Coulomb Energy Density Functionals for Nuclear Systems

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February 27, 2018

One-day workshop on “New Vistas on Nuclear Dynamics: Shapes, Spin, and Isospin”
Università degli Studi di Milano / Istituto Nazionale di Fisica Nucleare, Sezione di Milano
I Don’t Know!! (^o^)
I Don’t Know!! (^o^)

It’s Joke...
Who Am I?

- 2nd year of the master course student in Dept. Phys., U. Tokyo (Condensed Matter Theory)
- Student trainee in RIKEN Nishina Center (Nuclear Theory)

Research Topics

- Basic ideas of density functional theory
- Coulomb energy density functional in nuclear physics to understand isospin symmetry breaking of nuclear force
- Relativistic density functional theory in electronic systems to understand atomic properties of super-heavy elements
My “General” Research Motivations

I Want to Understand

- Fundamental symmetries (CPT symmetries) in many-body problem
- Relativistic effects in many-body problems
- Similarity and difference between nuclear physics, atomic physics, and condensed matter physics
  difference between these systems: mainly the interaction

My Motivation: Calculate Well-understood Things with High-accuracy

Electro-magnetic interaction/QED: well-understood
→ should be calculate with high-accuracy
  in order to find “unknown” physics and estimate uncertainly
  (e.g. estimation of isospin breaking of nuclear force)

At first, due to the wider applicability
I have used the DFT for nuclear systems and electron systems
Coulomb Energy Density Functionals in Nuclear Systems

Treatment of the Coulomb int. exactly in nuclear DFT

Relativistic Effects in Electronic Density Functional Theory

Treatment of the relativistic effects to calculate electronic structure of super-heavy elements (atoms, molecules, solids)

On-going Collaboration (selected)

- Inverse Kohn-Sham method (with D. Ohashi and H. Liang)
- FRG-DFT in electron systems (with T. Yokota)
- Many-body calculation toward measurement of EDM (with M. Kitaguchi and H. Nagahama)
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| 1 | Introduction |
| 2 | Coulomb Correlation Functional |
| 3 | Coulomb Exchange Functional |
| 4 | Conclusion and Perspectives |
Table of Contents

1 Introduction
2 Coulomb Correlation Functional
3 Coulomb Exchange Functional
4 Conclusion and Perspectives
• 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 charge-independence-breaking (CIB) force

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

are identical to 0, whereas
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• However, electromagnetic (EM) force also breaks isospin symmetry
Isospin Symmetry Breaking of Nuclear Force

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- 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
Mirror Nuclei Mass Difference

Isospin Symmetry Breaking of Nuclear Force  No
Electromagnetic Force  Off

Atomic Number: \( Z \)
Neutron Number: \( N \)

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Mirror Nuclei Mass Difference

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Atomic Number: $N$
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Motivations

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
Motivations

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.
Energy Density Functional for Electron Systems

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

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

\(T_0\): 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 \(E_{\text{gs}}\) 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 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, so far \( E_{\text{nucl}} \) 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

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

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- Under \( \rho_{ch} = \rho_p \) ansatz, the “exact-Fock” term should be used for \( E_{\text{Cx}} \)

\[ E_{\text{Cx}} = \frac{1}{2} \sum_{j, k \in \text{Proton}} \iint \frac{\psi_j^*(r) \psi_k^*(r') \psi_j(r') \psi_k(r)}{|r - r'|} \, dr \, dr' \]
Energy Density Functional for Electron Systems

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

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- Due to numerical cost, LDA \( E_{\text{Cx}} \) (Hartree-Fock-Slater approx.) is used or sometimes \( E_{\text{Cx}} \) is neglected
Density Gradient Effect in Atomic Nuclei

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

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


Density gradient effect is visible in surface region
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Previous Work

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

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<thead>
<tr>
<th>Nuclei</th>
<th>$E_{\text{C}_\text{x}}$ (MeV)</th>
<th>$E_{\text{C}_\text{c}}$ (MeV)</th>
<th>$E_{\text{C}<em>\text{c}}/E</em>{\text{C}_\text{x}}$</th>
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<td>−2.99</td>
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<td>−31.29</td>
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Our Work

In order to consider Coulomb correlation energy $E_{\text{C}_\text{c}}$ in self-consistent step, $E_{\text{C}_\text{c}}$ as a functional form is required
Coulomb Correlation Functional

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

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<tr>
<th>Nuclei</th>
<th>$E_{Cx}$ (MeV)</th>
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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.

→ $E_{Cc}$ is calculated as a test by functionals used in electron systems.
\[ \xi = \frac{\alpha mc}{\hbar} \left( \frac{3}{4\pi\rho} \right)^{1/3} \]

Evaluated from Analytical Formulae in LDA

Nuclei

Electron Systems

\[ \rho_0 \quad 0.001\rho_0 \]
### Energy (MeV)

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<tr>
<th>Nuclei</th>
<th>LDA $E_{Cx}$</th>
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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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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:

\[ E_{Cc} \text{ is around } -20\% \text{ of } E_{Cx} \]
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

\[ E_{Cc} \text{ is around } -20\% \text{ of } E_{Cx} \]

- 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
# Table of Contents

1. **Introduction**
2. **Coulomb Correlation Functional**
3. **Coulomb Exchange Functional**
4. **Conclusion and Perspectives**

---


### Energy (MeV)

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<tr>
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<th>LDA $E_{Cx}$</th>
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### Evaluation by Experimental $\rho_{\text{ch}}$

#### Hartree-Fock-Slater Approx.

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**Difference (600 keV): Non-negligible!**

**Hartree-Fock-Slater Approx.**

12% enhanced!!
Comparison to Exact Hartree-Fock Calculation

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

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


**Short Conclusion**

- GGA exchange functionals may work in nuclear system, where choice of functionals is not critical.
- GGA exchange enhanced from LDA:
  - 12% ($-80\,\text{keV}$) in $^4\text{He}$,
  - 2.3% ($-600\,\text{keV}$) in $^{208}\text{Pb}$.
- However, there are still some error:
  - → let us discuss modification for GGA functional.
PBE-GGA Coulomb Exchange Functional

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

\[ F (s) = 1 + \kappa - \frac{\kappa}{1 + \mu s^2 / \kappa}, \quad \mu = 0.21951, \quad \kappa = 0.804 \]


- \( \kappa \) is determined from Lieb-Oxford bound (analytical evaluation)
- \( \mu \) is determined from RPA calculation of homogeneous electron gas
Self-Consistent Calculation

PBE-GGA Coulomb Exchange Functional

\[
E_{\text{Cgx}}^{\text{GGA}} [\rho] = \int \varepsilon_{\text{Cgx}}^{\text{LDA}} (\rho (\mathbf{r})) \ F (s) \ \rho (\mathbf{r}) \ d\mathbf{r}, \quad s = \frac{\left| \nabla \rho \right|}{2 \left( 3 \pi^2 \right)^{1/3} \rho^{4/3}},
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PBE-GGA Coulomb Exchange Functional

\[
E_{\text{GGA}}^{\text{Cx}} [\rho] = \int \varepsilon_{\text{LDA}}^{\text{Cx}} (\rho (r)) \ F(s) \ \rho (r) \ dr, \quad s = \frac{|\nabla \rho|}{2 (3\pi^2)^{1/3} \rho^{4/3}},
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\[
F(s) = 1 + \kappa - \frac{\kappa}{1 + \lambda \mu s^2 / \kappa}, \quad \mu = 0.21951, \quad \kappa = 0.804
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- \( \mu \) is determined from RPA calculation of homogeneous electron gas
  \( \rightarrow \) \( \mu \) in nuclei can be different from in original one
**Self-Consistent Calculation**

**Setup for Self-consistent Skyrme Hartree-Fock Calculation**

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<tr>
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<th>Details</th>
</tr>
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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>
</tr>
</tbody>
</table>

**Calculation**

| Code                | Modified skyrme_rpa for GGA                                           |
| **Box Size**        | 0.1 fm × 150                                                          |
• $\lambda$ does not have an obvious isospin dependence

\[
F(s) = 1 + \kappa - \frac{\kappa}{1 + \lambda \mu s^2 / \kappa}
\]
• $\lambda$ does not have an obvious isospin dependence
• $\lambda = 1.25$ will reproduce well in mid/heavy-mass region
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• $\lambda = 1.25$ 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 → shell effect?

\[
F(s) = 1 + \kappa - \frac{\kappa}{1 + \lambda \mu s^2 / \kappa}
\]
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- GGA exchange enhanced from LDA
  12% (−80 keV) in $^4$He, 2.3% (−600 keV) in $^{208}$Pb → non-negligible
- “Modified” PBE-GGA Coulomb exchange functional with $\lambda = 1.25$
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- Numerical cost
  Exact-Fock $O(N^4)$
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  → Modified PBE-GGA should be used instead of the LDA!
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4. Conclusion and Perspectives
Recent Study of Coulomb Energy

- Studies which suggest **Coulomb repulsive is “strong”**
  - Skyrme HF without $E_{Cx}$ reproduces the mass globally
  - Effective charge of Coulomb EDF in Skyrme HF should be $e^2 \left( 1 + 0.45Z^{-2/3} \right)$ instead of $e^2$ in order to reproduce IMME
  - Coulomb correlation is $E_{Cc} < 0$

- Studies which suggest **Coulomb repulsive is “weak”**
  - Hartree term should be proportional to $Z(Z - 1)$ instead of $Z^2$
  - In the exact-Fock calculation, $E_{Cx} < 0$ is enhanced
  - In the GGA, $E_{Cx} < 0$ is enhanced
  - Finite-size effect decreases the Coulomb energy (On-going work)
Recent Study of Coulomb Energy

From fitting  Coulomb repulsive is **stronger** than expected
From first-principle  Coulomb repulsive is **weaker** than expected

Final Conclusion of Our Work

- GGA Coulomb exchange functionals in electron systems reproduces the exact-Fock energy, while numerical cost in GGA is almost the same as in LDA
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Grazie Mille!!