

**INT PROGRAM INT-13-3** 

**Quantitative Large Amplitude Shape Dynamics:** 

fission and heavy ion fusion

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# New generation of relativistic approach for nuclear structure

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 $\mathsf{EDF}-\mathsf{CDFT}-\mathsf{RMF}-\mathsf{RHF}-\mathsf{RBHF}$ 



## Outline

- **D** Introduction
- □ CDFT at the Hartree level (success)
- □ CDFT at the Hartree-Fock level (new learning)
- □ Full Dirac Brueckner-Hartree-Fock (expection)
- **D** DBHF calculation for  ${}^{16}O$ ,  ${}^{40}Ca$ ,  ${}^{48}Ca$  and  ${}^{56}Ni$
- □ 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!

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• Nuclear energy density functional has been introduced by effective Hamiltonians

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

- More degrees of freedom: spin, isospin, relativistic, pairing
- Nuclei are self-bound systems;  $\rho(r)$  here denotes the intrinsic density.
- Density functional is probably not exact, but a very good approximation.
- 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)
- > non-relativistic finite range forces of Gaussian shape (Gogny)
- relativistic (covariant) density functional theory (RMF)

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## $(\ \boldsymbol{\bar{\psi}} \ \textit{\textit{O}} \ \boldsymbol{\boldsymbol{\Gamma}} \ \boldsymbol{\psi}), \textit{\textit{O}} \in \{1, \vec{\tau}\}, \ \boldsymbol{\boldsymbol{\boldsymbol{\Gamma}}} \in \{1, \gamma_{\mu,} \ \gamma_{5,} \ \gamma_{5} \gamma_{\mu,} \ \sigma_{\mu\nu} \ \}$

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

$$\begin{split} L &= \overline{\psi}(i\gamma_{\mu}\partial^{\mu} - m)\psi \\ &- \frac{1}{2}\alpha_{s}(\overline{\psi}\psi)(\overline{\psi}\psi) - \frac{1}{2}\alpha_{v}(\overline{\psi}\gamma_{\mu}\psi)(\overline{\psi}\gamma^{\mu}\psi) - \frac{1}{2}\alpha_{Tv}(\overline{\psi}\overrightarrow{\tau}\gamma_{\mu}\psi)(\overline{\psi}\overrightarrow{\tau}\gamma^{\mu}\psi) \\ &- \frac{1}{3}\beta_{s}(\overline{\psi}\psi)^{3} - \frac{1}{4}\gamma_{s}(\overline{\psi}\psi)^{4} - \frac{1}{4}\gamma_{v}[(\overline{\psi}\gamma_{\mu}\psi)(\overline{\psi}\gamma^{\mu}\psi)]^{2} \\ &- \frac{1}{2}\delta_{s}\partial_{v}(\overline{\psi}\psi)\partial^{v}(\overline{\psi}\psi) - \frac{1}{2}\delta_{v}\partial_{v}(\overline{\psi}\gamma_{\mu}\psi)\partial^{v}(\overline{\psi}\gamma^{\mu}\psi) - \frac{1}{2}\delta_{Tv}\partial_{v}(\overline{\psi}\overrightarrow{\tau}\gamma_{\mu}\psi)\partial^{v}(\overline{\psi}\overrightarrow{\tau}\gamma_{\mu}\psi) \\ &- e\frac{1-\tau_{3}}{2}\overline{\psi}\gamma^{\mu}\psi A_{\mu} - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} \end{split}$$
 Higher order terms Localized 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.

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**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



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





β2, β3, …: Geng, Meng, Toki, 2007, Chinese Phys. Lett. 24-1865
 β2, γ, …: Meng, Peng, Zhang, Zhou, 2006, PRC 73-037303
 Lu, Zhao, Zhou, PRC85 (2012) 011301R



- 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

 $\beta_{\lambda\mu}$  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

Improve the mass description based on CDFT to  $\sigma \sim 0.5$  MeV. ΠT



## 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
- Nuclear saturation properties
- 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

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

▶ .....

Long PLB2006, Long PRC2007, Liang PRL2008, Liang PRC2009

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Single particle Hamiltonian:
 Kinetic energy: h<sup>k</sup>
 Local potentials: h

Non-local Potentials:

$$h^{\rm kin}(\mathbf{r}, \mathbf{r}') = [\boldsymbol{\alpha} \cdot \mathbf{p} + \beta M] \,\delta(\mathbf{r}, \mathbf{r}'),$$
  

$$h^{\rm D}(\mathbf{r}, \mathbf{r}') = [\boldsymbol{\Sigma}_T(\mathbf{r})\gamma_5 + \boldsymbol{\Sigma}_0(\mathbf{r}) + \beta \boldsymbol{\Sigma}_S(\mathbf{r})] \,\delta(\mathbf{r}, \mathbf{r}'),$$
  

$$h^{\rm E}(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} Y_G(\mathbf{r}, \mathbf{r}') & Y_F(\mathbf{r}, \mathbf{r}') \\ X_G(\mathbf{r}, \mathbf{r}') & X_F(\mathbf{r}, \mathbf{r}') \end{pmatrix}$$

Pairing Force: Gogny D1S

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

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



## Charge-exchange excitation modes

#### RH + RPA

- $\Rightarrow$   $\pi$ -meson is dominant in this resonance.
- ♦ zero-range pionic counter-term g' has to be refitted to reproduce the data.

#### RHF + RPA

- $\Rightarrow \text{ Isoscalar mesons } (\sigma, \omega) \text{ play an} \\ \text{essential role via the exchange terms.}$
- ♦ While, π-meson plays a minor role.
  ♦ g' = 1/3 is kept for self-consistency.





#### Lcalized form of Fock terms



The fine structure of spin-dipole excitations in O-16 is reproduced quite well in a 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)



- 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.

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



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



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

- without additional assumptions
- without additional parameters

## ab initio in nuclear physics

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





## ab initio calculation in nuclear physics

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## ab initio calculation for light nuclei



Pieper, Wiringa, et al.

Expt

### ab initio calculation for heavier nuclei

- Coupled Channel method
- BHF theory With HJ potential With Reid potential With Bonn potentials

thod Hagen PRL2009 Hjorth-Jensen Phys.Rep.1995 Dawson Ann.Phys.1962 Machleidt NPA1975 Muether PRC1990

	Bonn C	Bonn B	Bonn A	Exp.
$\varepsilon_{1s_{1/2}}$	-39.73	-44.37	-50.46	$-40\pm8$
$\varepsilon_{1p_{3/2}}$	-16.98	-19.49	-22.89	-18.4
$\varepsilon_{1p_{1/2}}$	-11.64	-13.24	-15.44	-12.1
Ē	-71.84	-85.60	-104.96	-127.68
r <sub>c</sub>	2.465	2.380	2.291	2.737

<sup>16</sup>O in BHF method in Bonn potential



## ab initio CDFT calculation for nucleus

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

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
 Density-dependent relativistic Hartree-Fock theory

Brockmann PRL1992 Fritz PRL1993



#### **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
- **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



100

50

**0.0** 

0.2

T-Matrix and G-Matrix

#### **Lippmann-Schwinger Equation** Lippmann Phys. Rev 1950 $T = V + V \frac{1}{E - H_0} T$ V is the realistic NN interaction $\succ$ *E* is the incident energy > T-matrix is for two-body scattering The corresponding EOS in HF 400 350 Relativeitc Hatteerto 300 E/A [MeV] 250 200 150 Non-relativsitc Hartree-Fock

0.6

0.8

0.4

ρ **[fm<sup>-3</sup>]** 

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

Brueckner Phys. Rev 1955

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

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

The corresponding EOS in HF





**Bethe-Goldstone equation** 

**Bethe-Goldstone equation in basis space** 

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

where  $\mathcal{E}_F$  is the Fermi energy,  $\mathcal{O} = \mathcal{E}_m + \mathcal{E}_n$  is the starting energy and i, j are intermediate states.

#### **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

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





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

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

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

$$G_{nn'}^{BHF} = G_{nmn'm'}\rho_{mm'} - G_{nmm'n'}\rho_{mm'}$$

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

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

where

$$\begin{split} A_{nn'}^{BHF} &= (\alpha \cdot p + \beta M)_{nn'} + \sum_{b} \sum_{m,m'} f_m^{(b)} f_{m'}^{(b)} (G_{nmn'm'} - G_{nmm'n'}) \\ B_{nn'}^{BHF} &= (\alpha \cdot p + \beta M)_{nn'} + \sum_{b} \sum_{m,m'} f_m^{(b)} g_{m'}^{(b)} (G_{nmn'm'} - G_{nmm'n'}) \\ C_{\tilde{n}n'}^{BHF} &= (\alpha \cdot p + \beta M)_{\tilde{n}n'} + \sum_{20} \sum_{m,m'} g_m^{(b)} g_{m'}^{(b)} (G_{\tilde{n}mn'm'} - G_{\tilde{n}mm'n'}) \end{split}$$

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Numerical check: RHF equation in HO &RHO basis

## Example

- ➢ 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

	r-space[1]	HO	RHO
E (MeV)	-49.44	-49.45	-49.45
<b>r</b> <sub>c</sub> (fm)	2.91	2.90	2.91
$\varepsilon_{1p_{1/2}} - \varepsilon_{1p_{3/2}}$ (MeV)	5.5	5.5	5.5

The properties of <sup>16</sup>O with different methods with Bouyssy interaction

[1] Bouyssy PRC1987

Hu, Meng, Ring, to be published.



## **Convergence of RBHF theory**

## Example

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

Machleidt ANP1987



**Convergence of RBHF calculation for <sup>16</sup>O** 

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<b>Properties of <sup>16</sup>O</b>								
	EXP.	RBHF	BHF	PK01				
	[1]	(N=28)	[2]	[3]				
E (MeV)	-127.62	-119.552	-104.96	-128.36				
<i>r<sub>c</sub></i> (fm)	2.737	2.6357	2.291	2.679				
$\varepsilon_{1 p_{1/2}} - \varepsilon_{1 p_{3/2}}$ (MeV)	6.3	4.1	7.5	6.3				

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

## **Energy components of <sup>16</sup>O in RBHF theory**

Methods	$\langle T \rangle$	$\langle V_m \rangle$	E <sub>coul</sub>	E <sub>c.m.</sub>	E <sub>tot</sub> .
PK01	209.176	-340.910	13.942	-10.572	-128.364
RBHF (N=28)	235.315	-357.898	14.037	-11.006	-119.552

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Hu, Meng, Ring, to be published.  $30^{30}$ 



#### Single proton energies for <sup>16</sup>O in RBHF theory

	EXP.	RBHF (N=28)	BHF	PKO1
$\varepsilon_{1s_{1/2}}$	$-40\pm8$	-34.085	-50.46	-34.682
$\varepsilon_{1p_{3/2}}$	-18.451	-16.954	-22.89	-17.719
$\varepsilon_{1p_{1/2}}$	-12.127	-12.872	-15.44	-11.417





The scalar and vector potentials in RMF and RBHF theories



**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

**DDRH\*** 

$$L = \overline{\psi}_{N} (i\gamma_{\mu}\partial^{\mu} - M_{N} - g_{\sigma N}(\rho)\sigma - g_{\omega N}(\rho)\gamma_{\mu}\omega^{\mu} - e\gamma_{\mu}\frac{1 - \tau^{3}}{2}A^{\mu})\psi_{N}$$
  
+ 
$$\frac{1}{2}\partial_{\mu}\sigma\partial^{\mu}\sigma - \frac{1}{2}m_{\sigma}^{2}\sigma^{2} - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_{\omega}^{2}\omega_{\mu}\omega^{\mu}$$
$$U_{S} = g_{\sigma B}(\rho)\sigma$$
$$U_{V} = g_{\omega B}(\rho)\omega$$

The Lagrangian of Density-dependent RHF (DDRHF) theory

Fritz PRL1993

$$L = \overline{\psi}_{N} (i\gamma_{\mu}\partial^{\mu} - M_{N} - g_{\sigma N}(\rho)\sigma - g_{\omega N}(\rho)\gamma_{\mu}\omega^{\mu} - \frac{f_{\pi N}}{m_{\pi}}(\rho)\tau^{a}\gamma_{5}\gamma_{\mu}\partial^{\mu}\pi^{a} - e\gamma_{\mu}\frac{1-\tau^{3}}{2}A^{\mu})\psi_{N}$$

$$+ \frac{1}{2}\partial_{\mu}\sigma\partial^{\mu}\sigma - \frac{1}{2}m_{\sigma}^{2}\sigma^{2} - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_{\omega}^{2}\omega_{\mu}\omega^{\mu}$$

$$+ \frac{1}{2}\partial_{\mu}\pi^{a}\partial^{\mu}\pi^{a} - \frac{1}{2}m_{\pi}^{2}\pi^{a2}$$

$$DDRHF^{*}$$

$$U_{S} = g_{\sigma B}(\rho)\sigma$$

$$U_{V} = g_{\omega B}(\rho)\omega$$



#### **Properties of <sup>16</sup>O**



[1] Audi NPA2003

\* DD couplings extracted from RBHF theory at nuclear matter

Hu, Meng, Ring, to be published.



#### Single particle levels in <sup>16</sup>O



Hu, Meng, Ring, to be published.

DDRH and DDRHF based on RBHF







#### Relation between binding energy and radii of <sup>16</sup>O





#### Relation between binding energy and radii





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

	E (MeV)				<i>r<sub>c</sub></i> (fm)			$\varepsilon_{1 p_{1/2}} - \varepsilon_{1 p_{3/2}} \text{ (MeV)}$		
	Exp.	RBHF	PKO1	Exp.	RBHF	PK01	Exp.	RBHF	PKO1	
<sup>14</sup> C	-105.73	-98.49	-106.66	2.50	2.42	2.45	<del></del>	4.6	6.6	
<sup>14</sup> O	-98.73	-91.51	-100.48	0. <u></u>	2.67	2.68	( <u> </u>	—		
<sup>40</sup> Ca	-342.05	-322.41	-341.93	3.48	3.37	3.43	7.2	5.7	6.5	
<sup>48</sup> Ca	-416.16	-385.62	-415.62	3.47	3.41	3.45	4.3	3.1	6.2	
<sup>56</sup> Ni	-483.95	-439.26	-484.61		3.62	3.67		1.2	1.8	

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

	<sup>14</sup> C	<sup>14</sup> 0	<sup>16</sup> 0	<sup>40</sup> Ca	<sup>48</sup> Ca	<sup>56</sup> Ni
$(E_{\mathrm{exp.}} - E_{RBHF})/E_{\mathrm{exp.}}$ (%)	6.85	7.31	6.32	5.74	7.34	9.23

➤The binding energy is reproduced within10% in RBHF

The spin-orbit splitting is small

Hu, Meng, Ring, to be published.



## **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.
- 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 <sup>14</sup>C, <sup>16</sup>O, <sup>40</sup>Ca, <sup>48</sup>Ca and <sup>56</sup>Ni are reproduced with RBHF within 10%, and RBHF results are comparable with the ones from PKO1.
- Calculation for heavier nuclei is in progress. Thank you for your attention!
  2013-10-10