDFT, i.e., Relativistic Brueckner-Hartree-Fock (RBHF) theory is developed for finite nuclei in HO basis.
- The code of RHF equation in HO basis is confirmed by reproduce the same results as in coordinate space.
- $\triangleright$  RBHF calculation for <sup>16</sup>O with Bonn potential has been check up to N fermion  $= 28$ .
- The experimental binding energy, charge radii and spin-orbit splitting for  ${}^{14}C$ ,  ${}^{16}O$ ,  ${}^{40}Ca$ ,  ${}^{48}Ca$  and  ${}^{56}Ni$  are reproduced with RBHF within 10%, and RBHF results are comparable with the ones from PKO1.
- 2013-10-10 $\blacktriangleright$ Calculation for heavier nuclei is in progress.<br>Thank you for your attention!