New generation of relativistic approach for nuclear structure

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EDF – CDFT – RMF – RHF – RBHF
Outline

- Introduction
- CDFT at the Hartree level (success)
- CDFT at the Hartree-Fock level (new learning)
- Full Dirac Brueckner-Hartree-Fock (exception)
- DBHF calculation for $^{16}O$, $^{40}Ca$, $^{48}Ca$ and $^{56}Ni$
- Summary & Perspectives
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 ground-state density of the interacting system can be reproduced by non-interacting particles moving in this local potential.

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

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

- Nuclear energy density functional has been introduced by effective Hamiltonians

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

- 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 (Skryme)
- non-relativistic finite range forces of Gaussian shape (Gogny)
- relativistic (covariant) density functional theory (RMF)
CDFT with non-linear point coupling interaction

\[ ( \bar{\psi} O \Gamma \psi ), O \in \{ 1, \bar{\tau} \}, \Gamma \in \{ 1, \gamma_\mu, \gamma_5, \gamma_5 \gamma_\mu, \sigma_{\mu \nu} \} \]

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

\[
L = \bar{\psi} (i \gamma_\mu \partial^\mu - m) \psi 
\]

\[
- \frac{1}{2} \alpha_s (\bar{\psi} \gamma_\mu \psi)(\bar{\psi} \gamma_\mu \psi) - \frac{1}{2} \alpha_v (\bar{\psi} \gamma_\mu \psi)(\bar{\psi} \gamma^\nu \gamma_\mu \psi) - \frac{1}{2} \alpha_{TV} (\bar{\psi} \gamma_{\mu \nu} \psi)(\bar{\psi} \gamma^\mu \psi) 
\]

\[
- \frac{1}{3} \beta_s (\bar{\psi} \psi)^3 - \frac{1}{4} \gamma_s (\bar{\psi} \psi)^4 - \frac{1}{4} \gamma_v [(\bar{\psi} \gamma_\mu \psi)(\bar{\psi} \gamma^\mu \psi)]^2 
\]

\[
- \frac{1}{2} \delta_s \partial_\nu (\bar{\psi} \gamma_\mu \psi) \partial^\nu (\bar{\psi} \psi) - \frac{1}{2} \delta_v \partial_\nu (\bar{\psi} \gamma_\mu \psi) \partial^\nu (\bar{\psi} \gamma^\mu \psi) - \frac{1}{2} \delta_{TV} \partial_\nu (\bar{\psi} \gamma_{\mu \nu} \psi) \partial^\nu (\bar{\psi} \gamma_{\mu \nu} \psi) 
\]

\[
- e \frac{1 - \tau_3}{2} \bar{\psi} \gamma^\mu \psi A_\mu - \frac{1}{4} F^{\mu \nu} F_{\mu \nu} 
\]

Higher order terms
Localized form of Fock terms
Fitting to 60 binding energies, 17 charge radii, and empirical pairing gaps of 60 selected spherical nuclei.
Deformed nuclei

Zhao, Li, Yao, Meng, PRC 82, 054319 (2010)
The structure of $^{240}$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 $\approx 2$ MeV, much closer to the available data. Li, Niksic, Vretenar, Ring, Meng, *Phys.Rev.C* 81, 064321 (2010)
$^{240}$Pu: 3D PES (\(\beta_{20}, \beta_{22}, \beta_{30}\)) in MD constraint CDFT

- 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

\(\beta_{2}, \beta_{3}, \ldots\): Geng, Meng, Toki, 2007, Chinese Phys. Lett. 24-1865

\(\beta_{2}, \gamma, \ldots\): Meng, Peng, Zhang, Zhou, 2006, PRC 73-037303

\(\beta_{\lambda,\mu}\) with even \(\mu\) are included automatically

Lu, Zhao, Zhou, PRC85 (2012) 011301R

\(\beta_{20} = 0.3, 0.6, 0.9, 1.3, 1.6\)
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
Nuclear Mass

Data for 2149 nuclei from Audi et al. NPA2003


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.
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

Preliminary!
Density of core & halo

deformed relativistic Hartree Bogoliubov in the continuum in a spherical Woods-Saxon basis

- Prolate core, but slightly oblate halo with sizable hexadecapole component!
- Decoupling of deformation between core & halo

Very successful in nuclear physics

- 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


In addition of the RMF advantages
- Pion contribution included
- Nuclear effective mass
- Fully self-consistent description for spin-isospin excitation
- ……

16

DDRHF(B): pion and Exchange term

- RHFB equation

\[
\int dr' \begin{pmatrix} h(r,r') - \lambda & \Delta(r,r') \\ \Delta(r,r') & -h(r,r') + \lambda \end{pmatrix} \begin{pmatrix} \psi_U(r') \\ \psi_V(r') \end{pmatrix} = E \begin{pmatrix} \psi_U(r) \\ \psi_V(r) \end{pmatrix}
\]

- Single particle Hamiltonian:
  - Kinetic energy:
  - Local potentials:
  - Non-local Potentials:

- Pairing Force: Gogny D1S

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

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

Long, Giai, Meng, Physics letters B640 (2006) 150
Long, Ring, Giai, Meng, PHYSICAL REVIEW C81 (2012) 024308
Long, Ring, Giai, Bertulani, Meng, PHYSICAL REVIEWC 81(2010) 031302
RH + RPA

- No contribution from isoscalar mesons ($\sigma, \omega$), because exchange terms are missing.
- $\pi$-meson is dominant in this resonance.
- Zero-range pionic counter-term $g'$ has to be refitted to reproduce the data.

RHF + RPA

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

Liang, Giai, Meng, PRL 101, 122502 (2008)
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.

- 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 spin-dipole excitation in Zr-90 is well reproduced with a RPA calculation.

Liang, Giai, Meng PRL 101, 122502 (2008)
Liang, Zhao, Meng Phys. Rev. C 85, 064302 (2012)
New generation CDFT: *ab initio* calculation
\textit{ab initio}----- “from the beginning”

- without additional assumptions
- without additional parameters

\textit{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

\textit{ab initio} in nuclear matter

- Variational method
- Green’s function method
- Chiral Perturbation theory
- Brueckner-Hartree-Fock (BHF) theory
- Relativistic BHF (RBHF) theory
- ............

\text{Akmal} \text{ PRC1998}
\text{Dickhoff} \text{ PPNP2004}
\text{Kaiser} \text{ NPA2002}
\text{Baldo} \text{ RPP2012}
\text{Brockmann} \text{ PRC1990}
**ab initio calculation for light nuclei**

- Gaussian Expansion Method  
  Hiyama PPNP2003
- Green Function Monte Carlo Method  
  Pieper PRC2004
- Lattice Chiral Effective Field Theory  
  Lee PPNP2009
- No-Core Shell Model  
  Barrett PPNP2012
- ...  

**ab initio calculation for heavier nuclei**

- Coupled Channel method  
  Hagen PRL2009
- BHF theory  
  Dawson Ann.Phys.1962  
  Machleidt NPA1975  
  Muether PRC1990

| 16O in BHF method in Bonn potential | | | | |
|---|---|---|---|
| ε_{1s/2} | ε_{1p3/2} | ε_{1p1/2} | E | r_c |
| -39.73 | -16.98 | -11.64 | -71.84 | 2.465 |
| -44.37 | -19.49 | -13.24 | -85.60 | 2.380 |
| -50.46 | -22.89 | -15.44 | -104.96 | 2.291 |
| -40 ± 8 | -18.29 | -12.68 | -127.68 | 2.737 |
Relativistic Brueckner Hartree-Fock: nuclear matter

- Nuclear matter
- Defining an effective medium dependent meson-exchange interaction based upon the nuclear matter G matrix

*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
Full ab initio CDFT

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
Lippmann-Schwinger Equation
Lippmann, Phys. Rev. 1950

\[ T = V + V \frac{1}{E - H_0} T \]

- \( V \) is the realistic NN interaction
- \( E \) is the incident energy
- \( T \)-matrix is for two-body scattering

The corresponding EOS in HF

Bethe-Goldstone Equation
Brueckner, Phys. Rev. 1955

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

- \( E \) is the starting energy
- \( Q \) is the Pauli operator
- \( G \)-matrix is for many-body problem

The corresponding EOS in HF
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 \( \varepsilon_F \) is the Fermi energy, \( \omega = \varepsilon_m + \varepsilon_n \) 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 Hartree-Fock (RHF) equation

\[ \sum_{n'} \left( \alpha \cdot p + \beta M + \beta \Gamma_{nn'}^{HF} \right) \psi_{n'} = \varepsilon_n \psi_n \]

where \( \Gamma_{nn'}^{HF} \) is related with the density matrix \( \rho_{nn'} \)

\[ \Gamma_{nn'}^{HF} = V_{nn'n'} \rho_{mm'} - V_{nnm'n'} \rho_{mm'} \]

RHF equation in HO basis

\[
\begin{pmatrix}
A_{nn'}^{RHF} & B_{nn'}^{RHF} \\
B_{nn'}^{RHF} & C_{nn'}^{RHF}
\end{pmatrix}
\begin{pmatrix}
(f_n^{(a)}) \\
(g_n^{(a)})
\end{pmatrix} = \varepsilon_a \begin{pmatrix}
(f_n^{(a)}) \\
(g_n^{(a)})
\end{pmatrix}
\]

where

\[
A_{nn'}^{RHF} = (\alpha \cdot p + \beta M)_{nn'} + \sum_b \sum_{m,m'} f_m^{(b)} f_{m'}^{(b)} (\nu_{nn'm'} - \nu_{nn'm'})
\]

\[
B_{nn'}^{RHF} = (\alpha \cdot p + \beta M)_{nn'} + \sum_b \sum_{m,m'} f_m^{(b)} g_{m'}^{(b)} (\nu_{nn'm'} - \nu_{nn'm'})
\]

\[
C_{nn'}^{RHF} = (\alpha \cdot p + \beta M)_{nn'} + \sum_b \sum_{m,m'} g_m^{(b)} g_{m'}^{(b)} (\nu_{nn'm'} - \nu_{nn'm'})
\]
Relativistic Brueckner Hartree-Fock (RBHF) equation

\[ \sum_{n'} \left( \alpha \cdot p + \beta M + \beta \Gamma_{nn'}^{BHF} \right) \psi_{n'} = \varepsilon_n \psi_n \]

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

\[ \Gamma_{nn'}^{BHF} = G_{nnm'm'} \rho_{mm'} - G_{nmnm'} \rho_{mm'} \]

RHF equation in HO basis

\[ \begin{pmatrix} A_{nn'}^{BHF} & B_{nn'}^{BHF} \\ B_{nn'}^{BHF} & C_{nn'}^{BHF} \end{pmatrix} \begin{pmatrix} f_{n'}^{(a)} \\ g_{n'}^{(a)} \end{pmatrix} = \varepsilon_a \begin{pmatrix} f_n^{(a)} \\ g_n^{(a)} \end{pmatrix} \]

where

\[ A_{nn'}^{BHF} = (\alpha \cdot p + \beta M)_{nn'} + \sum_b \sum_{m,m'} f_{m}^{(b)} f_{m'}^{(b)} (G_{nnm'm'} - G_{nmnm'}) \]

\[ B_{nn'}^{BHF} = (\alpha \cdot p + \beta M)_{nn'} + \sum_b \sum_{m,m'} f_{m}^{(b)} g_{m'}^{(b)} (G_{nmnm'} - G_{nmnm'}) \]

\[ C_{nn'}^{BHF} = (\alpha \cdot p + \beta M)_{nn'} + \sum_b \sum_{m,m'} g_{m}^{(b)} g_{m'}^{(b)} (G_{nnm'm'} - G_{nnmnm'}) \]
Example

- Object: $^{16}\text{O}$
- Interaction: Bouyssy C
- Basis: Harmonics Oscillator (HO) ($N=12$)
  Relativistic Harmonics Oscillator (RHO) ($N_F=12$, $N_D=8$)

The properties of $^{16}\text{O}$

<table>
<thead>
<tr>
<th></th>
<th>r-space[1]</th>
<th>HO</th>
<th>RHO</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (MeV)</td>
<td>$-49.44$</td>
<td>$-49.45$</td>
<td>$-49.45$</td>
</tr>
<tr>
<td>$r_c$ (fm)</td>
<td>$2.91$</td>
<td>$2.90$</td>
<td>$2.91$</td>
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<tr>
<td>$\varepsilon_{1p_{1/2}} - \varepsilon_{1p_{3/2}}$ (MeV)</td>
<td>$5.5$</td>
<td>$5.5$</td>
<td>$5.5$</td>
</tr>
</tbody>
</table>

The properties of $^{16}\text{O}$ with different methods with Bouyssy interaction

[1] Bouyssy PRC1987

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

- Object: $^{16}$O
- Interaction: Bonn A
- Basis: Harmonics Oscillator (HO)

Convergence of RBHF calculation for $^{16}$O

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

Machleidt ANP1987
Properties of $^{16}$O

<table>
<thead>
<tr>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

-127.62 -119.552 -104.96 -128.36
2.737 2.6357 2.291 2.679
6.3 4.1 7.5 6.3


Energy components of $^{16}$O in RBHF theory

<table>
<thead>
<tr>
<th>Methods</th>
<th>$\langle T \rangle$</th>
<th>$\langle V_m \rangle$</th>
<th>$E_{\text{coul}}$</th>
<th>$E_{\text{c.m.}}$</th>
<th>$E_{\text{tot.}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PKO1</td>
<td>209.176</td>
<td>-340.910</td>
<td>13.942</td>
<td>-10.572</td>
<td>-128.364</td>
</tr>
<tr>
<td>RBHF (N=28)</td>
<td>235.315</td>
<td>-357.898</td>
<td>14.037</td>
<td>-11.006</td>
<td>-119.552</td>
</tr>
</tbody>
</table>

Hu, Meng, Ring, *to be published.*
Single proton energies for $^{16}\text{O}$ in RBHF theory

<table>
<thead>
<tr>
<th></th>
<th>EXP.</th>
<th>RBHF ($N=28$)</th>
<th>BHF</th>
<th>PKO1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_{1s_{1/2}}$</td>
<td>$-40 \pm 8$</td>
<td>$-34.085$</td>
<td>$-50.46$</td>
<td>$-34.682$</td>
</tr>
<tr>
<td>$\varepsilon_{1p_{3/2}}$</td>
<td>$-18.451$</td>
<td>$-16.954$</td>
<td>$-22.89$</td>
<td>$-17.719$</td>
</tr>
<tr>
<td>$\varepsilon_{1p_{1/2}}$</td>
<td>$-12.127$</td>
<td>$-12.872$</td>
<td>$-15.44$</td>
<td>$-11.417$</td>
</tr>
</tbody>
</table>

Hu, Meng, Ring, *to be published.*
Spin-orbit splitting in RBHF theory

The scalar and vector potentials in RMF and RBHF theories

Spin-orbit force in RMF theory

\[ U_{S.O.} \propto (U_V - U_S) \vec{L} \cdot \vec{S} \]
The Lagrangian of Density-dependent RH (DDRH) theory

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

The Lagrangian of Density-dependent RHF (DDRHF) theory

\[ L = \bar{\psi}_N (i \gamma_\mu \partial^\mu - M_N - g_{\sigma N}(\rho)\sigma - g_{\omega N}(\rho)\gamma_\mu \omega^\mu - \frac{f_{\pi N}(\rho)\tau^a}{m_\pi} \gamma_5 \gamma_\mu \partial^\mu \pi^a - e\gamma_\mu \left( \frac{1 - \tau^3}{2} A^\mu \right)) \psi_N \]
\[ + \frac{1}{2} \partial_\mu \sigma \partial^\mu \sigma - \frac{1}{2} m_\sigma^2 \sigma^2 - \frac{1}{4} \Omega_{\mu \nu} \Omega^{\mu \nu} + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu \]
\[ + \frac{1}{2} \partial_\mu \pi^a \partial^\mu \pi^a - \frac{1}{2} m_\pi^2 \pi^{a2} \]

DDRH
\[ U_S = g_{\sigma B}(\rho)\sigma \]
\[ U_V = g_{\omega B}(\rho)\omega \]

DDRHF
\[ U_S = g_{\sigma B}(\rho)\sigma \]
\[ U_V = g_{\omega B}(\rho)\omega \]

Brockmann PRL1992

Fritz PRL1993
Properties of $^{16}\text{O}$

<table>
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<tr>
<th></th>
<th>EXP. [1]</th>
<th>DDRH*</th>
<th>DDRHF*</th>
<th>RBHF (N=28)</th>
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<td></td>
</tr>
</tbody>
</table>

-127.62 | -107.72 | -114.76 | -119.55
2.737   | 2.602   | 2.634   | 2.636
6.3     | 5.2     | 4.8     | 4.1

* DD couplings extracted from RBHF theory at nuclear matter

Hu, Meng, Ring, *to be published.*
Single particle levels in $^{16}\text{O}$

Hu, Meng, Ring, *to be published.*
Nucleon densities in $^{16}\text{O}$

- Charge density
- Nuclear density
- Proton density
- Neutron density

Parameters:
- $\rho_c$ [fm$^{-3}$]
- $\rho_v$ [fm$^{-3}$]
- $\rho_p$ [fm$^{-3}$]
- $\rho_n$ [fm$^{-3}$]
Relation between binding energy and radii of $^{16}\text{O}$

Hu, Meng, Ring, *to be published.*
Relation between binding energy and radii

Hu, Meng, Ring, to be published.
The binding energy is reproduced within 10% in RBHF

The spin-orbit splitting is small

Hu, Meng, Ring, *to be published.*
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 $^{16}$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.

Calculation for heavier nuclei is in progress.

Thank you for your attention!