Towards First-Principles Energy Density Functionals

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Energy Density Functional

- Density functional theory (DFT) gives the *exact* energy and density, if we know the *exact* energy density functional (EDF) $E_{\rm int}$

$$E\left[\rho\right] = T_0\left[\rho\right] + E_{\rm int}\left[\rho\right] + \int V_{\rm ext}\left(\boldsymbol{r}\right)\rho\left(\boldsymbol{r}\right)\, d\boldsymbol{r}$$

$$= \sum_j \varepsilon_j + E_{\rm int}\left[\rho\right] - \int V_{\rm int}\left(\boldsymbol{r}\right)\rho\left(\boldsymbol{r}\right)\, d\boldsymbol{r},$$

  where T_0 is the Kohn-Sham kinetic energy

- $F\left[\rho\right] = T_0\left[\rho\right] + E_{\rm int}\left[\rho\right]$ is the universal with respect to the interaction
- Ultimate goal: Derive *exact* $E_{\rm int}$

EDF in Electronic Systems

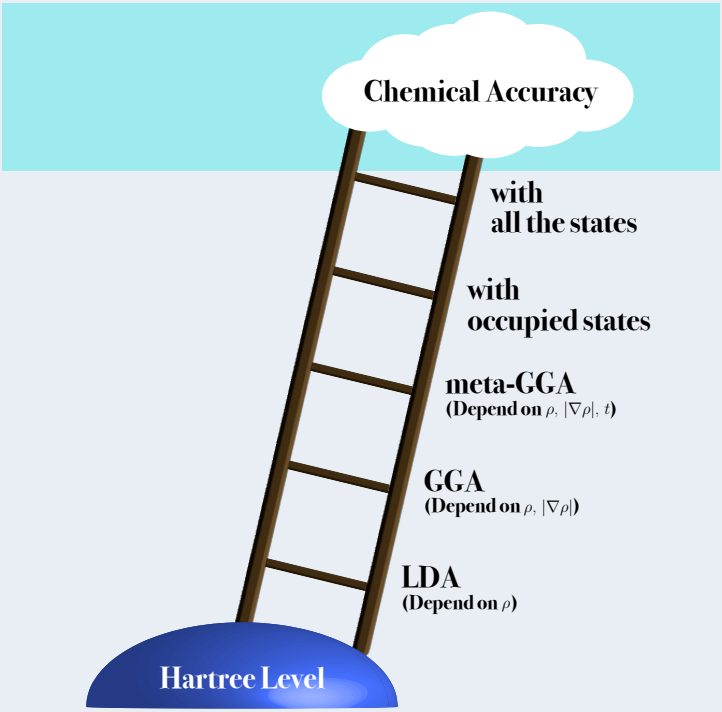
- The interaction is exactly known: Coulomb interaction
- E_{int} is further divided into two parts: $E_{\mathrm{int}}[\rho] = E_{\mathrm{H}}[\rho] + E_{\mathrm{xc}}[\rho]$
- The Hartree term E_{H} can be calculated exactly

$$E_{\mathrm{H}}[\rho] = \frac{1}{2}\iint \frac{\rho(\boldsymbol{r})\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\,d\boldsymbol{r}\,d\boldsymbol{r}'$$

- The remaining part "exchange-correlation functional" E_{xc} is unknown
- Energy density (energy per particle) $\varepsilon_{\mathrm{xc}}$ is defined by

$$E_{\mathrm{xc}}[\rho] = \int \varepsilon_{\mathrm{xc}}(\rho(\boldsymbol{r}), |\nabla\rho|(\boldsymbol{r}), \ldots)\rho(\boldsymbol{r})\,d\boldsymbol{r}$$

Jacob's Ladder in Electronic EDF



- Original Jacob's ladder
  a ladder an angel uses
  in Jacob's dream appeared
  in the Old Testament (旧約聖書)
- It represents the accuracy of EDFs
- The lowest level: depends only on ρ
- The second lowest: depends on ρ & $|\nabla\rho|$

Perdew and Schmidt. *AIP Conf. Proc.* **577**, 1 (2001)

Local Density Approximation (LDA) for Electronic E_{xc}

- LDA energy density $\varepsilon_{\mathrm{xc}}$ depends only on the local density ρ
- LDA $\varepsilon_{\mathrm{xc}}$ gives the exact value for the homogeneous electron gas
- Function form of $\varepsilon_{\mathrm{xc}}$ is assumed to satisfy the following results

High-density limit Analytically known
Gell-Mann-Brueckner resummation (diagrammatic calc)

Low-density limit Analytically known
Wigner crystal (electrons are crystallized)

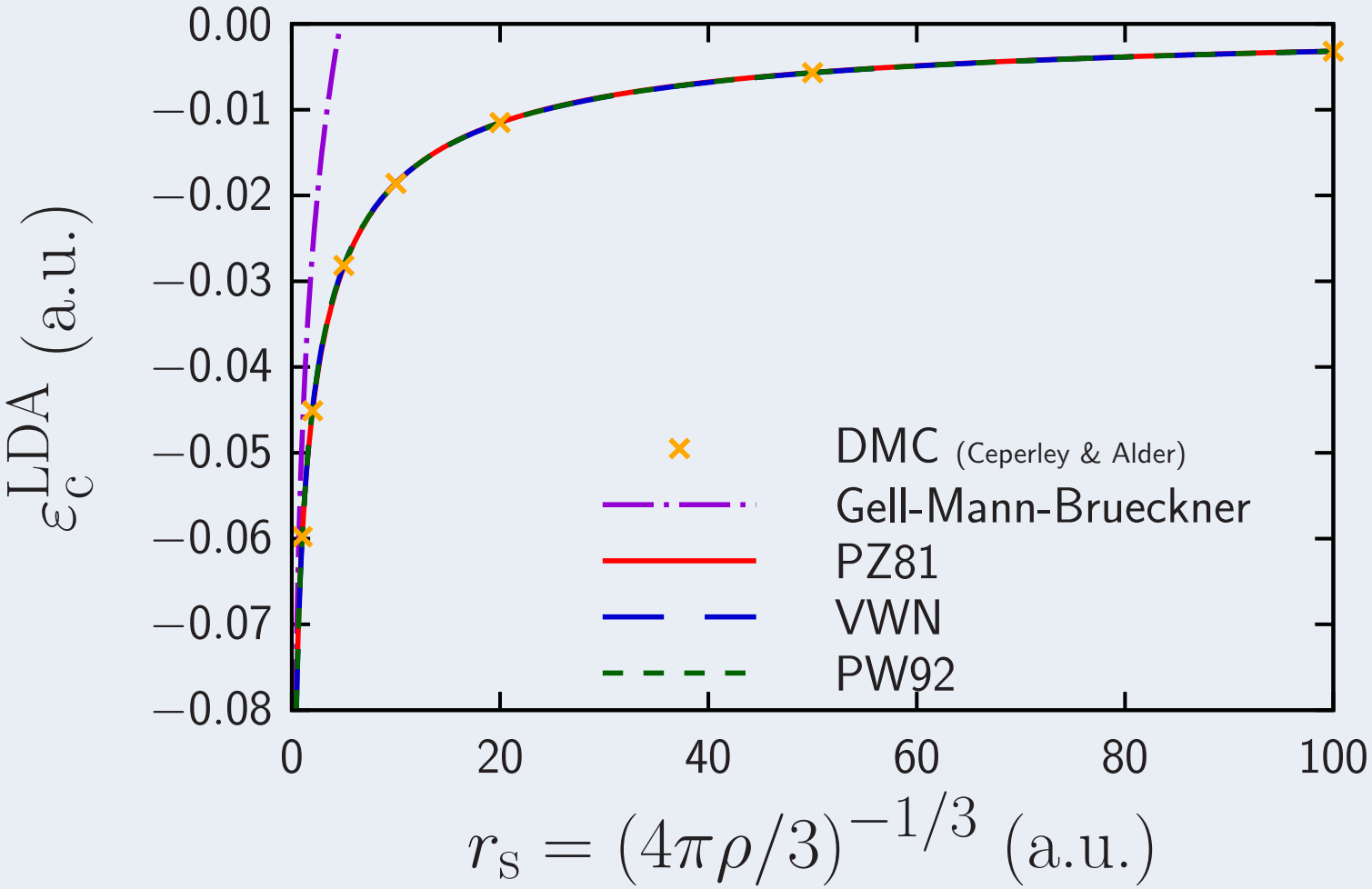
- Parameters are determined to reproduce the following results

Intermediate region $\varepsilon_{\mathrm{xc}}$ of homogeneous electron gas for a few ρ
calculated by diffusion Monte Carlo calculation

Gell-Mann and Brueckner. *Phys. Rev.* **106**, 364 (1957)

Ceperley and Alder. *Phys. Rev. Lett.* **45**, 566 (1980)

LDA E_{xc} for Electronic Systems



Ceperley and Alder. *Phys. Rev. Lett.* **45**, 566 (1980)
Vosko, Wilk, and Nusair. *Can. J. Phys.* **58**, 1200 (1980)
Perdew and Zunger. *Phys. Rev. B* **23**, 5048 (1981)
Perdew and Wang. *Phys. Rev. B* **45**, 13244 (1992)

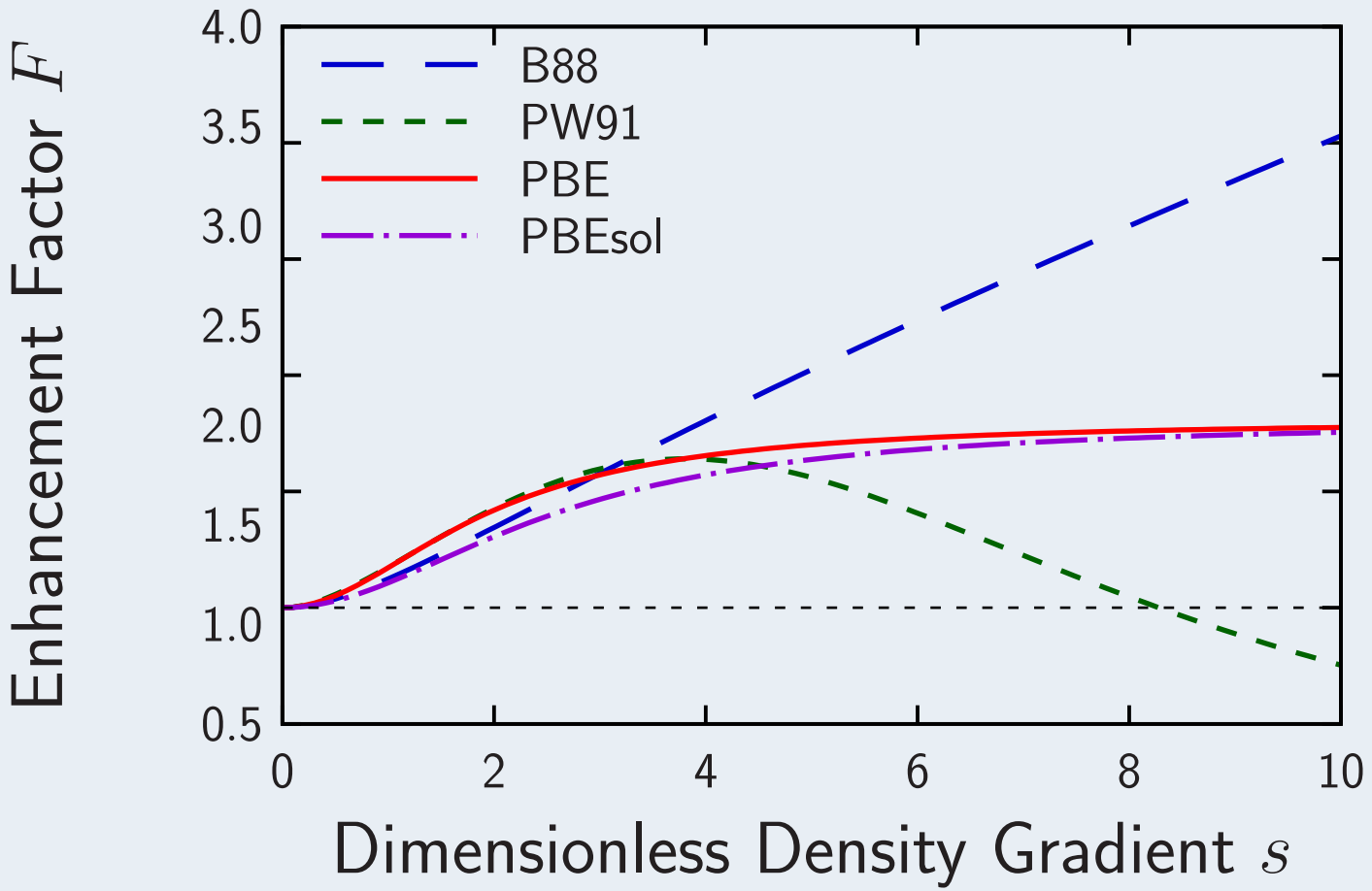
Generalized Gradient Approximation (GGA) for Electronic E_{xc}

- GGA energy density $\varepsilon_{\mathrm{xc}}$ depends on the local density ρ and $|\nabla\rho|$
- In contrast to the LDA, no first-priciples GGA E_{xc} is known
- Several assumption/conditions $\varepsilon_{\mathrm{xc}}$ satisfies are introduced
  - Uniform scaling $E_{\mathrm{Cx}}^{\mathrm{GGA}}\left[\lambda^3\rho\left(\lambda\boldsymbol{r}\right)\right] = \lambda E_{\mathrm{Cx}}^{\mathrm{GGA}}\left[\rho\left(\boldsymbol{r}\right)\right]$ determines the form most GGA exchange EDF satisfies: $\varepsilon_{\mathrm{x}}^{\mathrm{GGA}}\left(\rho, |\nabla\rho|\right) = \varepsilon_{\mathrm{x}}^{\mathrm{LDA}}\left(\rho\right) F\left(s\right),\ s = |\nabla\rho| \,/\, \left[2\left(3\pi^2\right)^{1/3}\rho^{4/3}\right]$
  - Trivial condition: $F\left(0\right) = 1$
  - The spin dependence: $E_{\mathrm{Cx}}^{\mathrm{GGA}}\left[\rho_\uparrow, \rho_\downarrow\right] = \frac{1}{2}E_{\mathrm{Cx}}^{\mathrm{GGA}}\left[\rho_\uparrow\right] + \frac{1}{2}E_{\mathrm{Cx}}^{\mathrm{GGA}}\left[\rho_\downarrow\right]$
  - Lieb-Oxford bound $E_{\mathrm{x}}\left[\rho\right] \geq E_{\mathrm{xc}}\left[\rho\right] \geq -1.679e^2 \int \left[\rho\left(\boldsymbol{r}\right)\right]^{4/3} d\boldsymbol{r}$
  - ...
- Different GGA E_{xc} introduces different assumption
  $\rightarrow$ Different GGA E_{xc} gives different behaviour

Lieb and Oxford. *Int. J. Quantum Chem.* **19**, 427 (1981)

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

s-Dependence of GGA E_{x}



Becke. *Phys. Rev. A* **38**, 3098 (1988)
Perdew *et al. Phys. Rev. B* **46**, 6671 (1992)
Perdew, Burke, and Ernzerhof. *Phys. Rev. Lett.* **77**, 3865 (1996)

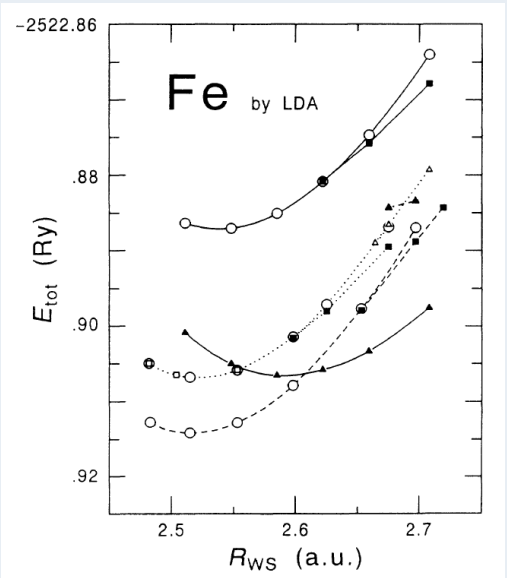
Perdew *et al. Phys. Rev. Lett.* **100**, 136406 (2008)

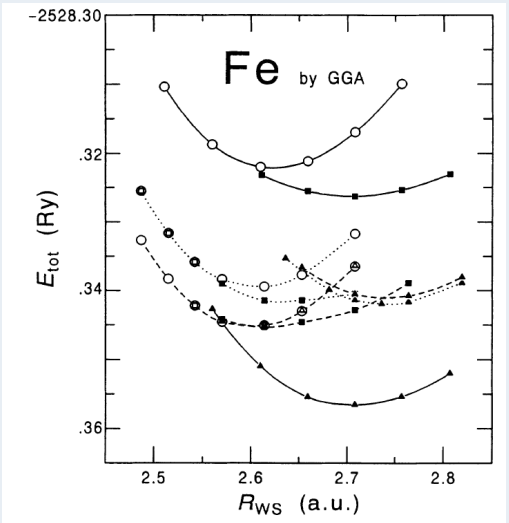
Remark of GGA

- Introduction of $|\nabla\rho|$ is crucial to predict crystal structures of metals
- Example: crystal structure of Fe (bcc feromagnetic)

  LDA (PZ81) Non-magnetic hexagonal close-packed (hcp)
  GGA (PW86) Ferromagnetic body-centered cubic (bcc)

  Solid line bcc
  Dotted line fcc
  Dashed line hcp
  Circle Non-mag.
  Triangle Ferro-mag.
  Square Anti-ferro-mag.
  Filled High spin
  Empty Low spin



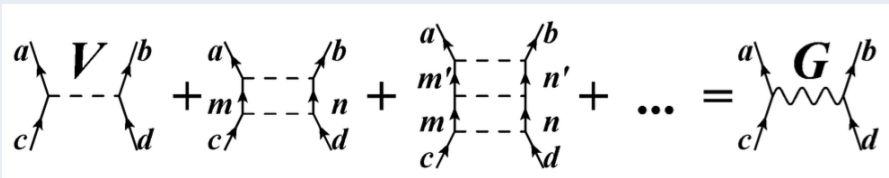


- Thanks to this success, first-principles DFT became widely used
- However, GGA often overestimates lattice const.,
  while LDA often underestimates it

Asada and Terakura. *Phys. Rev. B* **46**, 13599 (1992)

EDF in Nuclear Systems

- There are two interactions: nuclear & Coulomb ones ($v_{\rm nucl}$ & $v_{\rm Coul}$)
- $v_{\rm nucl}$ in vacuum is known by various methods
  scattering exp., deuteron properties, lattice QCD, chiral EFT
- $v_{\rm nucl}$ in medium is different from the bare one due to in-medium effect



- $v_{\rm nucl}$ in medium is still under discussion
- $E_{\rm int}$ is further divided into two parts: $E_{\rm int}[\rho] = E_{\rm nucl}[\rho] + E_{\rm Coul}[\rho]$
- Coulomb part $E_{\rm Coul}$ includes Hartree and exchange parts

$$E_{\rm Coul}[\rho] = E_{\rm CH}[\rho] + E_{\rm Cx}[\rho]$$

The figure is taken from a slide by S. Shen

Nuclear EDF E_{nucl}

- LDA E_{nucl} is not accurate enough to calculate nuclear properties
- Methods to derive EDFs
  1. Assume the functional form (GGA or meta-GGA level)
  2. Parameters are determined to reproduce experimental data, as well as homogeneous nucleon gas (nuclear matter)
- Since parameters are fitted to experimental data, the correlation energy is included implicitly in E_{nucl}
- Modern E_{nucl} EDF reproduces binding energies within 1–$5\,\mathrm{MeV}$ error
- For more detail: see Hinohara-san's talk

Questions

- Can we make *ab initio* EDFs?

For a specific channel Use a quantity which is only sensitive to the channel

CSB: Naito, Colò, Liang, Roca-Maza, Sagawa. *Phys. Rev. C* **105**, L021304 (2022)

- If we have more knowledge of density,
  can we construct more accurate EDFs?

- Is there a novel method to derive EDFs microscopically?

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  Another direction Inverse approach (First part of my talk)

- Is there a novel method to derive EDFs microscopically?

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- If we have more knowledge of density,
  can we construct more accurate EDFs?

  Possible direction Machine learning (Imoto-san's talk)

  Another direction Inverse approach (First part of my talk)

- Is there a novel method to derive EDFs microscopically?
  Functional renormalization group approach (Second part of my talk)

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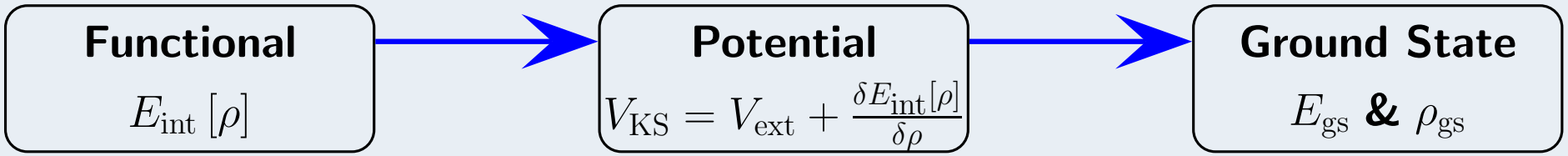
Collaborators in This Talk

- Giacomo Accorto (U. Zagreb, Croatia)
- Haozhao Liang (U. Tokyo/RIKEN, Japan)
- Tamara Nikšić (U. Zagreb, Croatia)
- Daisuke Ohashi (U. Tokyo/RIKEN → Private Company, Japan)
- Dario Vretenar (U. Zagreb, Croatia)

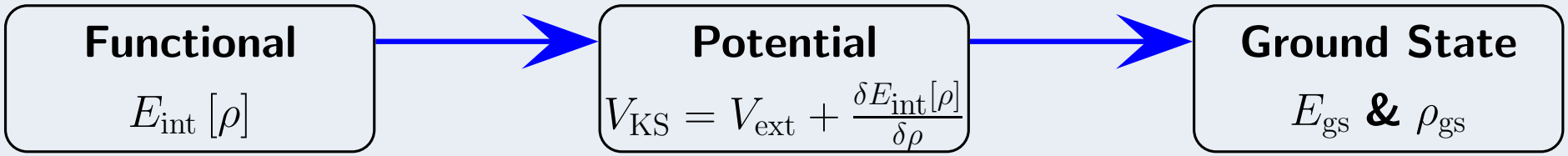
Naito, Ohashi, and Liang. *J. Phys. B* **52**, 245003 (2019)

Accorto, Naito, Liang, Nikšić, and Vretenar. *Phys. Rev. C* **103**, 044304 (2021)

Usual DFT Calculation

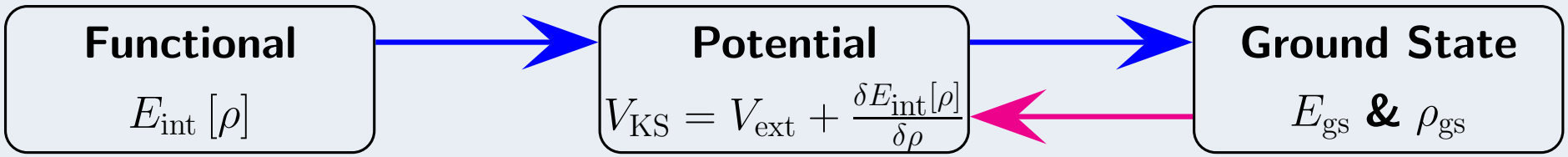


Usual DFT Calculation



Q1. If we know $\rho_{\rm gs}$, can we derive $V_{\rm KS}$?

Inverse Kohn-Sham Method



Q1. If we know $\rho_{\rm gs}$, can we derive $V_{\rm KS}$?

A1. Yes! Inverse Kohn-Sham Method

Inverse Kohn-Sham Method

- Assume that ρ_{gs} of a system (e.g., Ne atom) is known
- V_{KS} for the system (e.g., Ne atom) reads

$$V_{\mathrm{KS}}(\boldsymbol{r}) = \frac{\sum \varphi_j^*(\boldsymbol{r}) \left(\varepsilon_j + \frac{\hbar^2}{2M}\Delta\right) \varphi_j(\boldsymbol{r})}{\rho_{\mathrm{gs}}(\boldsymbol{r})}$$

Practically, V_{KS} is derived iteratively

$$V_{\mathrm{KS}}^n(\boldsymbol{r}) = \frac{\sum \varphi_j^{n*}(\boldsymbol{r}) \left(\varepsilon_j^n + \frac{\hbar^2}{2M}\Delta\right) \varphi_j^n(\boldsymbol{r})}{\rho_{\mathrm{gs}}(\boldsymbol{r})} = \frac{\rho^n(\boldsymbol{r})}{\rho_{\mathrm{gs}}(\boldsymbol{r})} V_{\mathrm{KS}}^{n-1}(\boldsymbol{r})$$

$$\left[-\frac{\hbar^2}{2M}\Delta + V_{\mathrm{KS}}^{n-1}(\boldsymbol{r})\right] \varphi_j^n(\boldsymbol{r}) = \varepsilon_j^n \varphi_j^n(\boldsymbol{r}) \qquad \rho^n(\boldsymbol{r}) = \sum \left|\varphi_j^n(\boldsymbol{r})\right|^2$$

- This potential V_{KS} can only be used for the system (e.g., Ne atom)
  $\rightarrow$ This V_{KS} cannot be used directly for another system (e.g., Ar atom)

Wang and Parr. *Phys. Rev. A* **47**, R1591 (1993)

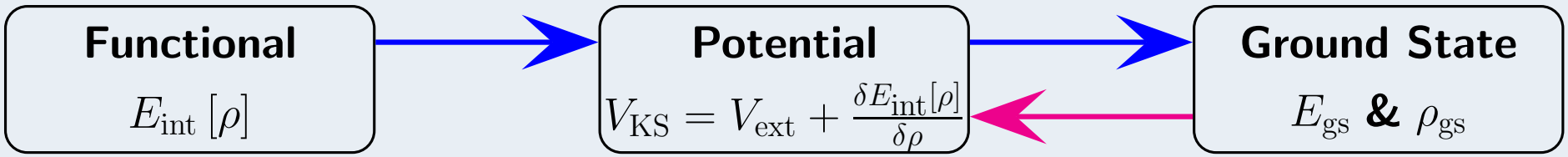
Inverse Kohn-Sham Method

- Since $V_{\rm KS}$ obtained by a system (e.g., $\rm Ne$ atom)
  is applicable only the system ($\rm Ne$ atom),
  IKS was usually used for the discussion of accuracy of $E_{\rm int}$, $V_{\rm KS}$ etc
- Also, numerical aspects of IKS has recently been discussed
- Recently, IKS has been highlighted again
  since such information can be combined with ML technique
- First application of IKS to nuclear systems was done by Milan group
  (Gianluca's talk)
- So far, as far as I know,
  $V_{\rm KS}$ obtained by IKS has not been applied yet to derive $E_{\rm int}$

Nuclear physics application: Accorto *et al. Phys. Rev. C* **101**, 024315 (2020)

Recent review: Shi and Wasserman. *J. Phys. Chem. Lett.* **12**, 5308 (2021)

Inverse Kohn-Sham Method



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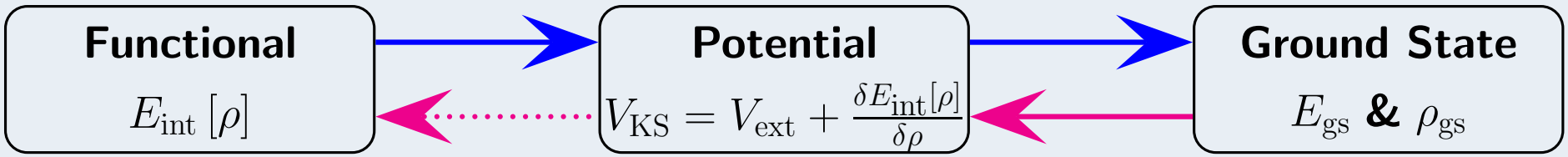
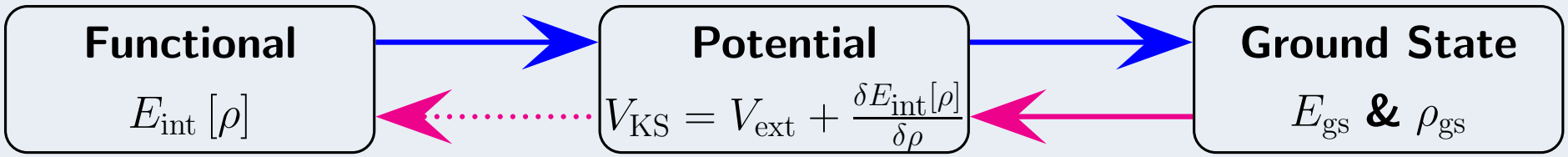


Q1. If we know $\rho_{\rm gs}$, can we derive $V_{\rm KS}$?

A1. Yes! Inverse Kohn-Sham Method

Q2. Can we derive $E_{\rm int}$ from $V_{\rm KS}$?

Inverse Kohn-Sham Method



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A1. Yes! Inverse Kohn-Sham Method

Q2. Can we derive $E_{\rm int}$ from $V_{\rm KS}$?

A2. Today's Topic!! "IKS-DFPT"

Problem of Derivation of E_{int} from V_{KS}

- Kohn-Sham potential V_{KS} is functional derivative of E_{int}

$$V_{\mathrm{KS}}(\boldsymbol{r}) = V_{\mathrm{ext}}(\boldsymbol{r}) + \left.\frac{\delta E_{\mathrm{int}}[\rho]}{\delta\rho}\right|_{\rho=\rho_{\mathrm{gs}}(\boldsymbol{r})}$$

- In principle, E_{int} can be derived
  if "functional integral" of V_{KS} can be done
- Even if E_{int} is derived by the functional integral,
  there is a problem: How can we determine "integral constant"?

Levy-Zahariev Formulation

- For an arbitrary scalar functional $c[\rho]$, the following equation holds

$$E[\rho] = \sum_j \left(\varepsilon_j + c[\rho]\right) + E_{\mathrm{int}}[\rho] - \int \left(V_{\mathrm{int}}(\boldsymbol{r}) + c[\rho]\right)\rho(\boldsymbol{r})\, d\boldsymbol{r}$$

- If we take

$$c[\rho] = \frac{E_{\mathrm{int}}[\rho] - \int V_{\mathrm{int}}(\boldsymbol{r})\rho(\boldsymbol{r})\, d\boldsymbol{r}}{\int \rho(\boldsymbol{r})\, d\boldsymbol{r}},$$

$$\tilde{V}_{\mathrm{int}}(\boldsymbol{r}) = V_{\mathrm{int}}(\boldsymbol{r}) + c[\rho],$$

  we obtain

$$E[\rho] = \sum_j \tilde{\varepsilon}_j$$

$$E_{\mathrm{int}}[\rho] = \int \tilde{V}_{\mathrm{int}}(\boldsymbol{r})\rho(\boldsymbol{r})\, d\boldsymbol{r}$$

- Nagai *et al.* used this formulation for ML EDF from IKS

Levy and Zahariev. *Phys. Rev. Lett.* **113**, 113002 (2014)

Nagai, Akashi, Sasaki, and Sugino. *J. Chem. Phys.* **148**, 241737 (2018)

Problem of Levy-Zahariev Formulation

- In the normal formulation, $V_{\mathrm{int}}^{N+\delta}(\boldsymbol{r}) - V_{\mathrm{int}}^{N-\delta}(\boldsymbol{r}) \neq 0$, where V_{int}^{N} is the Hxc potential for a N-particle system and $\delta > 0$ is an infinitesimal
- This is related to an ionic energy and an electron affinity
- In the LZ formulation $\tilde{V}_{\mathrm{int}}^{N+\delta}(\boldsymbol{r}) - \tilde{V}_{\mathrm{int}}^{N-\delta}(\boldsymbol{r}) = 0$
- Thus, $E_{\mathrm{int}}[\rho] = \int V_{\mathrm{int}}(\boldsymbol{r})\rho(\boldsymbol{r})\, d\boldsymbol{r}$ with V_{int} obtained by IKS corresponds to EDF in the LZ formulation
- Therefore, total energies obtained by this E_{int} should not be correct, while "relative energies" should be correct
- In nuclear physics, absolute energies are needed
  $\rightarrow$ Alternative method should be developed

Perdew, Parr, Levy, and Balduz. *Phys. Rev. Lett.* **49**, 1691 (1982)

Levy and Zahariev. *Phys. Rev. Lett.* **113**, 113002 (2014)

Brief Idea of IKS-DFPT

- DFT calculation with a "known" EDF $\tilde{E}_{\rm int}$ is succeeded
  $\rightarrow$ We assume that the "known" EDF $\tilde{E}_{\rm int}$ is good enough
- Improve $\tilde{E}_{\rm int}$ using some "exact" G.S. densities
- Difference between $\tilde{E}_{\rm int}$ & $E_{\rm int}^{\rm exact}$ is treated as 1st order perturbation
- Idea of **Density Functional Perturbation Theory (DFPT)** is used
  Original DFPT is usually used for phonon calculation for solid
  with considering pertubation for $V_{\rm ext}$
- $E_{\rm gs}$ is formally derived by two methods
  - Inverse Kohn-Sham method
  - Density functional perturbation theory
- Using the fact that two $E_{\rm gs}$ should be identical, $E_{\rm int}^{\rm exact} - \tilde{E}_{\rm int}$ is derived

Naito, Ohashi, and Liang. *J. Phys. B* **52**, 245003 (2019)

Perturbation Expansion for E_{int}, ρ, φ_j

$$E_{\mathrm{int}}^{\mathrm{exact}}[\rho] = \tilde{E}_{\mathrm{int}}[\rho] + \lambda E_{\mathrm{int}}^{(1)}[\rho] + O\left(\lambda^2\right)$$
$$V_{\mathrm{ext}}^{\mathrm{exact}}(\boldsymbol{r}) = \tilde{V}_{\mathrm{ext}}(\boldsymbol{r})$$
$$\rho_{\mathrm{gs}}^{\mathrm{exact}}(\boldsymbol{r}) = \tilde{\rho}_{\mathrm{gs}}(\boldsymbol{r}) + \lambda \rho_{\mathrm{gs}}^{(1)}(\boldsymbol{r}) + O\left(\lambda^2\right)$$
$$\varphi_j^{\mathrm{exact}}(\boldsymbol{r}) = \tilde{\varphi}_j(\boldsymbol{r}) + \lambda \varphi_j^{(1)}(\boldsymbol{r}) + O\left(\lambda^2\right)$$

Note: $\rho_{\mathrm{gs}}^{\mathrm{exact}}$ is known

Assumption: Orthogonal Condition

$$\int \tilde{\varphi}_j^*(\boldsymbol{r})\, \varphi_j^{(1)}(\boldsymbol{r})\, d\boldsymbol{r} = 0$$

Density

$$\tilde{\rho}_{\mathrm{gs}}(\boldsymbol{r}) = \sum \left|\tilde{\varphi}_j(\boldsymbol{r})\right|^2$$
$$\rho_{\mathrm{gs}}^{(1)}(\boldsymbol{r}) = \sum \left[\varphi_j^{(1)*}(\boldsymbol{r})\, \tilde{\varphi}_j(\boldsymbol{r}) + \tilde{\varphi}_j^*(\boldsymbol{r})\, \varphi_j^{(1)}(\boldsymbol{r})\right]$$

Ground-State Energy from IKS

$$E_{\mathrm{gs}}^{\mathrm{exact}} = \sum \varepsilon_j^{\mathrm{exact}} + E_{\mathrm{int}}^{\mathrm{exact}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] - \int \frac{\delta E_{\mathrm{int}}^{\mathrm{exact}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right)\, d\boldsymbol{r}$$

$$=$$

$\varepsilon_j^{\mathrm{exact}}$ can be derived by inverse Kohn-Sham method

Ground-State Energy from IKS

$$
\begin{aligned}
E_{\mathrm{gs}}^{\mathrm{exact}} &= \sum \varepsilon_j^{\mathrm{exact}} + E_{\mathrm{int}}^{\mathrm{exact}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] - \int \frac{\delta E_{\mathrm{int}}^{\mathrm{exact}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right)\, d\boldsymbol{r} \\
&= \sum \varepsilon_j^{\mathrm{exact}} + \tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] + \lambda E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] \\
&\quad - \int \frac{\delta \tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right)\, d\boldsymbol{r} - \lambda \int \frac{\delta E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right)\, d\boldsymbol{r} + O\left(\lambda^2\right)
\end{aligned}
$$

$\varepsilon_j^{\mathrm{exact}}$ can be derived by inverse Kohn-Sham method

Ground-State Energy from DFPT

$$E_{\mathrm{gs}}^{\mathrm{exact}} = \tilde{E}_{\mathrm{gs}} + \lambda \left. \frac{dE_{\mathrm{int}}^{\mathrm{exact}}\left[\tilde{\rho}_{\mathrm{gs}}\right]}{d\lambda} \right|_{\lambda=0} + O\left(\lambda^2\right)$$

$$=$$

$$=$$

Please see our paper for the derivation of this equation, since it is complicated

Ground-State Energy from DFPT

$$E_{\mathrm{gs}}^{\mathrm{exact}} = \tilde{E}_{\mathrm{gs}} + \lambda \left. \frac{dE_{\mathrm{int}}^{\mathrm{exact}}\left[\tilde{\rho}_{\mathrm{gs}}\right]}{d\lambda} \right|_{\lambda=0} + O\left(\lambda^2\right)$$

$$= \tilde{E}_{\mathrm{gs}} + \lambda E_{\mathrm{int}}^{(1)}\left[\tilde{\rho}_{\mathrm{gs}}\right] + O\left(\lambda^2\right)$$

$$=$$

Please see our paper for the derivation of this equation, since it is complicated

Ground-State Energy from DFPT

$$
\begin{aligned}
E_{\mathrm{gs}}^{\mathrm{exact}} &= \tilde{E}_{\mathrm{gs}} + \lambda \left. \frac{dE_{\mathrm{int}}^{\mathrm{exact}}\left[\tilde{\rho}_{\mathrm{gs}}\right]}{d\lambda} \right|_{\lambda=0} + O\left(\lambda^2\right) \\
&= \tilde{E}_{\mathrm{gs}} + \lambda E_{\mathrm{int}}^{(1)}\left[\tilde{\rho}_{\mathrm{gs}}\right] + O\left(\lambda^2\right) \\
&= \sum \tilde{\varepsilon}_j + \tilde{E}_{\mathrm{int}}\left[\tilde{\rho}_{\mathrm{gs}}\right] - \int \frac{\delta \tilde{E}_{\mathrm{int}}\left[\tilde{\rho}_{\mathrm{gs}}\right]}{\delta \rho\left(\boldsymbol{r}\right)} \tilde{\rho}_{\mathrm{gs}}\left(\boldsymbol{r}\right) d\boldsymbol{r} + \lambda E_{\mathrm{int}}^{(1)}\left[\tilde{\rho}_{\mathrm{gs}}\right] + O\left(\lambda^2\right)
\end{aligned}
$$

Please see our paper for the derivation of this equation, since it is complicated

Equation for IKS-DFPT

Compare two expression and neglect $O\left(\lambda^2\right)$ term

$$\tilde{E}_{\mathrm{gs}} + \lambda E_{\mathrm{int}}^{(1)}\left[\tilde{\rho}_{\mathrm{gs}}\right] \simeq \sum \varepsilon_j^{\mathrm{exact}} + \tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] + \lambda E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] - \int \frac{\delta \tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right) d\boldsymbol{r} - \lambda \int \frac{\delta E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right) d\boldsymbol{r}$$

Therefore, We Should Solve

$$\lambda E_{\mathrm{int}}^{(1)}\left[\tilde{\rho}_{\mathrm{gs}}\right] - \lambda E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] + \lambda \int \frac{\delta E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right) d\boldsymbol{r}$$

$$\simeq \sum \varepsilon_j^{\mathrm{exact}} + \tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] - \int \frac{\delta \tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right) d\boldsymbol{r} - \tilde{E}_{\mathrm{gs}}$$

Equation for IKS-DFPT

Compare two expression and neglect $O\left(\lambda^2\right)$ term

$$\tilde{E}_{\mathrm{gs}} + \lambda E_{\mathrm{int}}^{(1)}\left[\tilde{\rho}_{\mathrm{gs}}\right] \simeq \sum \varepsilon_j^{\mathrm{exact}} + \tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] + \lambda E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] - \int \frac{\delta \tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right) d\boldsymbol{r} - \lambda \int \frac{\delta E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right) d\boldsymbol{r}$$

Therefore, We Should Solve

$$\lambda E_{\mathrm{int}}^{(1)}\left[\tilde{\rho}_{\mathrm{gs}}\right] - \lambda E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] + \lambda \int \frac{\delta E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right) d\boldsymbol{r}$$

$$\simeq \sum \varepsilon_j^{\mathrm{exact}} + \tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] - \int \frac{\delta \tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right) d\boldsymbol{r} - \tilde{E}_{\mathrm{gs}} = C\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]$$

Right-hand side can be calculated exactly as $C\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]$ (constant)

Our Task

Deribe $\lambda E_{\mathrm{int}}^{(1)}$ from

$$\lambda E_{\mathrm{int}}^{(1)}\left[\tilde{\rho}_{\mathrm{gs}}^{\mathrm{exact}}\right]-\lambda E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]+\lambda\int\frac{\delta E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)}\rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right)\,d\boldsymbol{r}=C\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]$$

This equation is a functional equation: Difficult to solve!!

How to Solve It?

Inverse Kohn-Sham Method and Perturbation Theory

Our Task

Deribe $\lambda E_{\mathrm{int}}^{(1)}$ from

$$\lambda E_{\mathrm{int}}^{(1)}\left[\tilde{\rho}_{\mathrm{gs}}^{\mathrm{exact}}\right] - \lambda E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right] + \lambda \int \frac{\delta E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)} \rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right) d\boldsymbol{r} = C\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]$$

This equation is a functional equation: Difficult to solve!!

How to Solve It?

1. Assume the form of $\lambda E_{\mathrm{int}}^{(1)}$
2. If $\lambda E_{\mathrm{int}}^{(1)}$ has n parameters,
   substitute ρ_{gs} and ε_j of n kind of systems to the equation
3. Solve simultaniously

Inverse Kohn-Sham Method and Perturbation Theory

Assumption for $\lambda E_{\mathrm{int}}^{(1)}$

$$\lambda E_{\mathrm{int}}^{(1)}[\rho] = \lambda A \int [\rho(\boldsymbol{r})]^{\alpha} \, d\boldsymbol{r}$$

Unknown parameters: λA and α

Equation for IKS-DFPT1

$$\lambda A \int \left\{ \left[\tilde{\rho}_{\mathrm{gs}}(\boldsymbol{r}) \right]^{\alpha} + (\alpha - 1) \left[\rho_{\mathrm{gs}}^{\mathrm{exact}}(\boldsymbol{r}) \right]^{\alpha} \right\} d\boldsymbol{r} = C\left[\rho_{\mathrm{gs}}\right]$$

To derive λA and α, two densities are required

Iterative IKS-DFPT: Calculated Functional at n-th Step

$$E_{\mathrm{int}}^{n\text{-th}}[\rho] = \tilde{E}_{\mathrm{int}}[\rho] + \sum_{j=1}^{n} \lambda A_j \int [\rho(\boldsymbol{r})]^{\alpha_j} \, d\boldsymbol{r}$$

EDF for Electronic Systems

$$E_{\mathrm{int}}[\rho] = E_{\mathrm{H}}[\rho] + E_{\mathrm{x}}[\rho] + E_{\mathrm{c}}[\rho]$$

E_{H} Coulomb Hartree EDF

E_{x} Coulomb exchange EDF (LDA is used in this work)

E_{c} Coulomb correlation EDF (LDA is used in this work)

Setup

- Noble gas atoms are used for ρ_{gs}
- Two patterns are tested

Pattern 1

Known $\tilde{E}_{\mathrm{int}}$ E_{H}

"Exact" E_{int} $E_{\mathrm{H}} + E_{\mathrm{x}}$

Can we reproduce E_{x}?

Pattern 2

Known $\tilde{E}_{\mathrm{int}}$ $E_{\mathrm{H}} + E_{\mathrm{x}}$

"Exact" E_{int} $E_{\mathrm{H}} + E_{\mathrm{x}} + E_{\mathrm{c}}$

Can we reproduce E_{c}?

Energy: $E_{\mathrm{int}}^{\mathrm{exact}}$ is Hartree & LDA exchange (from Xe & Rn)

n	α_n	λA_n	$E_{\mathrm{gs}}^{n\text{-th}}$			
			Xe	Rn	Ne	Ar
0			−7054.6485	−21479.344		
Target	1.3333333	−0.7385588	−7223.1853	−21848.954	−127.49109	−524.51427

- Energy: 2.3 % (Xe) & 1.7 % (Rn) → 0.0017 % (Xe) & 0.0003 % (Rn)
- α_1: 0.16 %, A_n: 2.3 %

Naito, Ohashi, and Liang. *J. Phys. B* **52**, 245003 (2019)

Hartree Atomic Unit

$$m_e = 1, \qquad \hbar = 1, \qquad e^2 = 1, \qquad 4\pi\varepsilon_0 = 1, \qquad c = \frac{1}{\alpha}$$

Energy: $E_{\mathrm{int}}^{\mathrm{exact}}$ is Hartree & LDA exchange (from Xe & Rn)

n	α_n	λA_n	$E_{\mathrm{gs}}^{n\text{-th}}$			
			Xe	Rn	Ne	Ar
0			−7054.6485	−21479.344		
1	1.3311445	−0.7558229	−7224.9365	−21852.010		
Target	1.3333333	−0.7385588	−7223.1853	−21848.954	−127.49109	−524.51427

- Energy: 2.3 % (Xe) & 1.7 % (Rn) → 0.0017 % (Xe) & 0.0003 % (Rn)
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n	α_n	λA_n	$E_{\mathrm{gs}}^{n\text{-th}}$			
			Xe	Rn	Ne	Ar
0			−7054.6485	−21479.344		
1	1.3311445	−0.7558229	−7224.9365	−21852.010		
2	1.0436323	0.0306234	−7223.0601	−21848.894		
Target	1.3333333	−0.7385588	−7223.1853	−21848.954	−127.49109	−524.51427

- Energy: 2.3 % (Xe) & 1.7 % (Rn) → 0.0017 % (Xe) & 0.0003 % (Rn)
- α_1: 0.16 %, A_n: 2.3 %

Naito, Ohashi, and Liang. *J. Phys. B* **52**, 245003 (2019)

Hartree Atomic Unit

$$m_e = 1, \qquad \hbar = 1, \qquad e^2 = 1, \qquad 4\pi\varepsilon_0 = 1, \qquad c = \frac{1}{\alpha}$$

Energy: $E_{\mathrm{int}}^{\mathrm{exact}}$ is Hartree & LDA exchange (from Xe & Rn)

n	α_n	λA_n	$E_{\mathrm{gs}}^{n\text{-th}}$			
			Xe	Rn	Ne	Ar
0			−7054.6485	−21479.344	−116.99029	−497.38577
1	1.3311445	−0.7558229	−7224.9365	−21852.010	−127.69337	−524.94234
2	1.0436323	0.0306234	−7223.0601	−21848.894	−127.38285	−524.36807
Target	1.3333333	−0.7385588	−7223.1853	−21848.954	−127.49109	−524.51427

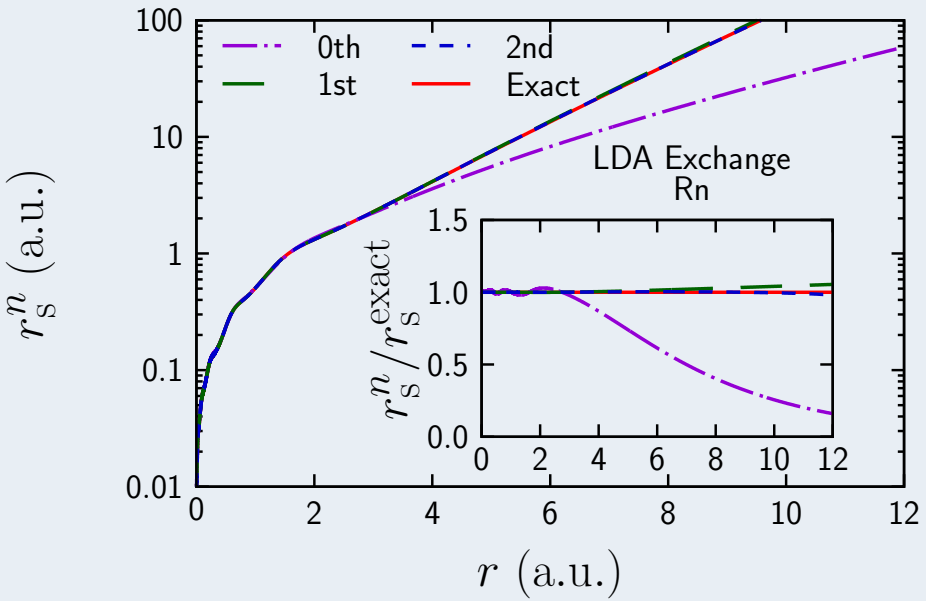
- Energy: 2.3 % (Xe) & 1.7 % (Rn) → 0.0017 % (Xe) & 0.0003 % (Rn)
- α_1: 0.16 %, A_n: 2.3 %

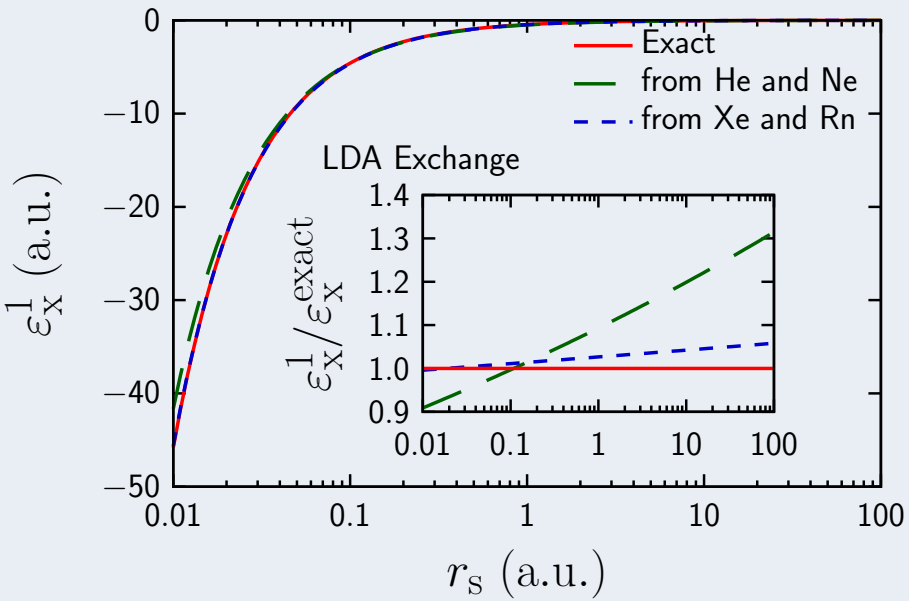
Naito, Ohashi, and Liang. *J. Phys. B* **52**, 245003 (2019)

Hartree Atomic Unit

$$m_e = 1, \qquad \hbar = 1, \qquad e^2 = 1, \qquad 4\pi\varepsilon_0 = 1, \qquad c = \frac{1}{\alpha}$$

Density and energy density: $E_{\mathrm{int}}^{\mathrm{exact}}$ is Hartree & LDA exchange





Naito, Ohashi, and Liang. *J. Phys. B* **52**, 245003 (2019)

$$r_{\mathrm{s}} = \left(\frac{3}{4\pi\rho}\right)^{1/3}, \qquad E_{\mathrm{x}}[\rho] = \int \varepsilon_{\mathrm{x}}^{1}(r_{\mathrm{s}}(\boldsymbol{r}))\,\rho(\boldsymbol{r})\,d\boldsymbol{r}$$

Energy: $E_{\mathrm{int}}^{\mathrm{exact}}$ is Hartree & LDA exchange-correlation (from Xe & Rn)

n	α_n	λA_n	$E_{\mathrm{gs}}^{n\text{-th}}$			
			Xe	Rn	Ne	Ar
0	—	—	−7223.1853	−21848.954		
Target	PZ81	PZ81	−7228.3628	−21857.954	−128.22766	−525.93461

- Energy: 0.072 % (Xe) & 0.041 % (Rn) → 0.0005 % (Xe) & 0.0001 % (Rn)

Naito, Ohashi, and Liang. *J. Phys. B* **52**, 245003 (2019)

Hartree Atomic Unit

$$m_e = 1, \qquad \hbar = 1, \qquad e^2 = 1, \qquad 4\pi\varepsilon_0 = 1, \qquad c = \frac{1}{\alpha}$$

Energy: $E_{\mathrm{int}}^{\mathrm{exact}}$ is Hartree & LDA exchange-correlation (from Xe & Rn)

n	α_n	λA_n	$E_{\mathrm{gs}}^{n\text{-th}}$			
			Xe	Rn	Ne	Ar
0	—	—	−7223.1853	−21848.954		
1	1.0862074	−0.0737520	−7228.4020	−21857.981		
Target	PZ81	PZ81	−7228.3628	−21857.954	−128.22766	−525.93461

- Energy: 0.072 % (Xe) & 0.041 % (Rn) → 0.0005 % (Xe) & 0.0001 % (Rn)

Naito, Ohashi, and Liang. *J. Phys. B* **52**, 245003 (2019)

Hartree Atomic Unit

$$m_e = 1, \qquad \hbar = 1, \qquad e^2 = 1, \qquad 4\pi\varepsilon_0 = 1, \qquad c = \frac{1}{\alpha}$$

Energy: $E_{\mathrm{int}}^{\mathrm{exact}}$ is Hartree & LDA exchange-correlation (from Xe & Rn)

n	α_n	λA_n	$E_{\mathrm{gs}}^{n\text{-th}}$			
			Xe	Rn	Ne	Ar
0	—	—	−7223.1853	−21848.954	−127.49109	−524.51427
1	1.0862074	−0.0737520	−7228.4020	−21857.981	−128.25792	−525.97900
Target	PZ81	PZ81	−7228.3628	−21857.954	−128.22766	−525.93461

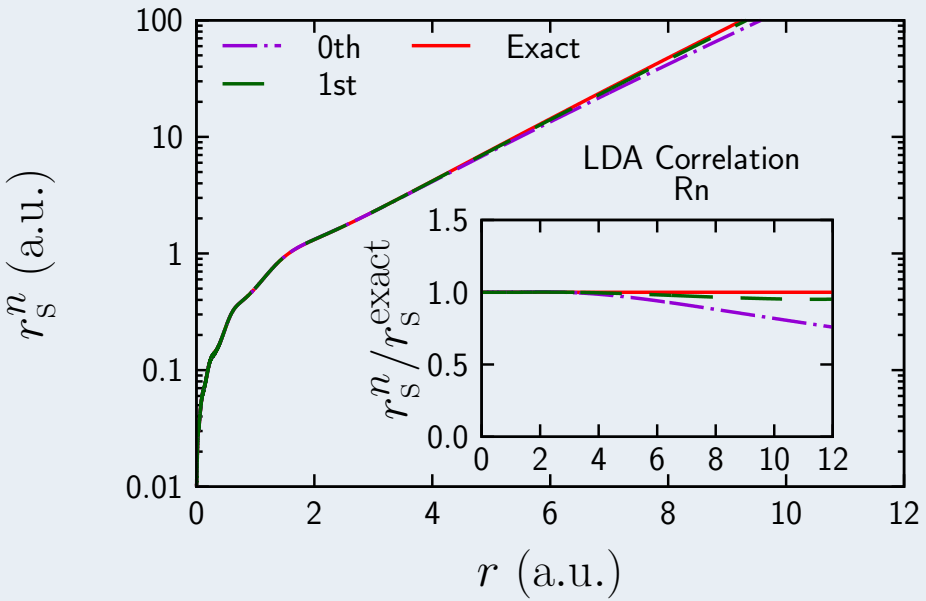
- Energy: 0.072 % (Xe) & 0.041 % (Rn) → 0.0005 % (Xe) & 0.0001 % (Rn)

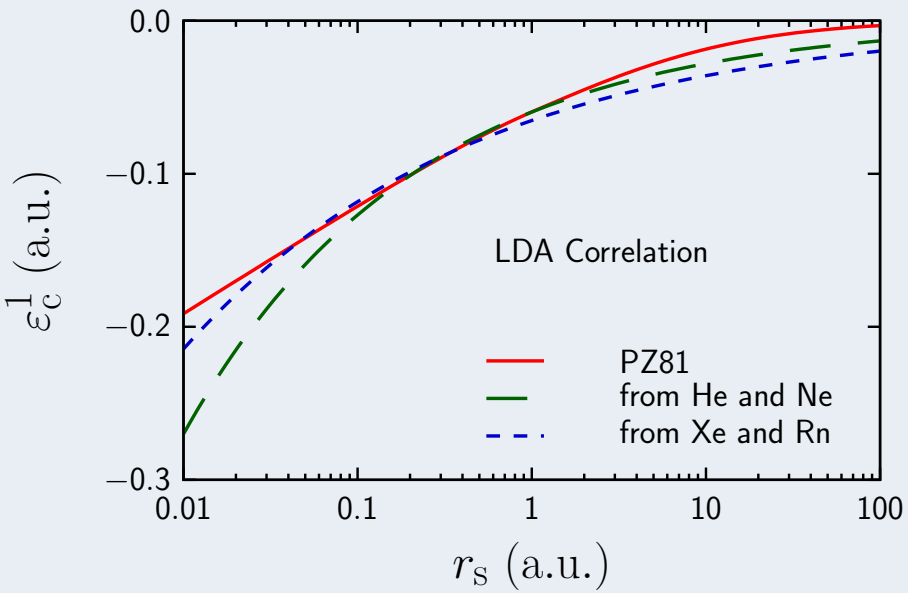
Naito, Ohashi, and Liang. *J. Phys. B* **52**, 245003 (2019)

Hartree Atomic Unit

$$m_e = 1, \qquad \hbar = 1, \qquad e^2 = 1, \qquad 4\pi\varepsilon_0 = 1, \qquad c = \frac{1}{\alpha}$$

Density and energy density: $E_{\mathrm{int}}^{\mathrm{exact}}$ is Hartree & LDA exchange-correlation





Naito, Ohashi, and Liang. *J. Phys. B* **52**, 245003 (2019)

$$r_{\mathrm{s}} = \left(\frac{3}{4\pi\rho}\right)^{1/3}, \qquad E_{\mathrm{c}}[\rho] = \int \varepsilon_{\mathrm{c}}^{1}(r_{\mathrm{s}}(\boldsymbol{r}))\,\rho(\boldsymbol{r})\,d\boldsymbol{r}$$

Short Conclusion

- IKS-DFPT can reproduce the target EDF with good accuracy in atomic systems
- How about nuclear systems??
- Can we extend this IKS-DFPT to relativistic systems?

Dirac Equation

$$\left[\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta\left(m+S\left(\boldsymbol{r}\right)\right)+V\left(\boldsymbol{r}\right)\right]\psi_j=\varepsilon_j\psi_j$$

$$\begin{pmatrix} m+S\left(\boldsymbol{r}\right)+V\left(\boldsymbol{r}\right) & \boldsymbol{\sigma}\cdot\boldsymbol{p} \\ \boldsymbol{\sigma}\cdot\boldsymbol{p} & -m-S\left(\boldsymbol{r}\right)+V\left(\boldsymbol{r}\right) \end{pmatrix}\begin{pmatrix}\psi_{\mathrm{U}j}\\ \psi_{\mathrm{L}j}\end{pmatrix}=\varepsilon_j\begin{pmatrix}\psi_{\mathrm{U}j}\\ \psi_{\mathrm{L}j}\end{pmatrix}$$

- $c=1$ is assumed
- S: scalar potential, V: vector potential
- In atomic systems, $S\equiv 0$ and V is the Coulomb potential

Relativistic Extension of Kohn-Sham Equation

- There are scalar KS potential S_{KS} and vector KS potential V_{KS}
- There are scalar density ρ_{S} and vector density ρ_{V}

$$\rho_{\mathrm{S}}\left(\boldsymbol{r}\right)=\sum\varphi_j^{\dagger}\left(\boldsymbol{r}\right)\beta\varphi_j\left(\boldsymbol{r}\right)=\sum\overline{\varphi}_j\left(\boldsymbol{r}\right)\varphi_j\left(\boldsymbol{r}\right)\qquad\rho_{\mathrm{V}}\left(\boldsymbol{r}\right)=\sum\varphi_j^{\dagger}\left(\boldsymbol{r}\right)\varphi_j\left(\boldsymbol{r}\right)$$

- S.P. orbital obeys $\left[\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta\left(m+S_{\mathrm{KS}}\left(\boldsymbol{r}\right)\right)+V_{\mathrm{KS}}\left(\boldsymbol{r}\right)\right]\varphi_j\left(\boldsymbol{r}\right)=\varepsilon_j\left(\boldsymbol{r}\right)$

Inverse Kohn-Sham Method and Perturbation Theory

Non-Relativistic Inverse Kohn-Sham Method

$$V_{\mathrm{KS}}(\boldsymbol{r}) = -\frac{1}{\rho(\boldsymbol{r})} \sum \varphi_j^*(\boldsymbol{r}) \left(-\frac{\hbar^2}{2M} \Delta - \varepsilon_j \right) \varphi_j(\boldsymbol{r})$$

Wang and Parr. *Phys. Rev. A* **47**, R1591 (1993)

Relativistic Inverse Kohn-Sham Method

$$V_{\mathrm{KS}}(\boldsymbol{r}) + S_{\mathrm{KS}}(\boldsymbol{r}) = -M - \frac{1}{\rho_{\mathrm{V}}(\boldsymbol{r}) + \rho_{\mathrm{S}}(\boldsymbol{r})} \sum \left[\varphi_j^\dagger(\boldsymbol{r}) + \overline{\varphi}_j(\boldsymbol{r}) \right] \left(\boldsymbol{\alpha} \cdot \boldsymbol{p} - \varepsilon_j \right) \varphi_j(\boldsymbol{r})$$

$$V_{\mathrm{KS}}(\boldsymbol{r}) - S_{\mathrm{KS}}(\boldsymbol{r}) = +M - \frac{1}{\rho_{\mathrm{V}}(\boldsymbol{r}) - \rho_{\mathrm{S}}(\boldsymbol{r})} \sum \left[\varphi_j^\dagger(\boldsymbol{r}) - \overline{\varphi}_j(\boldsymbol{r}) \right] \left(\boldsymbol{\alpha} \cdot \boldsymbol{p} - \varepsilon_j \right) \varphi_j(\boldsymbol{r})$$

Accorto, Naito, Liang, Nikšić, and Vretenar. *Phys. Rev. C* **103**, 044304 (2021)

Non-Relativistic IKS-DFPT

$$\lambda E_{\mathrm{int}}^{(1)}\left[\tilde{\rho}_{\mathrm{gs}}\right]-\lambda E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]+\lambda\int\frac{\delta E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)}\rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right)\,d\boldsymbol{r}$$

$$\simeq\sum\varepsilon_{j}^{\mathrm{exact}}-\tilde{E}_{\mathrm{gs}}+\tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]-\int\frac{\delta\tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{gs}}^{\mathrm{exact}}\right]}{\delta\rho\left(\boldsymbol{r}\right)}\rho_{\mathrm{gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right)\,d\boldsymbol{r}$$

Naito, Ohashi, and Liang. *J. Phys. B* **52**, 245003 (2019)

Relativistic IKS-DFPT

$$\lambda E_{\mathrm{int}}^{(1)}\left[\tilde{\rho}_{\mathrm{V,\,gs}},\tilde{\rho}_{\mathrm{S,\,gs}}\right]-\lambda E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{V,\,gs}}^{\mathrm{exact}},\rho_{\mathrm{S,\,gs}}^{\mathrm{exact}}\right]$$

$$+\lambda\int\frac{\delta E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{V,\,gs}}^{\mathrm{exact}},\rho_{\mathrm{S,\,gs}}\right]}{\delta\rho_{\mathrm{V}}\left(\boldsymbol{r}\right)}\rho_{\mathrm{V,\,gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right)\,d\boldsymbol{r}+\lambda\int\frac{\delta E_{\mathrm{int}}^{(1)}\left[\rho_{\mathrm{V,\,gs}}^{\mathrm{exact}},\rho_{\mathrm{S,\,gs}}\right]}{\delta\rho_{\mathrm{S}}\left(\boldsymbol{r}\right)}\rho_{\mathrm{S,\,gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right)\,d\boldsymbol{r}$$

$$\simeq\sum\varepsilon_{j}^{\mathrm{exact}}-\tilde{E}_{\mathrm{gs}}+\tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{V,\,gs}}^{\mathrm{exact}},\rho_{\mathrm{S,\,gs}}^{\mathrm{exact}}\right]$$

$$-\int\frac{\delta\tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{V,\,gs}}^{\mathrm{exact}},\rho_{\mathrm{S,\,gs}}^{\mathrm{exact}}\right]}{\delta\rho_{\mathrm{V}}\left(\boldsymbol{r}\right)}\rho_{\mathrm{V,\,gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right)\,d\boldsymbol{r}-\int\frac{\delta\tilde{E}_{\mathrm{int}}\left[\rho_{\mathrm{V,\,gs}}^{\mathrm{exact}},\rho_{\mathrm{S,\,gs}}^{\mathrm{exact}}\right]}{\delta\rho_{\mathrm{S}}\left(\boldsymbol{r}\right)}\rho_{\mathrm{S,\,gs}}^{\mathrm{exact}}\left(\boldsymbol{r}\right)\,d\boldsymbol{r}$$

Accorto, Naito, Liang, Nikšić, and Vretenar. *Phys. Rev. C* **103**, 044304 (2021)

DD-PC1 (without Coulomb)

$$S_{\text{DD-PC1}}\left[\rho_{\text{V}}, \rho_{\text{S}}, \vec{\rho}_{\text{TV}}\right] = \alpha_{\text{S}}\left(\rho_{\text{V}}\right)\rho_{\text{S}} + \delta_{\text{S}}\,\Delta\rho_{\text{S}}$$

$$V_{\text{DD-PC1}}\left[\rho_{\text{V}}, \rho_{\text{S}}, \vec{\rho}_{\text{TV}}\right] = \alpha_{\text{V}}\left(\rho_{\text{V}}\right)\rho_{\text{V}} + \alpha_{\text{TV}}\left(\rho_{\text{V}}\right)\vec{\rho}_{\text{TV}}$$

$$\Sigma_{\text{R}}\left[\rho_{\text{V}}, \rho_{\text{S}}, \vec{\rho}_{\text{TV}}\right] = \frac{1}{2}\frac{\partial\alpha_{\text{S}}}{\partial\rho}\rho_{\text{S}}^2 + \frac{1}{2}\frac{\partial\alpha_{\text{V}}}{\partial\rho}\rho_{\text{V}}^2 + \frac{1}{2}\frac{\partial\alpha_{\text{TV}}}{\partial\rho}\rho_{\text{TV}}^2$$

$$\alpha_{\text{S}}\left(\rho_{\text{V}}\right) = a_{\text{S}} + \left(b_{\text{S}} + c_{\text{S}}\frac{\rho_{\text{V}}}{\rho_{\text{sat}}}\right)e^{-d_{\text{S}}\rho_{\text{V}}/\rho_{\text{sat}}}$$

$$\alpha_{\text{V}}\left(\rho_{\text{V}}\right) = a_{\text{V}} + b_{\text{V}}e^{-d_{\text{V}}\rho_{\text{V}}/\rho_{\text{sat}}}$$

$$\alpha_{\text{TV}}\left(\rho_{\text{V}}\right) = b_{\text{TV}}e^{-d_{\text{TV}}\rho_{\text{V}}/\rho_{\text{sat}}}$$

Nikšić, Vretenar, and Ring. *Phys. Rev. C* **78**, 034318 (2008)

Benchmark Calculation

Start "LDA terms (only a_{S} and a_{V})" of DD-PC1

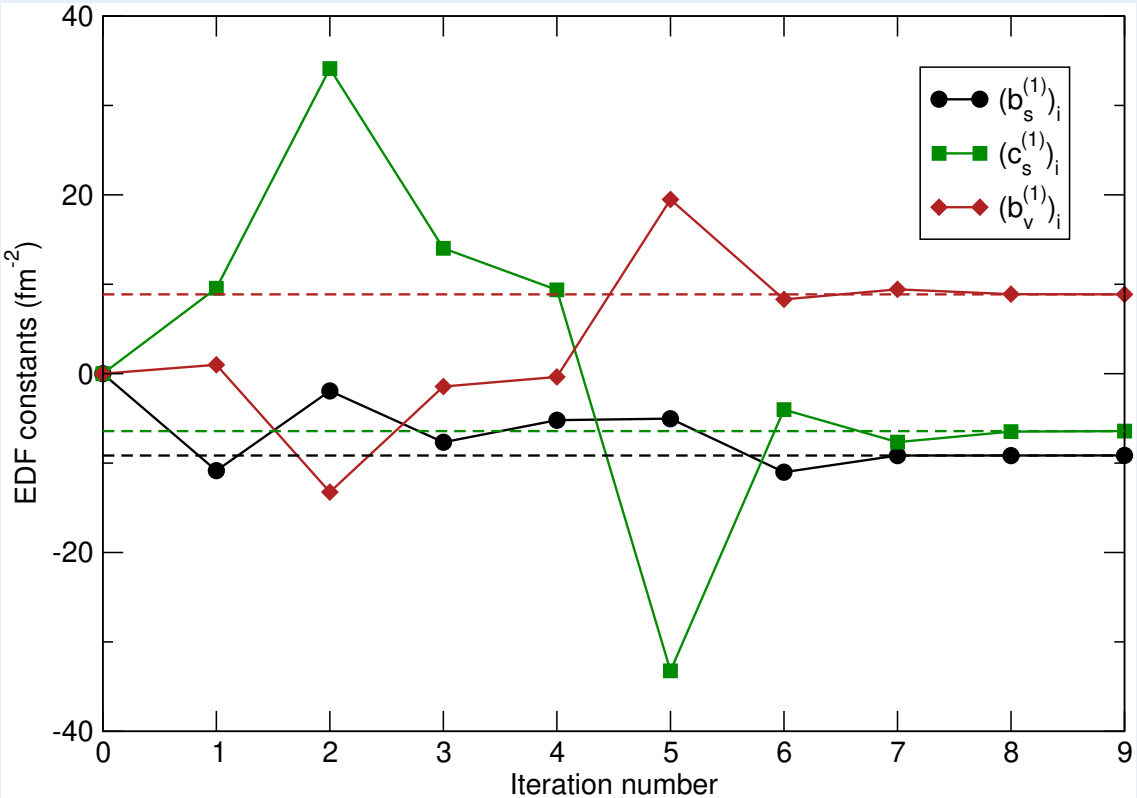
Goal All terms of DD-PC1 Can we repdoduce b and c? (d are fixed)

Systems: $N = Z$ nuclei w/o Coulomb (${}^{8}_{8}16$, ${}^{28}_{28}56$, ${}^{50}_{50}100$)

Benchmark Results

Iterative method is used

$$b_{\mathrm{S}} = \sum_k b_{\mathrm{S}}^{k\text{-th}} \qquad c_{\mathrm{S}} = \sum_k c_{\mathrm{S}}^{k\text{-th}} \qquad b_{\mathrm{V}} = \sum_k b_{\mathrm{V}}^{k\text{-th}}$$

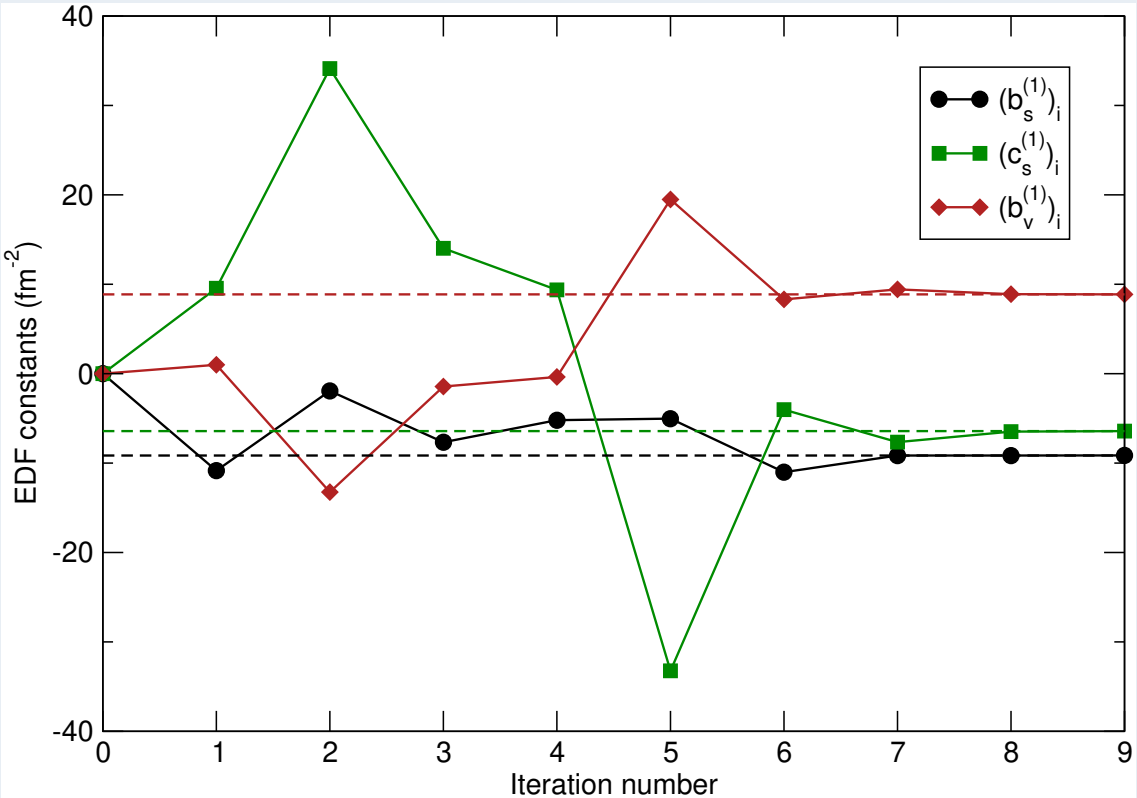


Accorto, Naito, Liang, Nikšić, and Vretenar. *Phys. Rev. C* **103**, 044304 (2021)

Benchmark Results

Iterative method is used

$$b_{\mathrm{S}} = \sum_k b_{\mathrm{S}}^{k\text{-th}} \qquad c_{\mathrm{S}} = \sum_k c_{\mathrm{S}}^{k\text{-th}} \qquad b_{\mathrm{V}} = \sum_k b_{\mathrm{V}}^{k\text{-th}}$$



Well reproduced!!

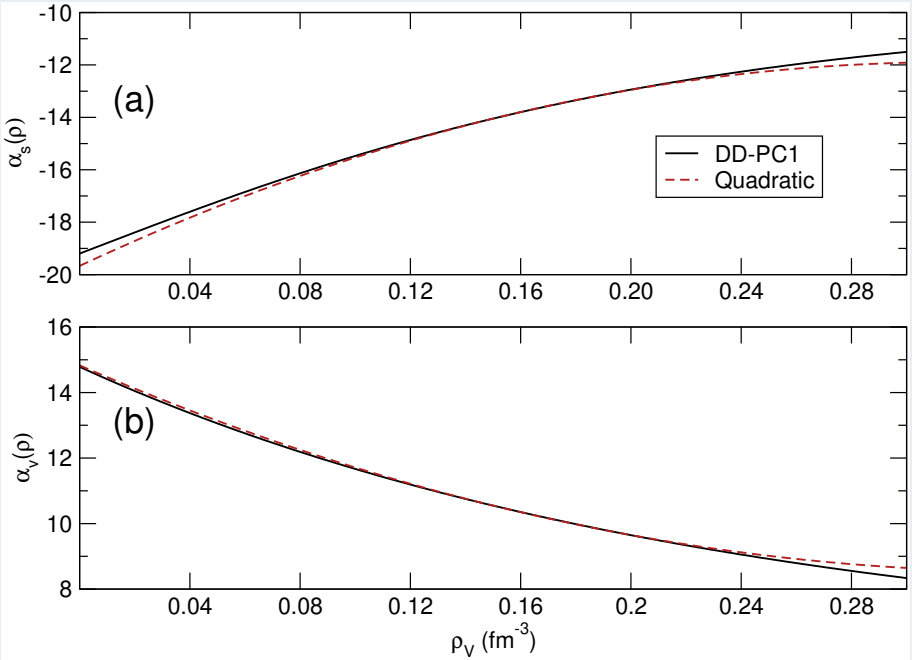
Accorto, Naito, Liang, Nikšić, and Vretenar. *Phys. Rev. C* **103**, 044304 (2021)

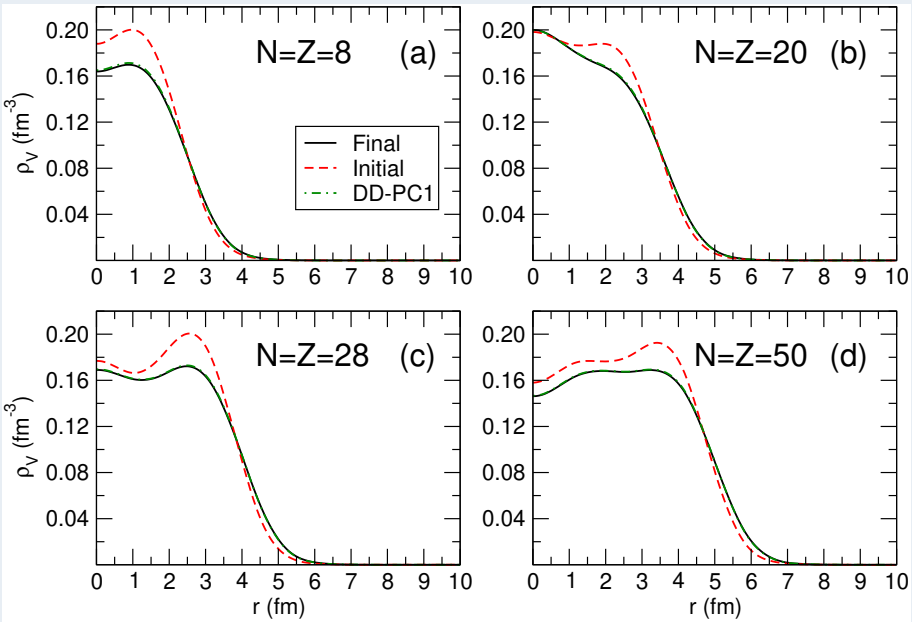
Benchmark Results (2)

Iterative method with **different ansatz** is used

$$\alpha_{\mathrm{S}}(\rho_{\mathrm{V}}) = a_{\mathrm{S}} + \sum_k b_{\mathrm{S}}^{k\text{-th}} \left(\frac{\rho_{\mathrm{V}}}{\rho_{\mathrm{sat}}} - 1\right) + \sum_k c_{\mathrm{S}}^{k\text{-th}} \left(\frac{\rho_{\mathrm{V}}}{\rho_{\mathrm{sat}}} - 1\right)^2$$

$$\alpha_{\mathrm{V}}(\rho_{\mathrm{V}}) = a_{\mathrm{V}} + \sum_k b_{\mathrm{V}}^{k\text{-th}} \left(\frac{\rho_{\mathrm{V}}}{\rho_{\mathrm{sat}}} - 1\right) + \sum_k c_{\mathrm{V}}^{k\text{-th}} \left(\frac{\rho_{\mathrm{V}}}{\rho_{\mathrm{sat}}} - 1\right)^2$$





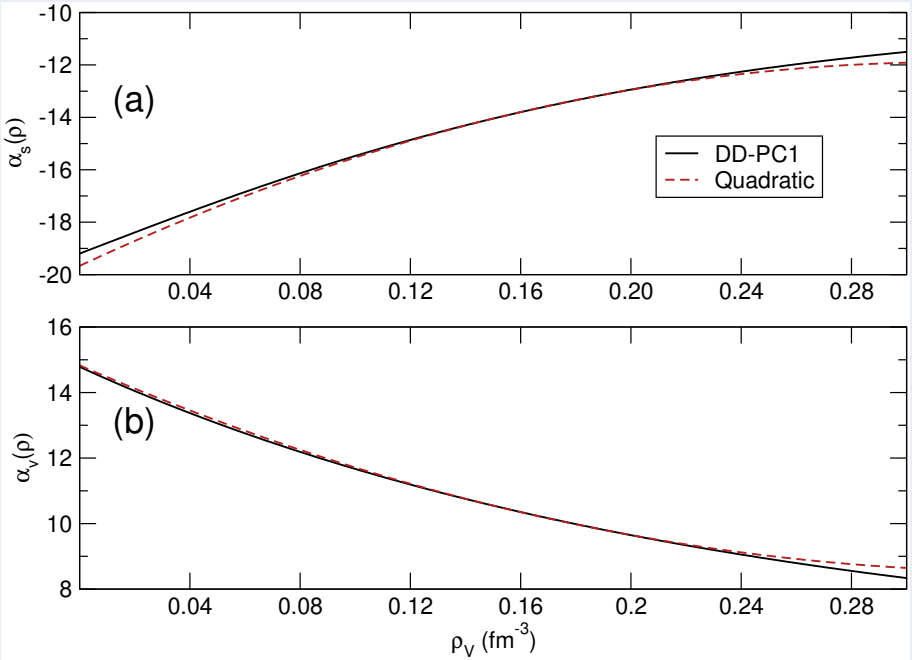
Accorto, Naito, Liang, Nikšić, and Vretenar. *Phys. Rev. C* **103**, 044304 (2021)

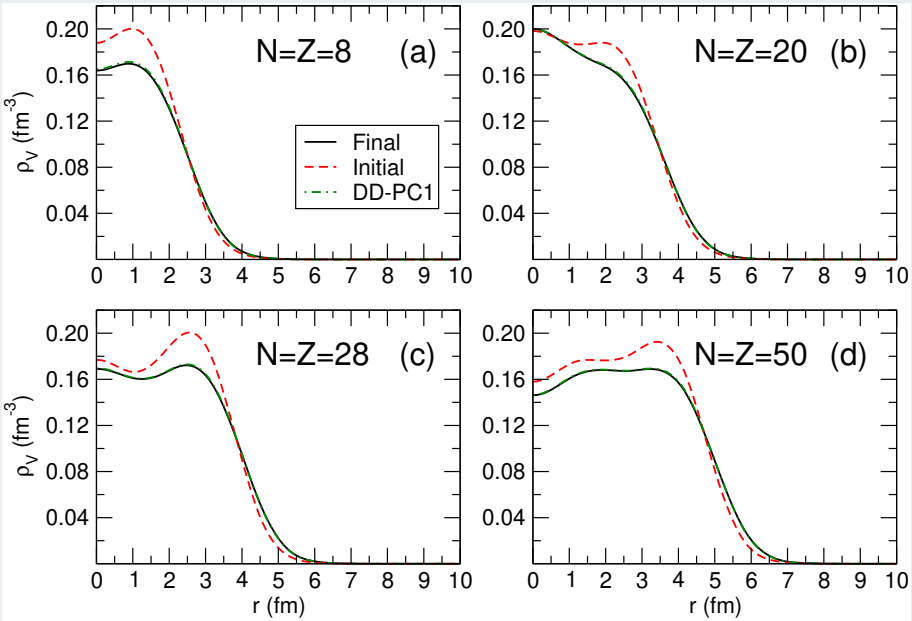
Benchmark Results (2)

Iterative method with **different ansatz** is used

$$\alpha_S(\rho_V) = a_S + \sum_k b_S^{k\text{-th}} \left(\frac{\rho_V}{\rho_{sat}} - 1\right) + \sum_k c_S^{k\text{-th}} \left(\frac{\rho_V}{\rho_{sat}} - 1\right)^2$$

$$\alpha_V(\rho_V) = a_V + \sum_k b_V^{k\text{-th}} \left(\frac{\rho_V}{\rho_{sat}} - 1\right) + \sum_k c_V^{k\text{-th}} \left(\frac{\rho_V}{\rho_{sat}} - 1\right)^2$$





Even with different ansatz, well reproduced!!

Accorto, Naito, Liang, Nikšić, and Vretenar. *Phys. Rev. C* **103**, 044304 (2021)

Inverse Kohn-Sham Method and Perturbation Theory

Conclusion

- Inverse Kohn-Sham method: starting from density, one can obtain V_{KS}
- A method to improve an EDF using known *exact* densities : **IKS-DFPT**
- Inverse KS method and IKS-DFPT are extended to relativsitc systems
- IKS-DFPT works well both for atomic systems and for nuclear systems in benchmark calculations
- Once accurate ρ_{gs} and E_{gs} are obtained by *ab initio* methods a known EDF can be improved

Perspectives

- How can we constrain spin-orbit potential?
- Can we go beyond benchmark calculations?
- Can we find a better ansatz?
- Milan group also works for the inverse Kohn-Sham method (Gianluca's talk)

Table of Contents

Collaborator in This Talk

- Takeru Yokota (RIKEN)

Yokota and Naito. *Phys. Rev. B* **99**, 115106 (2019)
Yokota and Naito. *Phys. Rev. Research* **3**, L012015 (2021)

Yokota and Naito. *Phys. Rev. B* **105**, 035105 (2022)

Previous Stage of This Work Done by

- Teiji Kunihiro (YITP, Kyoto U.)
- Takeru Yokota (RIKEN)
- Kenichi Yoshida (Kyoto U.)

Yokota, Yoshida, and Kunihiro. *Phys. Rev. C* **99**, 024302 (2019)

Yokota, Yoshida, and Kunihiro. *Prog. Theor. Exp. Phys.* **2019**, 011D01 (2019)

Effective Action Γ

- Effective action Γ is an action with the quantum fluctuation
- Effective action Γ can be calculated from the classical action S

Baym. *Phys. Rev.* **127**, 1391 (1962)

Effective Action for Density $\Gamma[\rho]$ (Two-Particle Point-Irreducible (2PPI) Formalism)

$$Z[J] = \int \exp\left[J(\tau, \boldsymbol{x})\,\rho_\psi(\tau, \boldsymbol{x}) - S\left[\psi^*, \psi\right]\right] \mathcal{D}\psi^*\,\mathcal{D}\psi \qquad \text{(Partition function)}$$

$$W[J] = \log Z[J] \qquad \text{(Generating functional of connected density correlation function)}$$

$$\rho(\tau, \boldsymbol{x}) = \sup_J \left.\frac{\delta W[J[\rho]]}{\delta J}\right|_{J=J(\tau,\boldsymbol{x})}$$

$$\Gamma[\rho] = \sup_J \left\{\int_{\tau=0}^{\tau=\beta} \int J[\rho]\,\rho(\tau, \boldsymbol{x})\; d\boldsymbol{x}\, d\tau - W[J[\rho]]\right\} \qquad \text{(Effective action)}$$

S: Action, $\rho_\psi = \psi^*\psi$: Density field J: External field, τ: Imaginary time

Fukuda, Kotani, Suzuki, and Yokojima. *Prog. Theor. Phys.* **92**, 833 (1994)

Variational Principle

$$\left.\frac{\delta\Gamma\left[\rho\right]}{\delta\rho}\right|_{\rho=\rho_{\mathrm{gs}}(\tau,\boldsymbol{x})} = \mu$$

$$\begin{aligned}
\rho_{\mathrm{gs}}\left(\tau,\boldsymbol{x}\right) &= \left.\frac{\delta W\left[J\right]}{\delta J}\right|_{J=\mu} \\
&= \left.\frac{\delta \log Z\left[J\right]}{\delta J}\right|_{J=\mu} \\
&= \frac{1}{Z\left[\mu\right]}\int \rho_{\psi}\left(\tau,\boldsymbol{x}\right)\exp\left[\mu\rho_{\psi}\left(\tau,\boldsymbol{x}\right) - S\left[\psi^{*},\psi\right]\right]\mathcal{D}\psi^{*}\,\mathcal{D}\psi
\end{aligned}$$

$$\begin{aligned}
\Gamma\left[\rho_{\mathrm{gs}}\right] &= \int_{\tau=0}^{\tau=\beta}\int \mu\rho_{\mathrm{gs}}\left(\tau,\boldsymbol{x}\right)\,d\tau\,d\boldsymbol{x} - \log Z\left[\mu\right] \\
&= \beta F_{\mathrm{Helmholtz}}
\end{aligned}$$

Relationship between $E[\rho]$ and $\Gamma[\rho]$

$$E[\rho] = \lim_{\beta\to\infty} \frac{\Gamma[\rho]}{\beta}$$

- If $\Gamma[\rho]$ can be calculated, an EDF $E[\rho]$ can be obtained
- Γ can be calculated using the functional renormalization group (FRG)

Fukuda, Kotani, Suzuki, and Yokojima. *Prog. Theor. Phys.* **92**, 833 (1994)

Relationship between $E[\rho]$ and $\Gamma[\rho]$

$$E[\rho] = \lim_{\beta\to\infty} \frac{\Gamma[\rho]}{\beta}$$

- If $\Gamma[\rho]$ can be calculated, an EDF $E[\rho]$ can be obtained
- Γ can be calculated using the functional renormalization group (FRG)
- FRG-DFT is a way to calculate $\Gamma[\rho]$,
  and accordingly the ground-state energy E_{gs} from the action

Fukuda, Kotani, Suzuki, and Yokojima. *Prog. Theor. Phys.* **92**, 833 (1994)

History of FRG-DFT (DFT-RG) for Finite Systems

2002 Electron-photon systems (formulation)

Polonyi and Sailer. *Phys. Rev. B* **66**, 155113 (2002)

2004 Self-bound fermionic systems (formulation)

Schwenk and Polonyi. arXiv:nucl-th/0403011

2013 $(0+0)$ and $(1+0)$-D anharmonic oscillator

Kemler and Braun. *J. Phys. G* **40**, 085105 (2013)

2017 $(1+1)$-D finite nuclei

Kemler, Pospiech, and Braun. *J. Phys. G* **44**, 015101 (2017)

2017 $(1+1)$-D finite systems with δ interaction

Kemler. PhD thesis, Tech. U. Darmstadt (2017)

2018 $(0+0)$-D anharmonic oscillator (KS-FRG)

Liang, Niu, and Hatsuda. *Phys. Lett. B* **779**, 430 (2018)

History of FRG-DFT (DFT-RG) for Infinite Systems

2019 $(1+1)$-D infinite nuclear matter

Yokota, Yoshida, and Kunihiro. *Phys. Rev. C* **99**, 024302 (2019)

Sakakibara. Master thesis, U. Tokyo (2020)

2019 $(1+1)$-D Non-linear Tomonaga-Luttinger liquid (excited state)

Yokota, Yoshida, and Kunihiro. *Prog. Theor. Exp. Phys.* **2019**, 011D01 (2019)

2019 $(2+1)$-D infinite homogeneous electron gas

Yokota and Naito. *Phys. Rev. B* **99**, 115106 (2019)

2021 Superfluid system

Yokota, Kasuya, Yoshida, and Kunihiro. *Prog. Theor. Exp. Phys.* **2021**, 013A03 (2021)

2021 $(3+1)$-D infinite homogeneous electron gas

Yokota and Naito. *Phys. Rev. Research* **3**, L012015 (2021)

2022 Spin-polarized infinite homogeneous electron gas

Yokota and Naito. *Phys. Rev. B* **105**, 035105 (2022)

History of FRG-DFT (DFT-RG) for Infinite Systems

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Yokota and Naito. *Phys. Rev. Research* **3**, L012015 (2021)

2022 Spin-polarized infinite homogeneous electron gas

Yokota and Naito. *Phys. Rev. B* **105**, 035105 (2022)

How to Calculate the Effective Action Γ? (Brief idea)

1. Introduce strength of interaction $\lambda \in [0, 1]$: $U_\lambda = \lambda V_{\mathrm{int}}$
2. Write effective action Γ in 2PPI formalism
3. Derive the flow equatoin $\partial_\lambda \Gamma_\lambda [\rho]$ formally
4. Solve the flow equation, where $\Gamma_{\lambda=0}$ can be calculated analytically
5. Introduce some truncations
   since flow equation is functional differential eq. (difficult to solve)
   - Second-order vertex expansion (Taylor expansion around $\rho_{\mathrm{gs},\lambda}$)
   - A coefficient is fixed during the flow
     (The coeff. for non-interacting system is used)

Action for Homogeneous Electron Gas: Interaction is gradually turning on

Interaction V_{int} is gradually turning on with parameter λ:

$$U_\lambda(X, X') = \lambda\delta(\tau - \tau')\, V_{\mathrm{int}}(\boldsymbol{x} - \boldsymbol{x}') = \lambda\delta(\tau - \tau')\, \frac{1}{|\boldsymbol{x} - \boldsymbol{x}'|}$$

Corresponding action is

$$S_\lambda[\psi^*, \psi] = S_{\mathrm{el}\lambda}[\psi^*, \psi] + S_{\text{el-i}\lambda}[\psi^*, \psi] + S_{\mathrm{i}\lambda}[\psi^*, \psi]$$

Starting from S_λ, one can calculate the effective action Γ_λ

$S_{\lambda=0}$, $\Gamma_{\lambda=0}$ Non-interacting Fermi Gas

$S_{\lambda=1}$, $\Gamma_{\lambda=1}$ Real (Interacting) Fermi Gas

$S_{\mathrm{el}\lambda}$: action for electrons, S_{i}: action for background charge,

$S_{\text{el-i}\lambda}$: action for electron-background, $X = (\tau, \boldsymbol{x})$

Owing to the background ion, divergence due to the Hartree term does not occur

n-Point Correlation Function

$$G_{\lambda}^{(n)}[J](X_1,\ldots,X_n) = \frac{\delta^n W_\lambda[J]}{\delta J(X_1)\ \ldots\ \delta J(X_n)}$$

Chemical Potential μ_λ

$$\left.\frac{\delta\Gamma_\lambda[\rho]}{\delta\rho}\right|_{\rho=\rho_{\mathrm{gs},\lambda}(X)} = J_\lambda\left[\rho_{\mathrm{gs},\lambda}\right](X) = \mu_\lambda, \qquad \rho_{\mathrm{gs},\lambda} \equiv n$$

- To fix electron density as n, λ-dependence is introduced in μ
- $\mu_{\lambda=0} = \left(3\pi^2 n\right)^{2/3}/2$
- In spin-polarized systems, μ_λ also has s dependence

Yokota, Yoshida, and Kunihiro. *Phys. Rev. C* **99**, 024302 (2019)

Change of Γ_λ: "Flow Equation"

Renormalization-group flow equation gives change of Γ_λ with respect to λ as

$$\partial_\lambda \Gamma_\lambda [\rho] = \frac{1}{2} \iint \partial_\lambda U_\lambda (X, X') \left[\rho(X) - n_\mathrm{i}\right] \left[\rho(X') - n_\mathrm{i}\right] dX\, dX'$$
$$+ \frac{1}{2} \iint \partial_\lambda\, U_\lambda (X, X') \left[\left(\frac{\delta^2 \Gamma_\lambda [\rho]}{\delta\rho\, \delta\rho} \right)^{-1} (X_\varepsilon, X') - \rho(X)\, \delta(\boldsymbol{x} - \boldsymbol{x}') \right] dX\, dX'$$

Schwenk and Polonyi. arXiv:nucl-th/0403011 (2004)
Kemler, Pospiech, and Braun. *J. Phys. G* **44**, 015101 (2017)
Yokota and Naito. *Phys. Rev. B* **99**, 115106 (2019)

In principle, $\Gamma_{\lambda=1}$ is obtained by solving above equation, starting from $\Gamma_{\lambda=0}$
However, it is difficult to solve this eq., since it is a functional differential eq.

Truncation: Vertex Expansion (Taylor Expansion around $\rho_{\mathrm{gs},\lambda}$)

$$\Gamma_\lambda[\rho] = \Gamma_\lambda\left[\rho_{\mathrm{gs},\lambda}\right] + \mu_\lambda \int \left[\rho(X) - \rho_{\mathrm{gs},\lambda}(X)\right] dX$$
$$+ \sum_{n=2}^{\infty} \frac{1}{n!} \int \cdots \int \Gamma_\lambda^{(n)}\left[\rho_{\mathrm{gs},\lambda}\right](X_1, \ldots X_n)$$
$$\times \left[\rho(X_1) - \rho_{\mathrm{gs},\lambda}(X_1)\right] \cdots \left[\rho(X_n) - \rho_{\mathrm{gs},\lambda}(X_n)\right] dX_1 \ldots dX_n,$$
$$\Gamma_\lambda^{(n)}[\rho](X_1, \ldots, X_n) = \frac{\delta^n \Gamma_\lambda[\rho]}{\delta\rho(X_1) \ldots \delta\rho(X_n)}$$

Truncated Flow Equation

Flow equation for $\Gamma_\lambda^{(n)}$ depends on $\Gamma_\lambda^{(m)}$ $(m \leq n+2)$
$\rightarrow$ Additional truncation is needed for practice

- Second-order vertex expansion
- $C_\lambda \simeq C_{\lambda=0}$ (detail is shown later)

Flow Equation for $E_{\mathrm{gs},\lambda}$

$$\begin{aligned}\partial_\lambda E_{\mathrm{gs},\lambda} = \lim_{\beta\to\infty}\frac{1}{\beta}\Bigg[&\int \mu_\lambda\,\partial_\lambda\rho_{\mathrm{gs},\lambda}(X)\,dX \\ &+\frac{1}{2}\iint \partial_\lambda U_\lambda(X,X')\left(\rho_{\mathrm{gs}\lambda}(X)-n_{\mathrm{i}}\right)\left(\rho_{\mathrm{gs}\lambda}(X')-n_{\mathrm{i}}\right)dX\,dX' \\ &+\frac{1}{2}\iint \partial_\lambda U_\lambda(X,X')\left(G^{(2)}_\lambda(X_{\varepsilon'},X')-\rho_{\mathrm{gs},\lambda}(X')\,\delta(\boldsymbol{x}-\boldsymbol{x}')\right)\Bigg]\,dX\,dX'\end{aligned}$$

In Momentum Representation

$$\partial_\lambda\frac{E_{\mathrm{gs},\lambda}}{N} = \frac{1}{2n}\frac{1}{(2\pi)^d}\int\tilde{U}(\boldsymbol{p})\left(\int e^{i\omega\varepsilon'}\tilde{G}^{(2)}_\lambda(P)\frac{d\omega}{2\pi}-n\right)d\boldsymbol{p}$$

Flow Equation for $\rho_{\mathrm{gs},\lambda}$

$$\partial_\lambda \rho_{\mathrm{gs},\lambda}(X) = \int G_\lambda^{(2)}(X,X') \left(\partial_\lambda \mu_\lambda - \int \partial_\lambda U_\lambda(X',X'') \left(\rho_{\mathrm{gs},\lambda}(X'') - n_{\mathrm{i}} \right) dX'' \right) dX' - \frac{1}{2} \iint \partial_\lambda U_\lambda(X',X'') \left(G_\lambda^{(3)}\left(X, X'_{\varepsilon'}, X''\right) - G_\lambda^{(2)}(X,X')\, \delta(\boldsymbol{x}' - \boldsymbol{x}'') \right) dX'\, dX''$$

n_{i}: Density for background charge

Since $\rho_{\mathrm{gs},\lambda} \equiv n$ $(\partial_\lambda \rho_{\mathrm{gs},\lambda} \equiv 0)$

$$\partial_\lambda \mu_\lambda = \frac{1}{(2\pi)^d} \frac{1}{2\tilde{G}_\lambda^{(2)}(0)} \int \tilde{U}(\boldsymbol{p}) \left(\frac{1}{2\pi} \int e^{i\omega\varepsilon'} \tilde{G}_\lambda^{(3)}(P,-P)\, d\omega - \tilde{G}_\lambda^{(2)}(0) \right) d\boldsymbol{p}$$

d: Spatial dimension, $\tilde{G}$: Fourier transformation of G, $\tilde{G}_\lambda^{(2)}(0) = \lim_{\boldsymbol{p}\to\boldsymbol{0}} \tilde{G}_\lambda^{(2)}(0,\boldsymbol{p})$

Flow Equation for $G_\lambda^{(2)}$

$$\begin{aligned}\partial_\lambda G_\lambda^{(2)}(X_1, X_2) = &\int G_\lambda^{(3)}(X_1, X_2, X') \\ &\times \left(\partial_\lambda \mu_\lambda - \int \partial_\lambda U_\lambda(X', X'') \left(\rho_{\mathrm{gs},\lambda}(X'') - n_\mathrm{i} \right) dX'' \right) dX' \\ &- \int \partial_\lambda U_\lambda(X', X'') \\ &\times \Big[G_\lambda^{(2)}(X_1, X') \, G_\lambda^{(2)}(X_2, X'') \\ &+ \frac{1}{2} \left(G_\lambda^{(4)}\left(X_1, X_2, X', X''_{\varepsilon'}\right) - G_\lambda^{(3)}(X_1, X_2, X'') \, \delta(\boldsymbol{x}' - \boldsymbol{x}'') \right) \Big] \, dX' \, dX''\end{aligned}$$

In Momentum Representation

$$\partial_\lambda \tilde{G}_\lambda^{(2)}(P) = -\tilde{U}(\boldsymbol{p}) \left[\tilde{G}_\lambda^{(2)}(P) \right]^2 + C_\lambda(P),$$

In this work, a truncation $C_\lambda \simeq C_{\lambda=0}$ is used

Final Result for E_{gs}

$$\frac{E_{\mathrm{gs},\lambda=1}}{N} = \frac{E_{\mathrm{gs},\lambda=0}}{N} + \frac{1}{2n}\frac{1}{(2\pi)^d}\int \tilde{U}(\boldsymbol{p})\left(\frac{1}{2\pi}\int e^{i\omega\varepsilon'}\tilde{G}^{(2)}_{\lambda=0}(P)\,d\omega - n\right)d\boldsymbol{p} + \frac{1}{2n}\int_0^1 d\lambda \frac{1}{(2\pi)^{d+1}}\iint e^{i\omega\varepsilon'}\tilde{U}(\boldsymbol{p})\left(\tilde{G}^{(2)}_{\lambda}(P) - \tilde{G}^{(2)}_{\lambda=0}(P)\right)d\omega\, d\boldsymbol{p}$$

1st Term Energy for free system
(identical to kinetic energy $(3/10)(9\pi/4)^{2/3} r_{\mathrm{s}}^{-2}$ in 3D case)

2nd Term Exchange Term
(identical to $-(3/4\pi)(9\pi/4)^{1/3} r_{\mathrm{s}}^{-1}$ in 3DHEG case)

3rd Term Correlation term

Technique

In 3DHEG case, the high-dimensional (6D) numerical integral is required

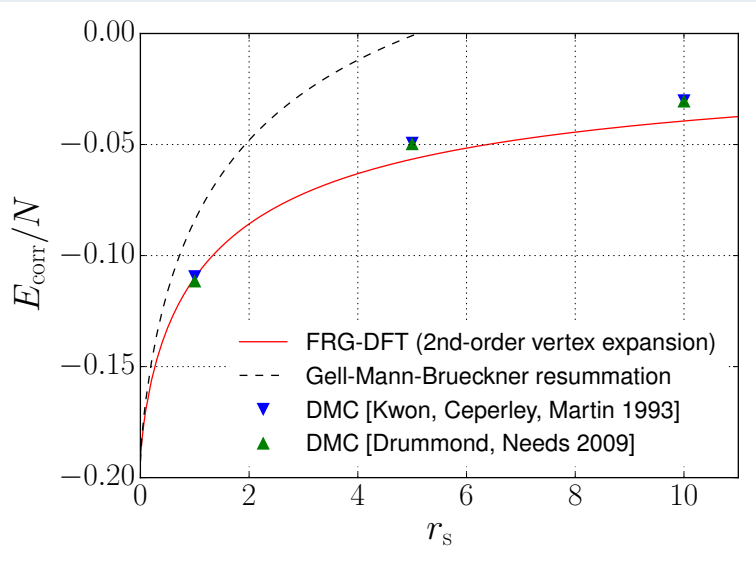
- Using cylindrical coordinates $\boldsymbol{p} = (p, p_\theta, p_z)$
- p-direction can be done analytically with the special functions
- p_θ-direction can be done analytically due to the isotropy
- Thus, only 2D numerical integral $(p_z,\ p_z')$ is needed!!

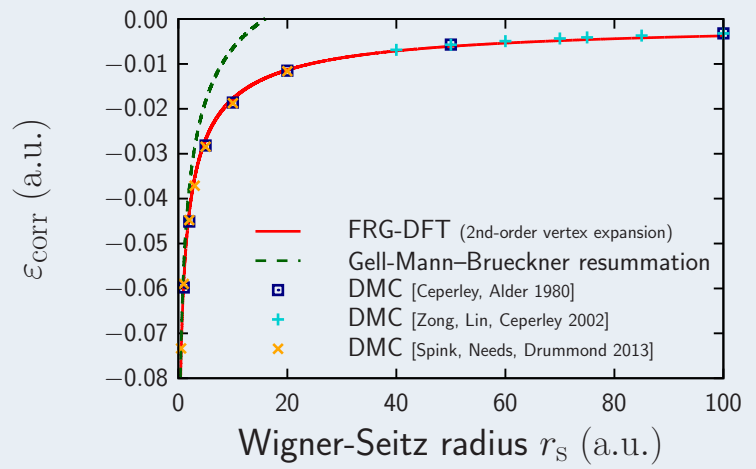
Thanks to this technique, finally, the FRG-DFT in 3DHEG can be performed

Calculation

- $\varepsilon_{\mathrm{corr}} = E_{\mathrm{corr}}/N$ for 65536 points in $r_{\mathrm{s}} \in \left[10^{-6}\,\mathrm{a.u.}, 100\,\mathrm{a.u.}\right)$ are calculated
- Thanks to the technique, such huge points can be calculated (cf: Monte Carlo calutlation usually provides more or less 10 points)

Correlation Energy in 2D & 3D HEG (LDA Correlation Functional)





- In $r_{\rm s} \to 0$,
  Gell-Mann-Brueckner limit
  is exactly reproduced
- DMC results are reproduced
  in the high-density region
- Deviation from DMC results
  in the low-density region
  → part of correlation is missing
- Correlation in 3D is smaller than in 2D
  → Results in 3D are better

Yokota and Naito. *Phys. Rev. B* **99**, 115106 (2019)

Yokota and Naito. *Phys. Rev. Research* **3**, L012015 (2021)

Functional Renormalization Group and Its Application to DFT

Way to Construct Conventional LDA Correlation Functional

- Fitting to the DMC calculation (Ceperley-Alder) with certain Ansätze
- In $\rho \to \infty$, Gell-Mann-Brueckner result should be reproduced

There are several LDA correlation functionals: “PZ81”, “VWN”, “PW92”

New Correlation Functional (Chachiyo, revChachiyo)

- Analytical formula is derived by 2nd-order Møller-Plesset
- The coefficient is determined by $\rho \to \infty$ limit

  (In “revChachiyo”, CA result with $r_s = 50\,\mathrm{Bohr}$ is also considered)

Our Correlation Functional

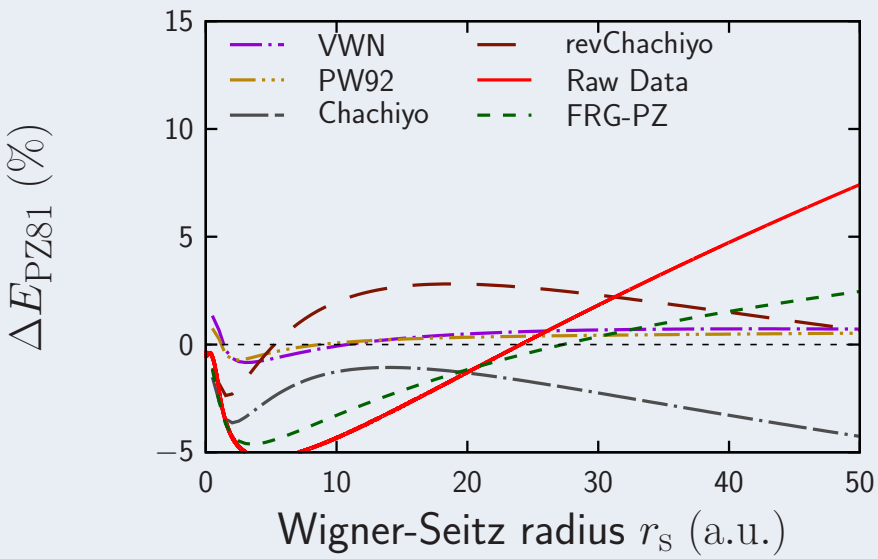
- We made functionals from FRG-DFT data
- We compared results among these functionals
- We also tested “fitting-free” method

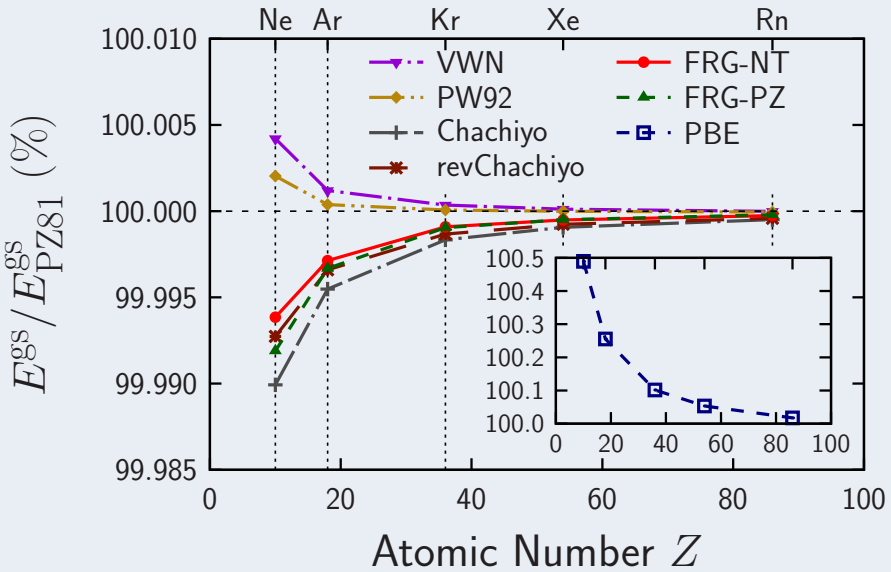
Fitting-free method

- ε_c and $d\varepsilon_c/dr_s$ for 65536 points in $0 < r_s < 100$ a.u. region is calculated by FRG-DFT
- Between two points, ε_c and $d\varepsilon_c/dr_s$ are calculated with linear interpolation
- In $r_s > 100$, ε_c and $d\varepsilon_c/dr_s$ are calculated with extrapolation
  (to derive the extrapolation function, data for $95 < r_s < 100$ a.u. are used)

Hereinafter, results in this method is shown as “NumTable” in legend

Error to PZ81 $\Delta E_{\mathrm{PZ}} = (E - E_{\mathrm{PZ}})/E_{\mathrm{PZ}})$ & DFT Calculation

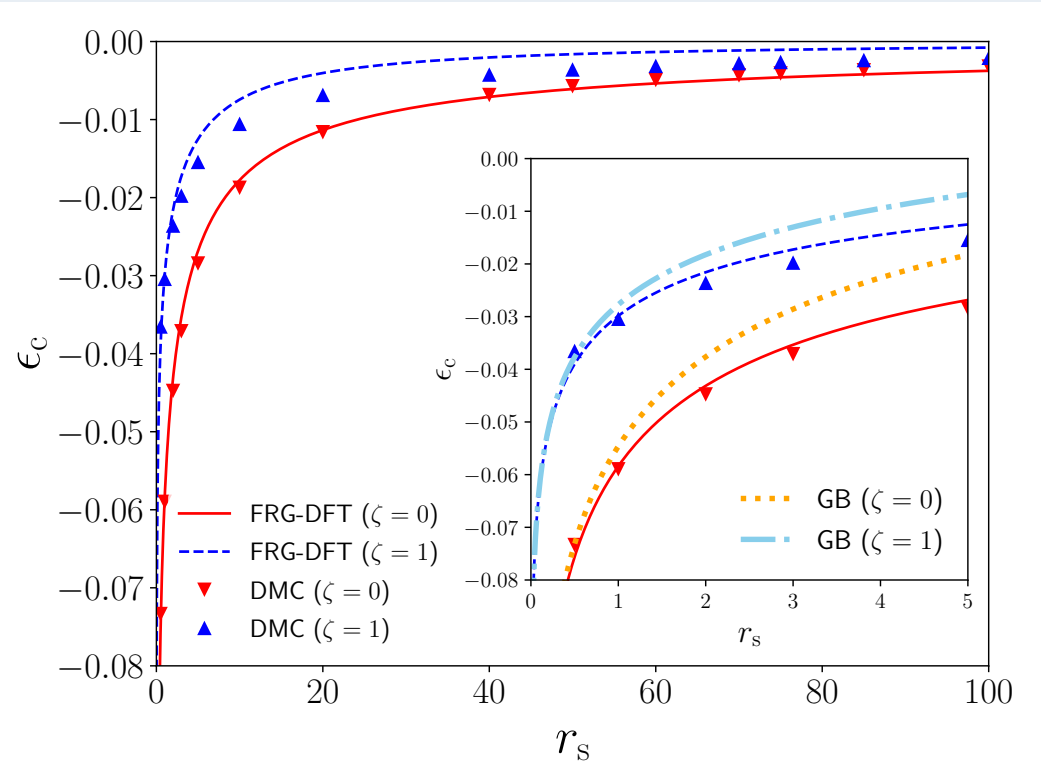




Yokota and Naito. *Phys. Rev. Research* **3**, L012015 (2021)

Extension to Spin-Polarized Systems

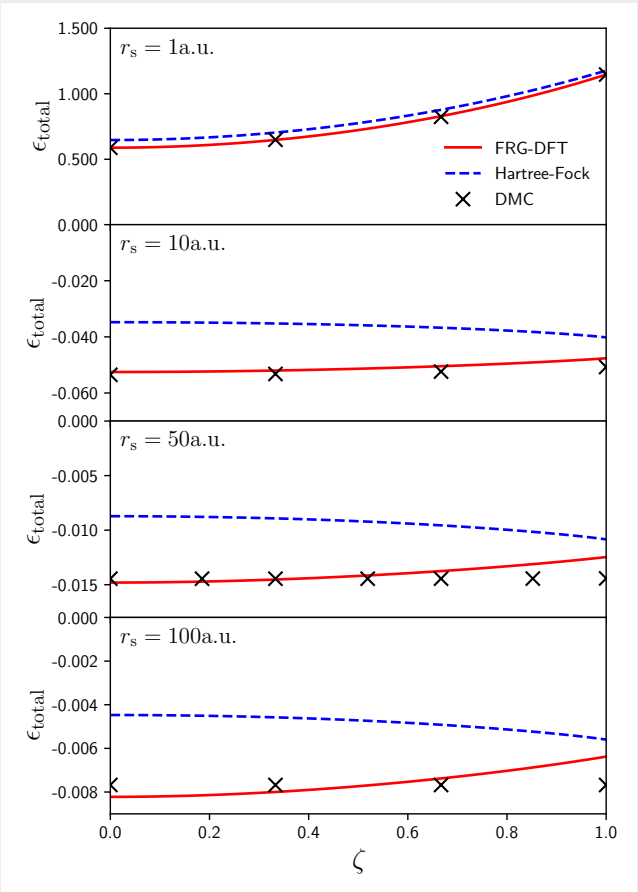
- To extend the FRG-DFT to the spin-polarized systems, the FRG-DFT is extended to multi-component systems
- $e_\uparrow$ and $e_\downarrow$ are treated as different particle
- $\zeta = (\rho_\uparrow - \rho_\downarrow)/\rho$
  $\zeta = 0$ for spin-unpolarized systems; $\zeta = 1$ for spin-polarized systems

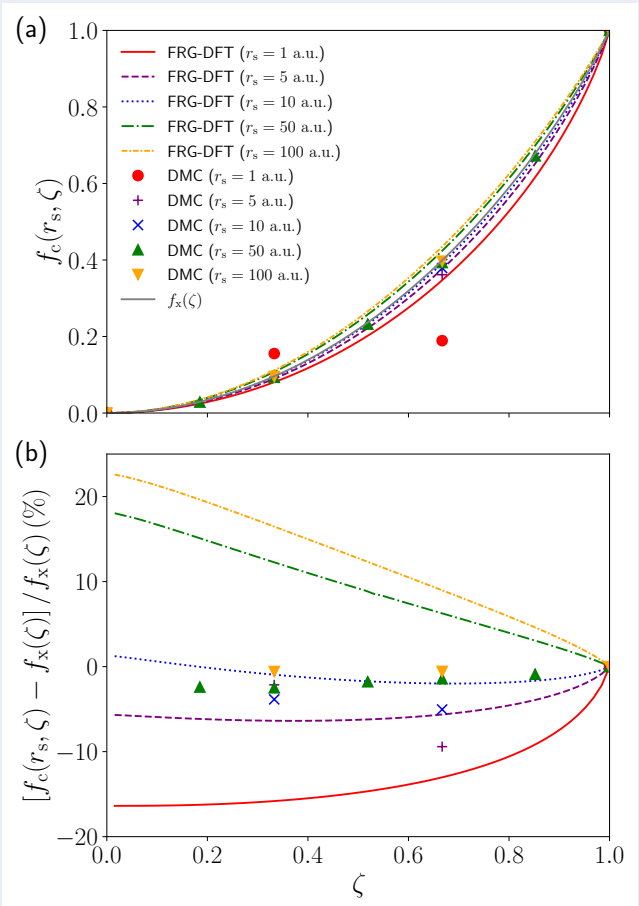


Yokota and Naito. *Phys. Rev. B* **105**, 035105 (2022)

Arbitrary Spin-Polarized Systems

- In DMC, limited numbers of ζ can be calculated
- Usually, interpolaration function f_c is assumed to be the same as f_x

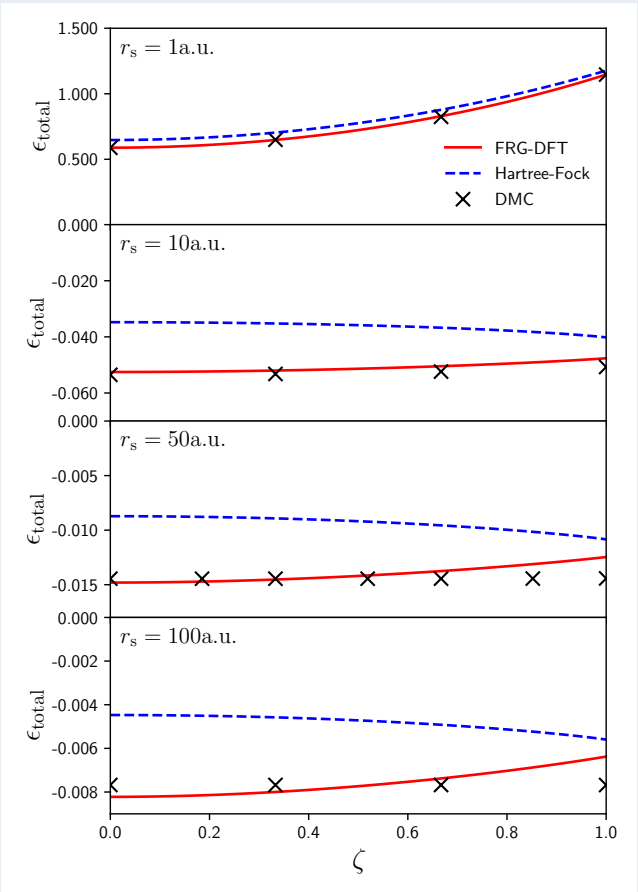


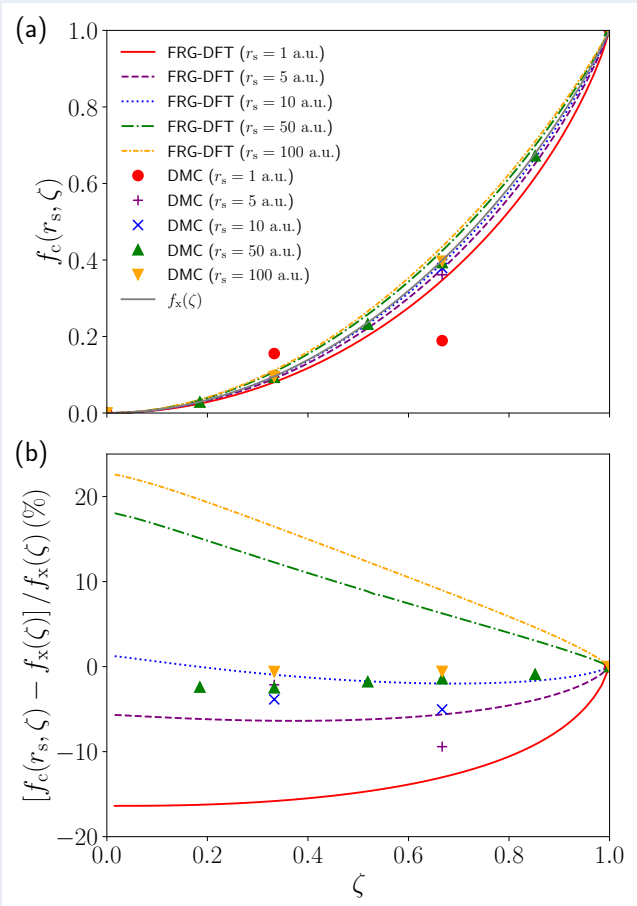


Yokota and Naito. *Phys. Rev. B* **105**, 035105 (2022)

Arbitrary Spin-Polarized Systems

- In DMC, limited numbers of ζ can be calculated
- Usually, interpolaration function f_{c} is assumed to be the same as f_{x}
- f_{c} may have ρ dependence?





Yokota and Naito. *Phys. Rev. B* **105**, 035105 (2022)

Towards Superconducting/Superfluid Density Functional Theory

- In principle, all the quantities are functionals of ρ (HK theorem)
- In practice, to describe the Cooper pairing,
  abnormal (pair) density κ is needed
  "Oliveira-Gross-Kohn theorem" (Hinohara-san & Akashi-san's talks)
- In normal FRG-DFT, there is an external potential ($J \leftrightarrow \rho$)
- In FRG-DFT with pairings, two more external fields are introduced
  $\left(\left(J_\rho, J_\kappa, J_{\kappa^*}\right) \leftrightarrow (\rho, \kappa, \kappa^*)\right)$
- Gauge invariance is broken by hand
- Using the Wick theorem, "density correlator" appeared in the flow eq. can be separated into three parts: pairing, exchange, and correlation

Oliveira, Gross, Kohn. *Phys. Rev. Lett.* **60**, 2430 (1988)

Yokota, Kasuya, Yoshida, and Kunihiro. *Prog. Theor. Exp. Phys.* **2021**, 013A03 (2021)

Conclusion

- FRG: Derive effective action with evolving V_{int}
- FRG-DFT is an alternative method to construct EDFs
  succeded to construct Coulomb LDA E_{c} with arbitrary spin polarization
- Pairing can also be considered in FRG-DFT
- Excited state can also be calculated using FRG-DFT
- Low numerical cost $\rightarrow$ Fitting-free DFT calculation

Perspectives

- Nuclear EDF
- Gradient effect (GGA)

Conclusion

Table of Contents

Conclusion

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  - Inverse Kohn-Sham & Density Functional Perturbation Theory (IKS-DFPT)
  - Functional Renormalization Group Aided Density Functional Theory (FRG-DFT)
- IKS-DFPT: Information of densities from *ab initio* calc. are needed
  $\rightarrow$ Improve "known" EDF
- FRG-DFT: Alternative method to derive EDF microscopically
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Conclusion

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Thank you for attention!!