Coulomb Energy Density Functionals for Nuclear Systems

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Motivation

Isospin Symmetry Breaking of Nuclear Force

- If nuclear force has fully isospin symmetry (i.e., nuclear force for $T = 1$ has no T_3 dependence), charge-symmetry-breaking (CSB) and charge-independence-breaking (CIB) force

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

  are identical to 0, whereas $V_{\mathrm{CSB}} \neq 0$ and $V_{\mathrm{CIB}} \neq 0$ are known
- Amount of isospin symmetry breaking (ISB) of nuclear force is related to CKM matrix V_{ud}

Electromagnetic Interaction and ISB Force

- Electromagnetic (EM) force breaks isospin symmetry of nuclei as well as ISB force
- EM force and ISB of nuclear force are entangled to each other, for example, in mirror nuclei and in energy of isobaric analog states

To understand isospin symmetry breaking of nuclear force, high-accuracy evaluation of electromagnetic force is required

Density Functional Theory (Kohn-Sham Scheme)

Ground-State Energy Density Functional

- Electron Systems

$$E_{\mathrm{gs}} = T_0\left[\rho_{\mathrm{gs}}\right] + \int V_{\mathrm{ext}}(\boldsymbol{r})\,\rho_{\mathrm{gs}}(\boldsymbol{r})\,d\boldsymbol{r} + E_{\mathrm{CH}}\left[\rho_{\mathrm{gs}}\right] + E_{\mathrm{Cx}}\left[\rho_{\mathrm{gs}}\right] + E_{\mathrm{Cc}}\left[\rho_{\mathrm{gs}}\right]$$

- In Nuclear Physics (Atomic Nuclei: Self-Bound System $V_{\mathrm{ext}} \equiv 0$)

$$E_{\mathrm{gs}} = T_0\left[\rho_{\mathrm{gs}}\right] + E_{\mathrm{nucl}}\left[\rho_{\mathrm{gs}}\right] + E_{\mathrm{CH}}\left[\rho_{\mathrm{gs}}\right] + E_{\mathrm{Cx}}\left[\rho_{\mathrm{gs}}\right]$$

This expression is the exact: Accuracy depends on E_{nucl}, E_{Cx}, E_{Cc}

E_{gs}: Ground-state energy, ρ_{gs}: Ground-state density, T_0: kinetic energy of non-interacting system, E_{nucl}: nuclear functional, E_{CH}: Coulomb Hartree functional, E_{Cx}: Coulomb exchange functional, E_{Cc}: Coulomb correlation functional

Approximation for E_{Cx} and E_{Cc}

- Local Density Approximation (LDA)

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

- Generalized Gradient Approximation (GGA)

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

Why Density Functional Theory??

Only the DFT can calculate microscopically for whole nuclear chart!!

What We Did

Toward an understanding of ISB of nuclear force in medium,

1. E_{Cx} and E_{Cc} for electron systems are tested by using experimental ρ_{ch} — T. Naito, R. Akashi, and H. Liang. *Phys. Rev. C* **97**, 044319 (2018)
2. Coulomb GGA exchange functionals for nuclear systems is developed — T. Naito, X. Roca-Maza, G. Colò, and H. Liang. *Phys. Rev. C* **99**, 024309 (2019)

Coulomb Correlation Functional ($E_{\mathrm{Cx}}^{\mathrm{LDA}}$ v.s. $E_{\mathrm{Cc}}^{\mathrm{LDA}}$)

Our work E_{Cc} is calculated as a test by functionals $E_{\mathrm{Cc}}[\rho]$ used in electron systems

Previous work E_{Cc} is calculated for some specific nuclei by using the responce function

Hartree-Fock-Slater — Consitent with $\varepsilon_{\mathrm{Cc}}/\varepsilon_{\mathrm{Cx}}$

Nuclei	Our Work (MeV)			Previous Work (MeV)		
	LDA E_{Cx}	LDA E_{Cc}	$E_{\mathrm{Cc}}^{\mathrm{LDA}}/E_{\mathrm{Cx}}^{\mathrm{LDA}}$	E_{Cx}	E_{Cc}	$E_{\mathrm{Cc}}/E_{\mathrm{Cx}}$
^{16}O	−2.638	−0.05218	1.978 %	−2.99	0.99	−33.1 %
^{40}Ca	−7.087	−0.1329	1.875 %	−7.92	3.18	−40.2 %
^{48}Ca	−7.113	−0.1332	1.873 %			
^{58}Ni	−10.28	−0.1879	1.828 %			
^{116}Sn	−18.41	−0.3361	1.826 %			
^{124}Sn	−18.24	−0.3356	1.840 %			
^{208}Pb	−30.31	−0.5524	1.823 %	−31.29	6.88	−22.0 %

Previous work: Bulgac and Shaginyan. *Nucl. Phys. A* **601**, 103 (1996)

Non-negligible!

Coulomb Exchange Functional ($E_{\mathrm{Cx}}^{\mathrm{LDA}}$ v.s. $E_{\mathrm{Cx}}^{\mathrm{GGA}}$)

PBE-GGA Coulomb Exchange Functional

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

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

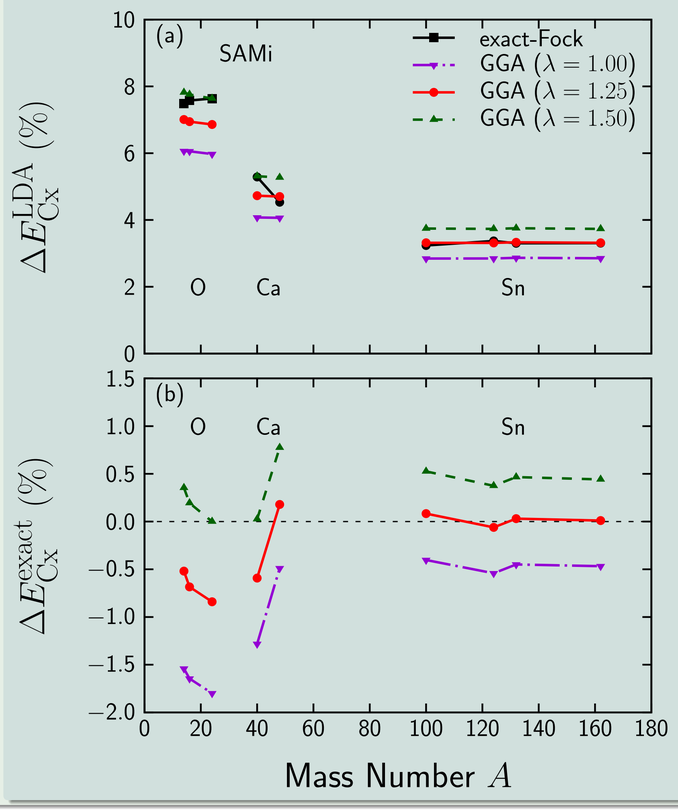
- κ is determined from Lieb-Oxford bound (analytical evaluation) → κ must be kept in any systems
- μ is determined from RPA calculation of homogeneous electron gas → μ in nuclei can be different from in original one

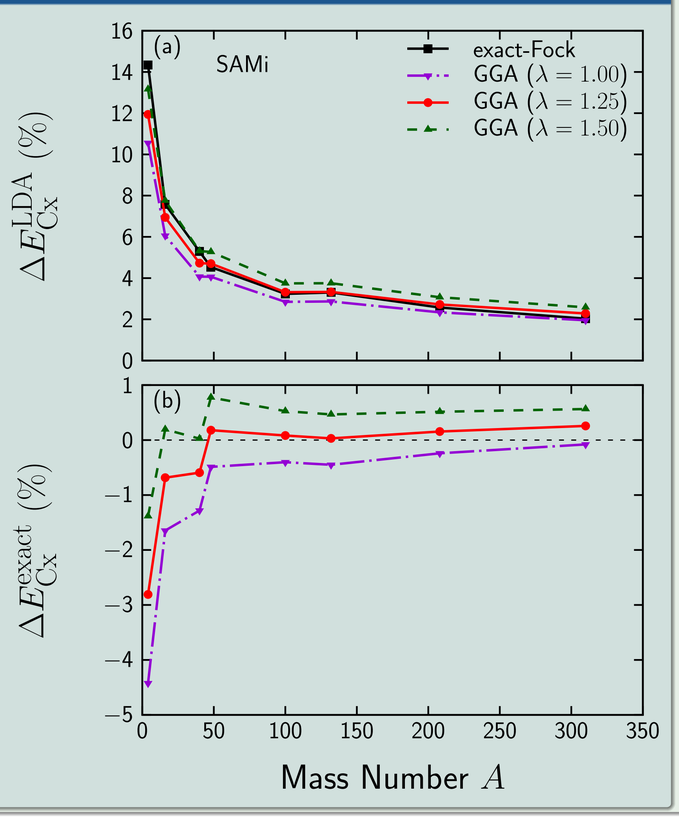
Perdew, Burke, and Ernzerhof. *Phys. Rev. Lett.* **77**, 3865 (1996)

Self-consistent Skyrme Hartree-Fock Calculation

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

$$\Delta E_{\mathrm{Cx}}^{\mathrm{exact}} = \frac{E_{\mathrm{Cx}} - E_{\mathrm{Cx}}^{\mathrm{exact}}}{E_{\mathrm{Cx}}}$$





PBE-GGA $E_{\mathrm{Cx}}[\rho]$ with $\lambda = 1.25$ reproduces the exact-Fock energy!!

Conclusion

Coulomb Correlation Functional

- Difference between the previous work and our work shows that the nuclear force should be considered in the Coulomb correlation functional
- Coulomb correlation functionals in electron systems are not applicable to atomic nuclei directly in contrast to the Coulomb exchange functional → Coulomb correlation functional should be constracted from scratch

Coulomb Exchange Functional

- "Modified" PBE-GGA Coulomb exchange functional with $\lambda = 1.25$ reproduces the exact-Fock energy almost whole nuclear chart
- λ does not have an obvious isospin dependence
- The numerical cost of the GGA is $O\left(N^3\right)$ (same as the LDA), whereas that of the exact-Fock is $O\left(N^4\right)$

Perspectives

- Compared to recent works
  - From fitting: Coulomb repulsive is **stronger** than expected (e.g. Dong *et al. Nucl. Phys. A* **983**, 133 (2019))
  - From first-principle: Coulomb repulsive is **weaker** than expected (e.g. our work, Agrawal *et al. Phys. Rev. C* **72**, 014310 (2005), Roca-Maza *et al. Phys. Rev. C* **94**, 044313 (2016))

  ISB term of nuclear force is stronger than expected??
  How Coulomb correlation EDF works??
- Next Step
  - Considering finite-size effect of nucleons (ρ_{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)
- Applications
  - Mirror nuclei mass difference
  - Isobaric analog state (IAS) energy
  - Superallowed β-decay → Unitarity check of CKM matrix