Coulomb Energy Density Functionals for Nuclear Systems

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Center for Computational Sciences, University of Tsukuba, Japan

Isospin Symmetry Breaking of Nuclear Force

- 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

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

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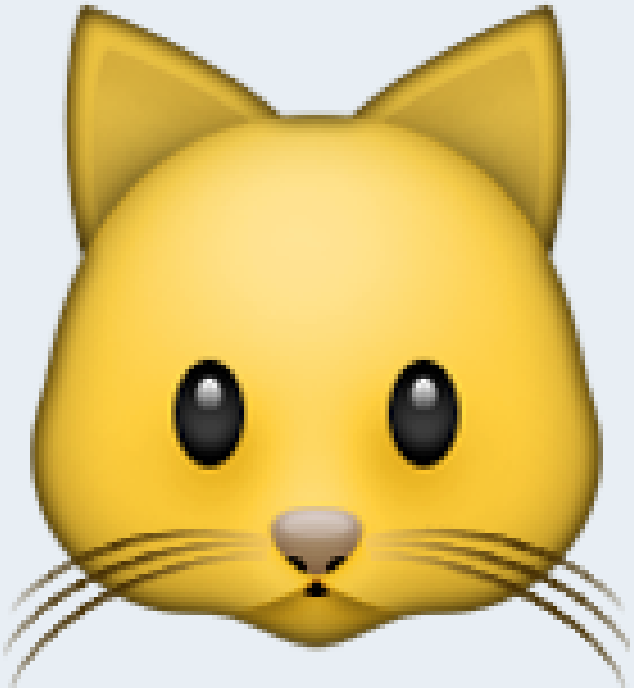
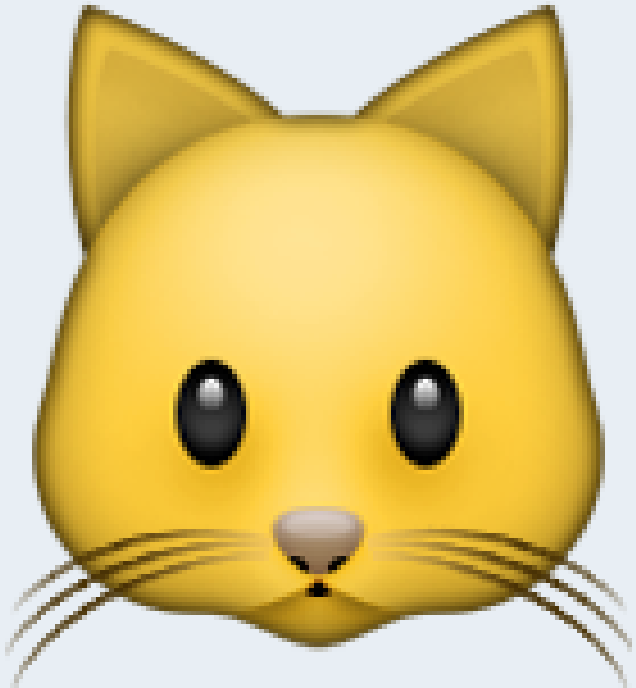
- However, electromagnetic (EM) force also breaks isospin symmetry
- EM force and ISB of nuclear force are entangled to each other,
  for example, in mirror nuclei and in isobaric analog states

Mirror Nuclei Mass Difference

Isospin Symmetry Breaking of Nuclear Force	**No**
Electromagnetic Force	**Off**



Atomic Number: Z
Neutron Number: N



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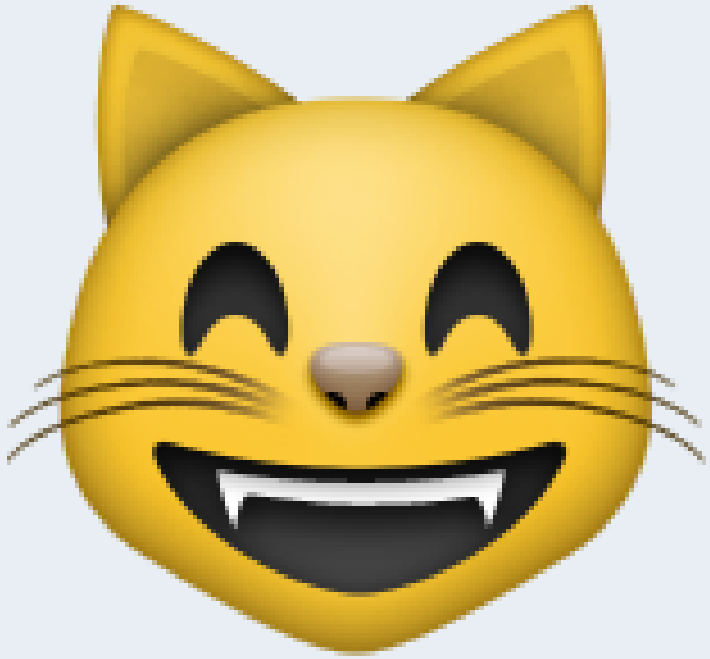

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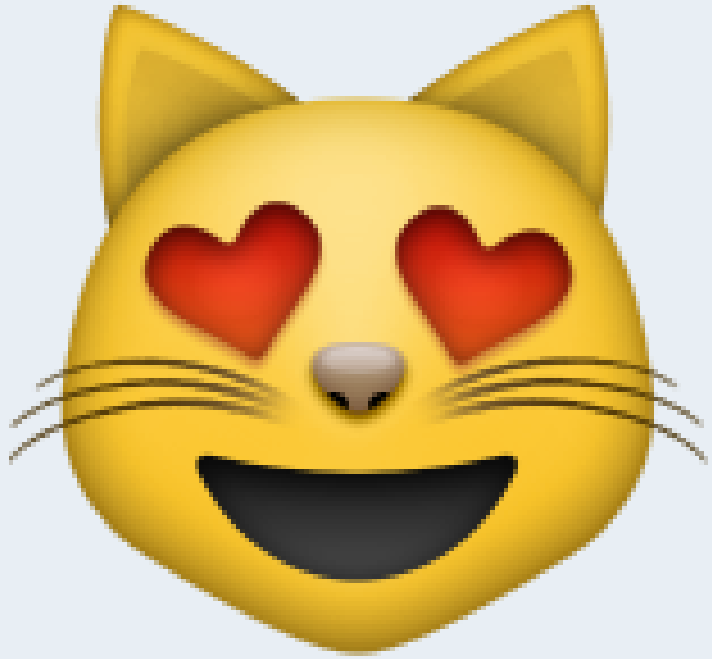

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Motivations

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

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

Energy Density Functional for Electron Systems

$$E_{\mathrm{gs}} = T_0\left[\rho_{\mathrm{gs}}\right] + \int V_{\mathrm{ext}}(\boldsymbol{r})\,\rho_{\mathrm{gs}}(\boldsymbol{r})\,d\boldsymbol{r} + E_{\mathrm{d}}\left[\rho_{\mathrm{gs}}\right] + E_{\mathrm{x}}\left[\rho_{\mathrm{gs}}\right] + E_{\mathrm{c}}\left[\rho_{\mathrm{gs}}\right]$$
$$= \sum_j \varepsilon_j - \int V_{\mathrm{xc}}(\boldsymbol{r})\,\rho_{\mathrm{gs}}(\boldsymbol{r})\,d\boldsymbol{r} - E_{\mathrm{d}}\left[\rho_{\mathrm{gs}}\right] + E_{\mathrm{x}}\left[\rho_{\mathrm{gs}}\right] + E_{\mathrm{c}}\left[\rho_{\mathrm{gs}}\right]$$

T_0: kinetic energy of non-interacting system, ε_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
  $\rightarrow$ LDA gives the exact energy for homogeneous systems
- E_{x} in LDA is the known as Hartree-Fock-Slater approximation
- Energy density ε depends only on $\rho(\boldsymbol{r})$

$$E_i[\rho] = \int \varepsilon_i(\rho(\boldsymbol{r}))\, \rho(\boldsymbol{r})\, d\boldsymbol{r} \quad (i = \mathrm{x},\, \mathrm{c})$$

Generalized Gradient Approximation (GGA)

- Energy density ε depends on $|\nabla\rho(\boldsymbol{r})|$ as well as $\rho(\boldsymbol{r})$

$$E_i[\rho] = \int \varepsilon_i(\rho(\boldsymbol{r}), |\nabla\rho(\boldsymbol{r})|)\, \rho(\boldsymbol{r})\, d\boldsymbol{r} \quad (i = \mathrm{x},\, \mathrm{c})$$

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Energy Density Functional in Nuclear Physics

$$E_{\mathrm{gs}} = T_0\left[\rho_p, \rho_n\right] + E_{\mathrm{nucl}}\left[\rho_p, \rho_n\right] + E_{\mathrm{Cd}}\left[\rho_{\mathrm{ch}}\right] + E_{\mathrm{Cx}}\left[\rho_{\mathrm{ch}}\right]$$

T_0: kinetic energy of non-interacting system, E_{nucl}: nuclear part functional,
E_{Cd}: direct Coulomb functional, E_{Cx}: exchange Coulomb functional,

$V_{\mathrm{ext}} \equiv 0$ 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_{nucl} is given by fitting to experimental data
  $\rightarrow$
- Usually, protons are assumed to be point particles ($\rho_{\mathrm{ch}} = \rho_p$)

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- Since exact effective nuclear force is still under discussion,
  E_{nucl} is given by fitting to experimental data
  $\rightarrow$ Coulomb correlation is included implicitly
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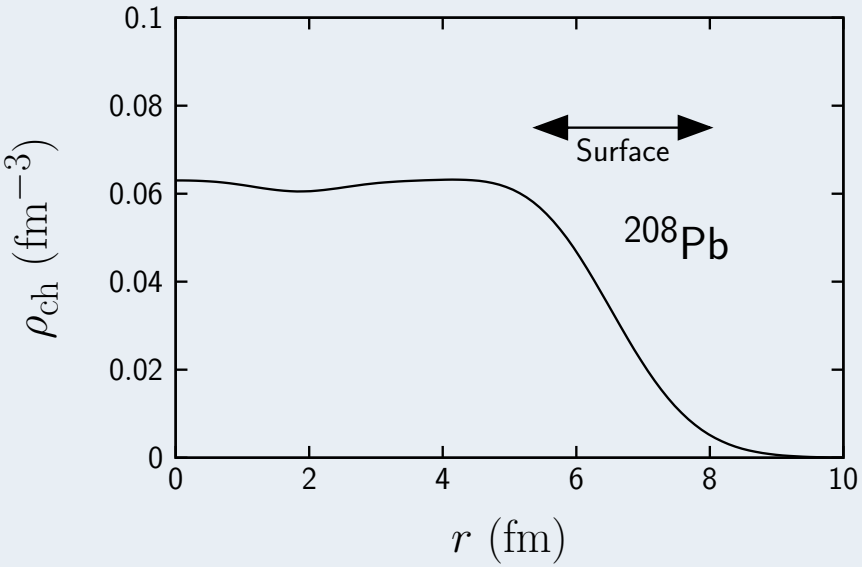
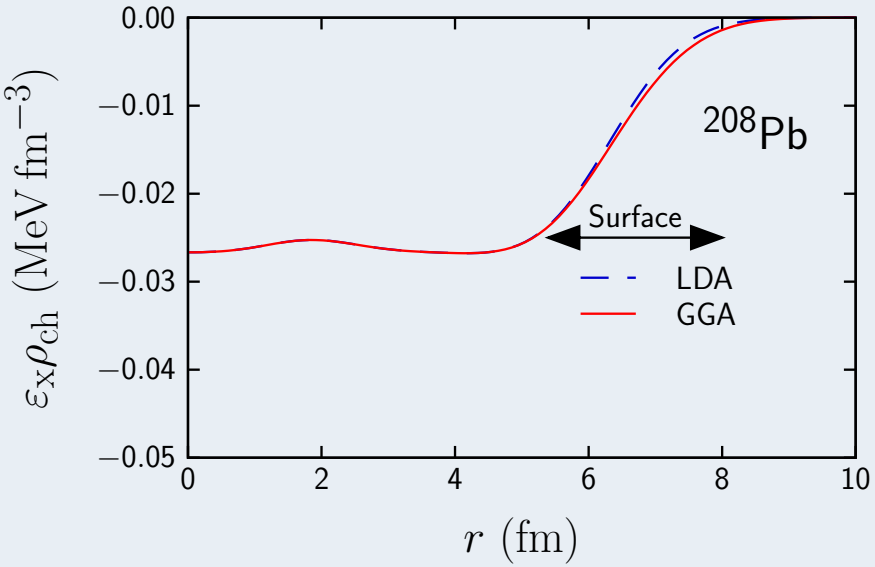
Density Gradient Effect in Atomic Nuclei

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





$$E_{\rm Cx}\left[\rho_{\rm ch}\right] = \int \varepsilon_{\rm x}\left(r\right)\,\rho_{\rm ch}\left(r\right)\,d\boldsymbol{r}$$

$\rho_{\rm ch}$ Data: Vries, Jager, and Vries. *At. Data Nucl. Data Tables* **36**, 495 (1987)

GGA: PBE functional (Perdew, Burke, and Ernzerhof. *Phys. Rev. Lett.* **77**, 3865 (1996))

Density gradient effect is visible in surface region

Coulomb Correlation Functional


T. Naito, R. Akashi, and H. Liang. *Phys. Rev. C* **97**, 044319 (2018)

Coulomb Correlation Functional

Previous Work

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

Nuclei	E_{Cx} (MeV)	E_{Cc} (MeV)	$E_{\mathrm{Cc}}/E_{\mathrm{Cx}}$
^{16}O	−2.99	0.99	−33.1 %
^{40}Ca	−7.92	3.18	−40.2 %
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Bulgac and Shaginyan. *Nucl. Phys. A* **601**, 103 (1996), *Phys. Lett. B* **469**, 1 (1999)

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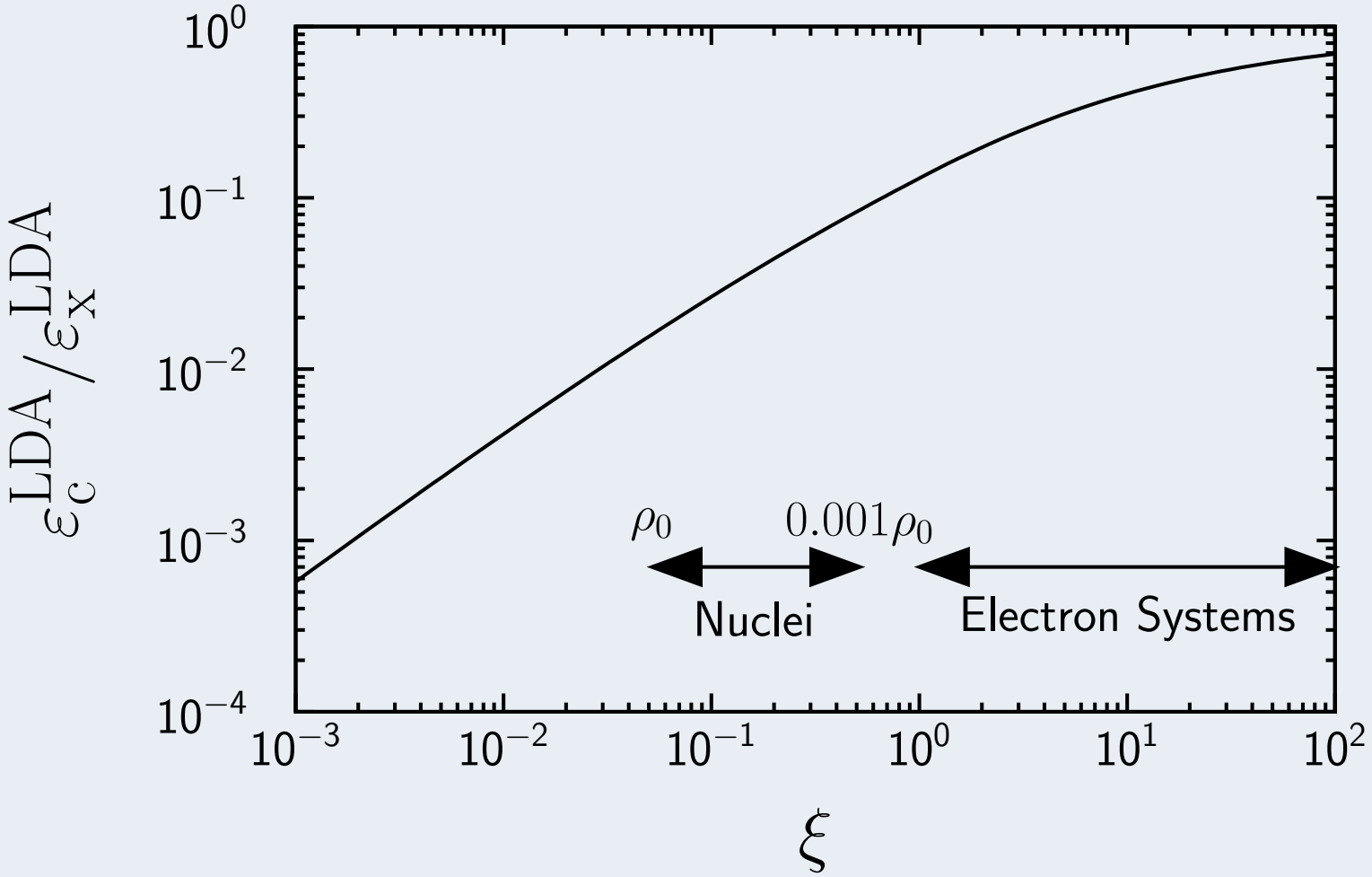
$\rightarrow$ E_{Cc} is calculated as a test by functionals used in electron systems

Evaluated from Analytical Formulae in LDA



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

Evaluation by Experimental ρ_{ch}

Energy (MeV)

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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
  $\rightarrow$ nuclear force causes main part of Coulomb correlation

  Our Work does not include effects from the nuclear force
  E_{Cc} is around $2\,\%$ 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




T. Naito, R. Akashi, and H. Liang. *Phys. Rev. C* **97**, 044319 (2018)

T. Naito, X. Roca-Maza, G. Colò, and H. Liang. arXiv:1810.02500 [nucl-th]

Evaluation by Experimental ρ_{ch}

Energy (MeV)

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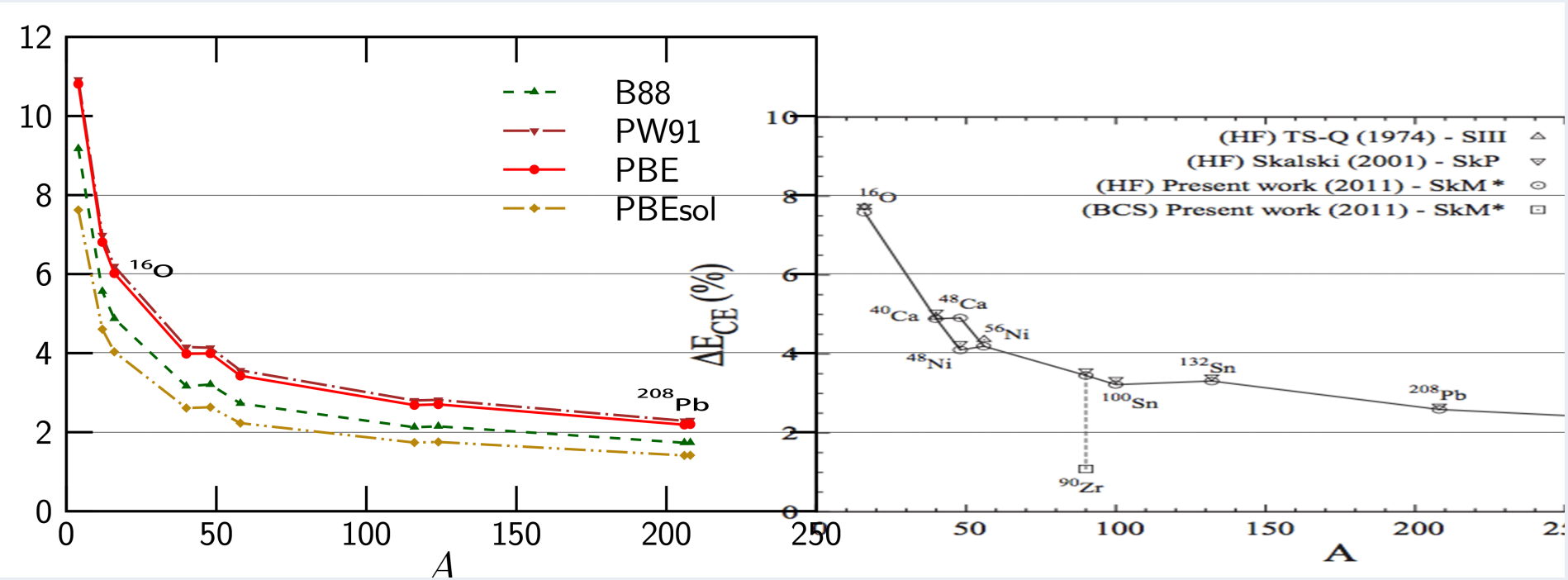
Difference (600 keV): Non-negligible!

Evaluation by Experimental ρ_{ch}

Comparison to Exact Hartree-Fock Calculation

$$\Delta E_{\mathrm{Cx}} = \frac{E_{\mathrm{Cx}}^{\mathrm{GGA}} - E_{\mathrm{Cx}}^{\mathrm{LDA}}}{E_{\mathrm{Cx}}^{\mathrm{GGA}}} \qquad \Delta E_{\mathrm{Cx}} = \frac{E_{\mathrm{Cx}}^{\mathrm{exactHF}} - E_{\mathrm{Cx}}^{\mathrm{LDA}}}{E_{\mathrm{Cx}}^{\mathrm{exactHF}}}$$



Left graph: Naito, Akashi, and Liang. *Phys. Rev. C* **97**, 044319 (2018)

Right graph: Le Bloas *et al.* *Phys. Rev. C* **84**, 014310 (2011)

Evaluation by Experimental ρ_{ch}

Short Conclusion

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

PBE-GGA Coulomb Exchange Functional

$$E_{\mathrm{Cx}}^{\mathrm{GGA}}[\rho] = \int \varepsilon_{\mathrm{Cx}}^{\mathrm{LDA}}(\rho(\boldsymbol{r}))\, F(s)\, \rho(\boldsymbol{r})\, d\boldsymbol{r}, \qquad s = \frac{|\nabla\rho|}{2(3\pi^2)^{1/3}\rho^{4/3}},$$

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

Perdew, Burke, and Ernzerhof. *Phys. Rev. Lett.* **77**, 3865 (1996)

- κ is determined from Lieb-Oxford bound (analytical evaluation)
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  $\rightarrow$ κ must be kept in any systems
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Self-Consistent Calculation

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- κ is determined from Lieb-Oxford bound (analytical evaluation)
  $\rightarrow$ κ must be kept in any systems
- μ is determined from RPA calculation of homogeneous electron gas
  $\rightarrow$ μ in nuclei can be different from in original one

Self-Consistent Calculation

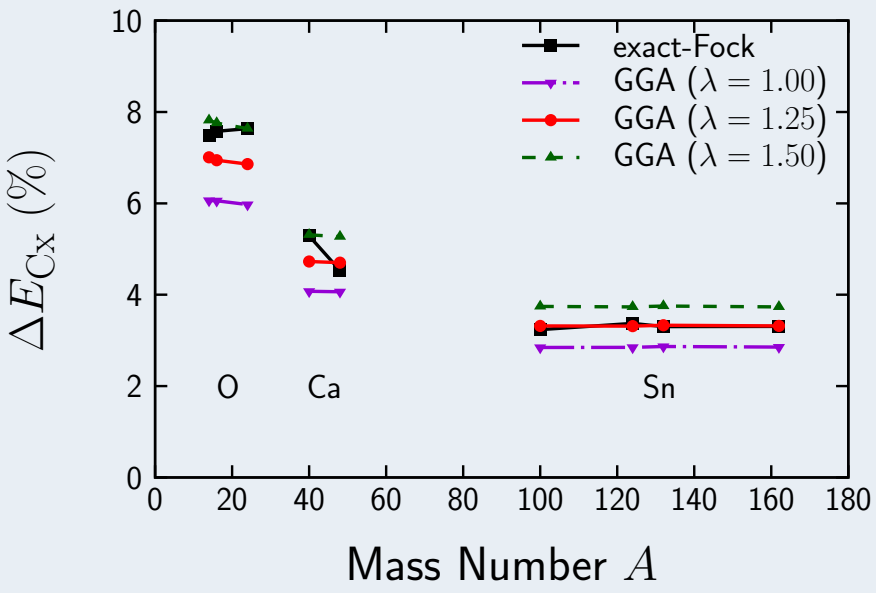
Setup for Self-consistent Skyrme Hartree-Fock Calculation

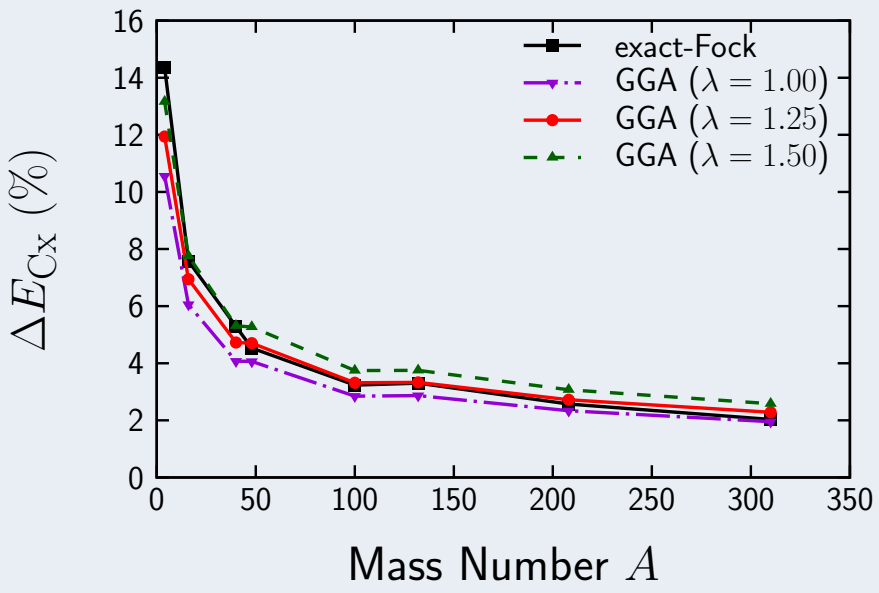
Nuclear Part	SAMi Functional (However, choice of functional of nuclear part is not critical)
Coulomb Part	LDA exchange is replaced to PBE Functional (GGA)
Correlation Part	Coulomb correlation part is not considerd
Pairing Correlation	Neglected

Calculation

Code	Modified `skyrme_rpa` for GGA Colò, Cao, Van Giai, and Capelli. *Comput. Phys. Commn.* **184**, 142 (2013)
Box Size	$0.1\,\mathrm{fm} \times 150$

Self-Consistent Calculation





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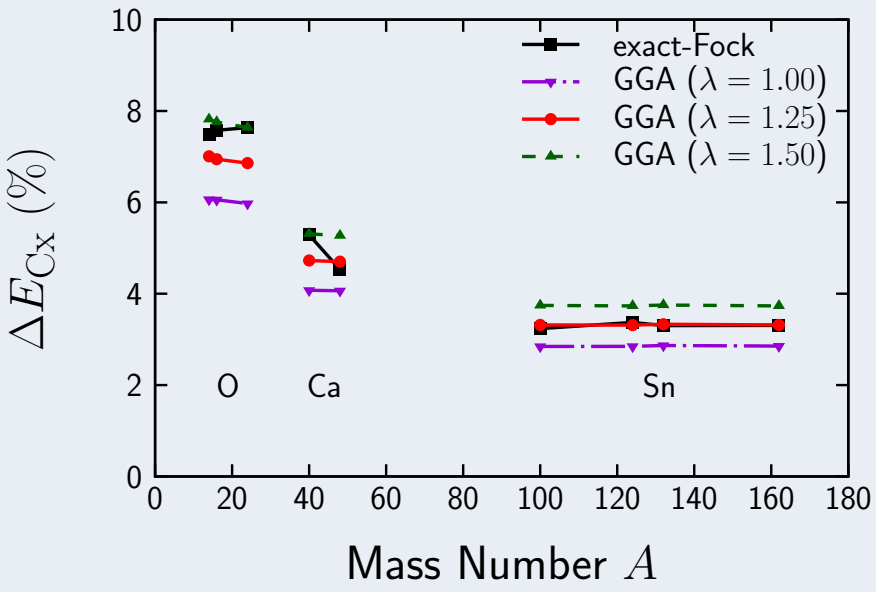

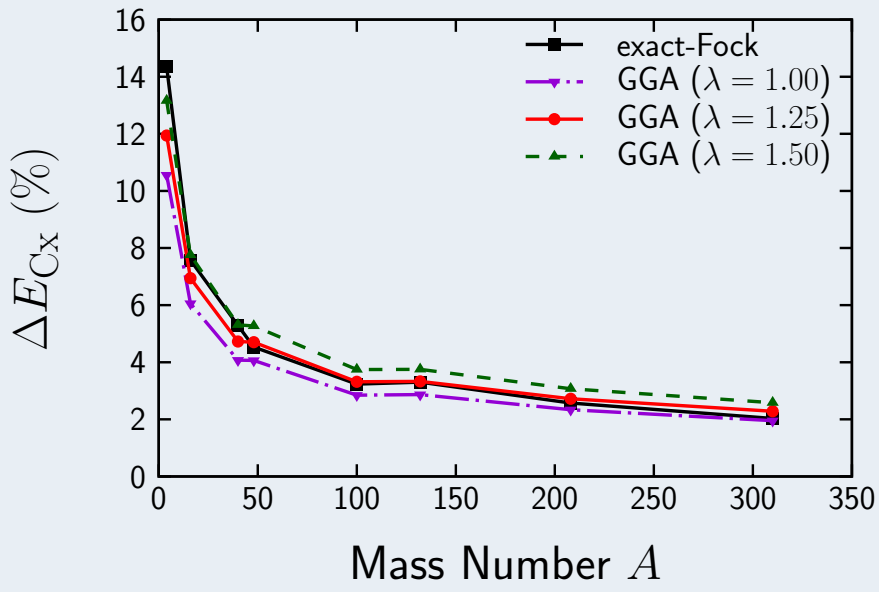

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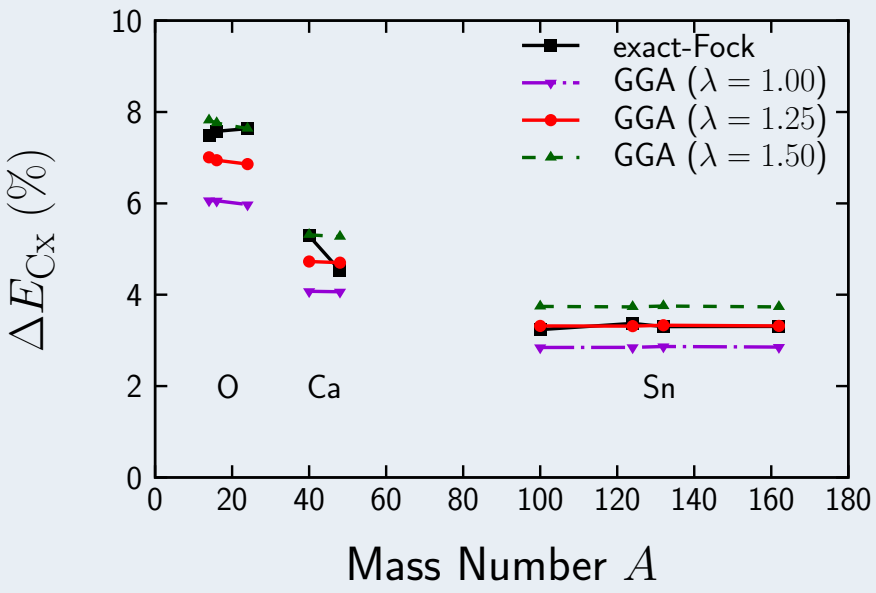

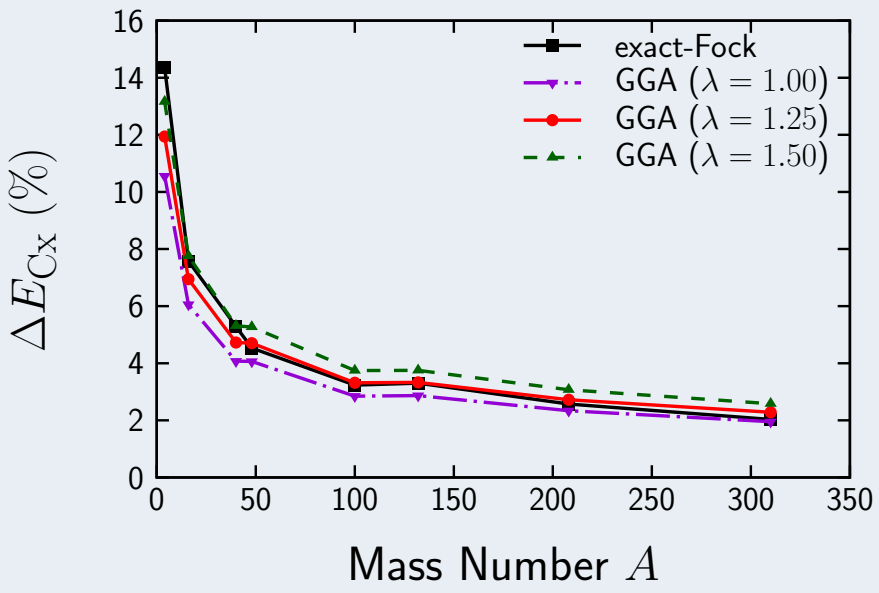

- λ does not have an obvious isospin dependence
- $\lambda = 1.25$ will reproduce well in mid/heavy-mass region
- For whole nuclear chart, $\lambda = 1.25$ is the most suitable
- In light nuclei, $\lambda = 1.25$ has still a little error $\rightarrow$ shell effect?

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

Coulomb Exchange Energy

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 $O\left(N^4\right)$

  LDA $O\left(N^3\right)$

  GGA Still $O\left(N^3\right)$

  $\rightarrow$

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  GGA Still $O\left(N^3\right)$

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

Roca-Maza, Colò, and Sagawa. *Phys. Rev. Lett.* **120**, 202501 (2018)

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

Application to the measurable quantities, for example

Mirror nuclei mass difference, Isobaric Analog State, Superallowed β-decay

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Thank you for attention!!