Coulomb Energy Density Functionals for Nuclear Systems

内藤 智也 (Tomoya Naito)

Department of Physics, Graduate School of Science, the University of Tokyo, JAPAN
RIKEN Nishina Center, JAPAN

December 12, 2018
Tsukuba-CCS workshop on “microscopic theories of nuclear structure and dynamics”
Center for Computational Sciences, University of Tsukuba, Japan
• Nuclear force for $T = 1$ has little $T_3$ dependence i.e., that for $p-p$, $n-n$, and $n-p$ ($T = 1$) are almost the same

Nuclear force has almost isospin symmetry

• If nuclear force has fully isospin symmetry, charge-symmetry-breaking (CSB) force and charde-independence-breaking (CIB) force

\[ V_{\text{CSB}} = V_{nn} - V_{pp}, \quad V_{\text{CIB}} = V_{np} - \frac{V_{nn} + V_{pp}}{2} \]

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Isospin Symmetry Breaking of Nuclear Force

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- However, electromagnetic (EM) force also breaks isospin symmetry
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• Amount of isospin symmetry breaking (ISB) of nuclear force is related to flavor symmetry breaking for quarks (CKM matrix $V_{ud}$)

• However, electromagnetic (EM) force also breaks isospin symmetry

• EM force and ISB of nuclear force are entangled to each other, for example, in mirror nuclei and in isobaric analog states
Isospin Symmetry Breaking of Nuclear Force
Electromagnetic Force

No
Off

Atomic Number: $Z$
Neutron Number: $N$

Atomic Number: $N$
Neutron Number: $Z$
Mirror Nuclei Mass Difference

Isospin Symmetry Breaking of Nuclear Force Yes
Electromagnetic Force Off

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Isospin Symmetry Breaking of Nuclear Force
Yes
Electromagnetic Force
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Importance of Electromagnetic Force

In order to understand isospin symmetry breaking of nuclear force, high-accuracy evaluation of electromagnetic force is required.

Electromagnetic Force in Condensed Matter Physics

Most phenomena are caused by the Coulomb force.
High-accuracy calculations have been developed for decades.

- In Density Functional Theory (DFT), Correlation is considered.
- Correlation is not considered in nuclear DFT.
- Density gradient effect is considered as GGA.
- Surface effect is important for nuclei.

Our Work

Coulomb correlation and Density gradient effect (GGA) in Coulomb term are considered in nuclear DFT.
### Motivations

#### Importance of Electromagnetic Force

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#### Our Work

Coulomb correlation and Density gradient effect (GGA) in Coulomb term are considered in nuclear DFT.
Energy Density Functional for Electron Systems

\[ E_{gs} = T_0 \rho_{gs} + \int V_{\text{ext}}(\mathbf{r}) \rho_{gs}(\mathbf{r}) \, d\mathbf{r} + E_d \rho_{gs} + E_x \rho_{gs} + E_c \rho_{gs} \]

\[ = \sum_j \varepsilon_j - \int V_{xc}(\mathbf{r}) \rho_{gs}(\mathbf{r}) \, d\mathbf{r} - E_d \rho_{gs} + E_x \rho_{gs} + E_c \rho_{gs} \]

- \( T_0 \): kinetic energy of non-interacting system,
- \( \varepsilon_j \): single-particle energy of KS-system,
- \( E_d \): direct (Hartree) functional,
- \( E_x \): exchange functional,
- \( E_c \): correlation functional

- \( E_d \) is exactly known
- Once \( E_x \) and \( E_c \) are known, the exact \( E_{gs} \) can be calculated
- Unfortunately, exact forms of \( E_x \) and \( E_c \) are unknown
- Approximation of \( E_x \) and \( E_c \) are required
Local Density Approximation (LDA)

- $E_x$ and $E_c$ are approximated to those of homogeneous systems $→$ LDA gives the exact energy for homogeneous systems
- $E_x$ in LDA is the known as Hartree-Fock-Slater approximation
- Energy density $\varepsilon$ depends only on $\rho (r)$

$$E_i [\rho] = \int \varepsilon_i (\rho (r)) \rho (r) \, dr \quad (i = x, c)$$

Generalized Gradient Approximation (GGA)

- Energy density $\varepsilon$ depends on $|\nabla \rho (r)|$ as well as $\rho (r)$

$$E_i [\rho] = \int \varepsilon_i (\rho (r), |\nabla \rho (r)|) \rho (r) \, dr \quad (i = x, c)$$
Energy Density Functional for Electron Systems

\[ E_{gs} = T_0 [\rho_{gs}] + \int V_{\text{ext}} (r) \rho_{gs} (r) \, dr + E_d [\rho_{gs}] + E_x [\rho_{gs}] + E_c [\rho_{gs}] \]

Energy Density Functional in Nuclear Physics

\[ E_{gs} = T_0 [\rho_p, \rho_n] + E_{\text{nucl}} [\rho_p, \rho_n] + E_{Cd} [\rho_{ch}] + E_{Cx} [\rho_{ch}] \]

- \( T_0 \): kinetic energy of non-interacting system,
- \( E_{\text{nucl}} \): nuclear part functional,
- \( E_{Cd} \): direct Coulomb functional,
- \( E_{Cx} \): exchange Coulomb functional,
- \( V_{\text{ext}} \equiv 0 \) since nuclear systems are self-bound systems

- Coulomb correlation functional \( E_{Cc} \) is not included explicitly
- Since exact effective nuclear force is still under discussion, \( E_{\text{nucl}} \) is given by fitting to experimental data
- Usually, protons are assumed to be point particles (\( \rho_{ch} = \rho_p \))
Energy Density Functional for Electron Systems

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- Coulomb correlation functional \( E_{Cc} \) is not included explicitly
- Since exact effective nuclear force is still under discussion, \( E_{\text{nucl}} \) is given by fitting to experimental data
  \( \rightarrow \) Coulomb correlation is included implicitly
- Usually, protons are assumed to be point particles \( (\rho_{\text{ch}} = \rho_p) \)
Density Gradient Effect in Atomic Nuclei

Evaluation of $^{208}$Pb by Using Experimental $\rho_{\text{ch}}$

![Graph showing density gradient effect](image)

$$E_{C_{\text{x}}} [\rho_{\text{ch}}] = \int \varepsilon_x (r) \rho_{\text{ch}} (r) \, dr$$


Density gradient effect is visible in surface region
Coulomb Correlation Functional

Coulomb Correlation Functional

Previous Work

Coulomb correlation energy is calculated for some specific nuclei by using the response function

\[
\begin{array}{cccc}
\text{Nuclei} & E_{\text{Cx}} (\text{MeV}) & E_{\text{Cc}} (\text{MeV}) & E_{\text{Cc}}/E_{\text{Cx}} \\
^{16}\text{O} & -2.99 & 0.99 & -33.1 \% \\
^{40}\text{Ca} & -7.92 & 3.18 & -40.2 \% \\
^{208}\text{Pb} & -31.29 & 6.88 & -22.0 \% \\
\end{array}
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In order to consider Coulomb correlation energy \( E_{\text{Cc}} \) in self-consistent step, \( E_{\text{Cc}} \) as a functional form is required
Coulomb Correlation Functional

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Our Work

In order to consider Coulomb correlation energy $E_{Cc}$ in self-consistent step, $E_{Cc}$ as a functional form is required

$\rightarrow E_{Cc}$ is calculated as a test by functionals used in electron systems
Evaluated from Analytical Formulae in LDA

$$\xi = \frac{\alpha mc}{\hbar} \left( \frac{3}{4\pi \rho} \right)^{1/3}$$
### Energy (MeV)

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## Evaluation by Experimental $\rho_{\text{ch}}$

Hartree-Fock-Slater Approx. Consistent with $\varepsilon_{\text{Cc}}/\varepsilon_{\text{Cx}}$

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Hartree-Fock-Slater Approx. Consistent with $\varepsilon_{Cc}/\varepsilon_{Cx}$

Non-negligible!
Short Conclusion

- Coulomb correlation energy is considered as a functional in our work.
- Nuclear force is strong attractive, Coulomb force is weak repulsive.
  → nuclear force causes main part of Coulomb correlation.

**Our Work** does not include effects from the nuclear force:
\[ E_{Cc} \text{ is around } 2\% \text{ of } E_{Cx} \]

**Previous Work** included effects from the nuclear force:
\[ E_{Cc} \text{ is around } -20\% \text{ of } E_{Cx} \]
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- This difference shows that the nuclear force should be considered in the Coulomb correlation functional.
- Thus, \( E_{Cc} \) in this work is not applicable for nuclear systems directly.
- The way to derive \( E_{Cc} \) in nuclear systems should be considered again.
Coulomb Exchange Functional


## Evaluation by Experimental $\rho_{\text{ch}}$

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<tr>
<td>$^{12}$C</td>
<td>-1.962</td>
<td>-2.105</td>
<td>-0.143</td>
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**Hartree-Fock-Slater Approx.**

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### Energy (MeV)

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<th>Nuclei</th>
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<tr>
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### Evaluation by Experimental $\rho_{ch}$

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**Hartree-Fock-Slater Approx.**

**12 % enhanced!!**

**Difference (600 keV): Non-negligible!**
Comparison to Exact Hartree-Fock Calculation

\[ \Delta E_{\text{Cx}} = \frac{E_{\text{GGA}}^{\text{GGA}} - E_{\text{LDA}}^{\text{LDA}}}{E_{\text{Cx}}^{\text{GGA}}} \]

\[ \Delta E_{\text{Cx}} = \frac{E_{\text{exactHF}}^{\text{exactHF}} - E_{\text{LDA}}^{\text{LDA}}}{E_{\text{Cx}}^{\text{exactHF}}} \]


**Short Conclusion**

- GGA exchange functionals may work in nuclear system, where choice of functionals is not critical.
- GGA exchange enhanced from LDA
  
  \[ 12\% \, (-80 \text{ keV}) \text{ in } ^4\text{He}, \, 2.3\% \, (-600 \text{ keV}) \text{ in } ^{208}\text{Pb} \]

- However, there are still some error
  
  → let us discuss modification for GGA functional.
The PBE-GGA Coulomb Exchange Functional is given by:

\[ E_{\text{Cx}}^{\text{GGA}} [\rho] = \int \varepsilon_{\text{Cx}}^{\text{LDA}} (\rho (r)) F(s) \rho (r) \, dr, \]

where

\[ s = \frac{|\nabla \rho|}{2 (3\pi^2)^{1/3} \rho^{4/3}}, \]

and

\[ F(s) = 1 + \kappa - \frac{\kappa}{1 + \mu s^2 / \kappa}, \]

with

\[ \mu = 0.21951, \quad \kappa = 0.804 \]


- \( \kappa \) is determined from Lieb-Oxford bound (analytical evaluation)
- \( \mu \) is determined from RPA calculation of homogeneous electron gas
PBE-GGA Coulomb Exchange Functional

\[ E_{\text{Cx}}^{\text{GGA}}[\rho] = \int \mathcal{E}_{\text{Cx}}^{\text{LDA}}(\rho(r)) \ F(s) \ \rho(r) \ dr, \quad s = \frac{|\nabla \rho|}{2 \left(3 \pi^2\right)^{1/3} \rho^{4/3}}, \]

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  \( \rightarrow \) \( \kappa \) must be kept in any systems

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Self-Consistent Calculation

PBE-GGA Coulomb Exchange Functional

\[ E_{\text{C}x}^{\text{GGA}} [\rho] = \int \varepsilon_{\text{C}x}^{\text{LDA}} (\rho (r)) \ F (s) \ \rho (r) \ dr, \]

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  \( \rightarrow \) \( \mu \) in nuclei can be different from in original one
### Setup for Self-consistent Skyrme Hartree-Fock Calculation

<table>
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<tr>
<th>Part</th>
<th>Description</th>
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</thead>
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<tr>
<td><strong>Nuclear Part</strong></td>
<td>SAMi Functional</td>
</tr>
<tr>
<td></td>
<td>(However, choice of functional of nuclear part is not critical)</td>
</tr>
<tr>
<td><strong>Coulomb Part</strong></td>
<td>LDA exchange is replaced to PBE Functional (GGA)</td>
</tr>
<tr>
<td><strong>Correlation Part</strong></td>
<td>Coulomb correlation part is not considered</td>
</tr>
<tr>
<td><strong>Pairing Correlation</strong></td>
<td>Neglected</td>
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### Calculation

- **Code**: Modified `skyrme_rpa` for GGA


- **Box Size**: $0.1 \text{ fm} \times 150$
• \( \lambda \) does not have an obvious isospin dependence
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- $\lambda = 1.25$ will reproduce well in mid/heavy-mass region

$$F(s) = 1 + \kappa - \frac{\kappa}{1 + \lambda \mu s^2 / \kappa}$$
• $\lambda$ does not have an obvious isospin dependence
• $\lambda = 1.25$ will reproduce well in mid/heavy-mass region
• For whole nuclear chart, $\lambda = 1.25$ is the most suitable
• In light nuclei, $\lambda = 1.25$ has still a little error $\rightarrow$ shell effect?

$$F (s) = 1 + \kappa - \frac{\kappa}{1 + \lambda \mu s^2 / \kappa}$$
Short Conclusion

- “Modified” PBE-GGA Coulomb exchange functional with $\lambda = 1.25$ reproduces the exact-Fock energy almost whole nuclear chart
- Numerical cost
  - Exact-Fock $O(N^4)$
  - LDA $O(N^3)$
  - GGA Still $O(N^3)$

$\rightarrow$
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  - LDA $O(N^3)$
  - GGA Still $O(N^3)$

→ Modified PBE-GGA should be used instead of the LDA!
Final Conclusion

- GGA Coulomb exchange functionals in electron systems reproduces the exact-Fock energy, while numerical cost in GGA is almost the same as in LDA.
- Coulomb correlation functionals in electron systems are not applicable to atomic nuclei directly.

Next Step for More Higher Accuracy Coulomb Energy

Considering finite-size effect of proton ($\rho_{ch}$ is used in each SCF step instead of $\rho_p$) since finite-size effect of proton is sometimes non-negligible.


Naito, Roca-Maza, Colò, and Liang. *In Progress*

Application to the measurable quantities, for example

Mirror nuclei mass difference, Isobaric Analog State, Superallowed $\beta$-decay.
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Thank you for attention!!