汎関数くりこみ群に基づいた密度汎関数理論による三次元電子ガス計算に基づく局所密度近似相関汎関数の第一原理的構築

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August 24, 2020
熱場の量子論とその応用 2020 (online)
高エネルギー加速器研究機構 素粒子原子核研究所 理論センター

Takeru Yokota and Tomoya Naito. *To Be Submitted.*

Table of Contents

Density Functional Theory (DFT)

Motivation: What Kind of Problems Do We Want to Solve?

- Target Systems: Quantum Many-Body Problem
  Atomic nuclei, Atoms, Molecules, Solids
- We Want to know E_{gs} and ρ_{gs} (At the first step)
- # of Particles: $50 \lesssim N \lesssim 10000$
  → Efficient method is required

Hamiltonian

We (assume to) know the Hamiltonian of the system

$$H = \sum_{j} t_j + \sum_{j} V_{\mathrm{ext}}\left(\boldsymbol{r}_j\right) + \sum_{j<k} V_{\mathrm{int}}\left(\boldsymbol{r}_j, \boldsymbol{r}_k\right)$$

t_j: single-particle kintetic operator $\boldsymbol{r}_j$: coordinate of particle j,

V_{ext}: external potential, V_{int}: interaction

Density Functional Theory (DFT)

Why Density Functional Theory??

- “Real interacting system” is mapped to “fictitious non-interacting system”
  → Problem is truncated to one-body problem: Efficient ($O\left(N^3\right)$)
  WFM is very accurate but numerical cost is huge ($O\left(N^7\right)$ for CCSD)
- In principle, DFT gives exact E_{gs} and ρ_{gs}

Basic theorem of DFT	Hohenberg-Kohn theorem
Realization (Practical way) of DFT	Kohn-Sham scheme

Usually, Kohn-Sham scheme is also refered as “DFT”

Density Functional Theory (DFT)

Hohenberg-Kohn Theorem

1. There is one-to-one correspondense between V_{ext} and ρ_{gs}
2. Ground-state energy is written as

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

   with the unique functional F with respect to V_{int}

3. Ground-state energy is given by the variational principle

$$E_{\mathrm{gs}} = \inf_{\Psi} \langle \Psi | H | \Psi \rangle = \inf_{\rho} \inf_{\Psi_\rho} \left\langle \Psi_\rho \middle| H \middle| \Psi_\rho \right\rangle$$

Hohemberg and Kohn. *Phys. Rev.* **146**, B864 (1964)
Levy. *Proc. Natl. Acad. Sci. USA* **76**, 6062 (1979)
Levy. *Phys. Rev. A* **26**, 1200 (1982)

Density Functional Theory (DFT)

Kohn-Sham Effective Potential

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

$$[t + V_{\mathrm{KS}}(\boldsymbol{r})]\, \varphi_j = \varepsilon_j \varphi_j$$

Ground-state Energy in Kohn-Sham Scheme

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

T_0: kinetic energy of non-interacting system, ε_j: single-particle energy of KS-system,
E_{d}: Hartree functional, E_{x}: exchange functional, E_{c}: correlation functional

Kohn and Sham. *Phys. Rev.* **140**, A1133 (1965)

Density Functional Theory (DFT)

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

Hartree Energy Density Functional E_{H}

$$E_{\mathrm{H}} \left[\rho \right] = \frac{1}{2} \iint V_{\mathrm{int}} \left(\boldsymbol{r}, \boldsymbol{r}' \right) \rho \left(\boldsymbol{r} \right) \rho \left(\boldsymbol{r}' \right) \, d\boldsymbol{r} \, d\boldsymbol{r}'$$

Once V_{int} is known, exact E_{H} can be calculated

Exchange/Correlation Energy Density Functional E_{x}, E_{c}

Exchange E_{x} Fock energy (in density functional form)

Correlation E_{c} "residue"

Even if V_{int} is known, exact E_{x} and E_{c} cannot be derived

(E_{x}: so far the functional form is not derived, E_{c}: impossible by definition)

→ Approximations for E_{x}, E_{c} are required

Density Functional Theory (DFT)

Local Density Approximation (LDA)

- Approximated to E_{x} and E_{c} for homogeneous systems
  Other highly-accurate methods provide E_{x} and E_{c},
  and functionals are given by the fitting to these data
- Energy density ε depends only on density $\rho(\boldsymbol{r})$

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

- Beyond the LDA is also known, while the LDA is still widely used

E_{xc} for Electron Systems in LDA Level

LDA-Exchange	Exact form is known
LDA-Correlation	Functional is fit to the E_{c} for homogeneous electron gas, calculated by using diffusion Monte Carlo method

Table of Contents

Hartree Atomic Unit

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

$$1\,\mathrm{Hartree} \simeq 27.2\,\mathrm{eV}, \qquad 1\,\mathrm{a.u.(length)} = a_{\mathrm{B}} \simeq 0.529\,\text{Å}$$

Functional-Renormalization-Group Aided DFT (FRG-DFT)

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

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

- This equation comes from the Legendre trans. between E & F
- Effective action Γ is the quantum counterparts of classical action S
- Γ includes qunatum fluctuations
- Γ can formally be calculated from S

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

If Γ can be calculated microscopically, E (E_{xc}) can be derived

One of the way to derive Γ is the FRG-DFT

In short. . .

FRG-DFT is a way to calculate ground-state energy from the action

Functional-Renormalization-Group Aided DFT (FRG-DFT)

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

2002 The formalism was proposed

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

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)

2015 $(1+1)$-D finite nuclei

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

2015 $(1+1)$-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)

Functional-Renormalization-Group Aided DFT (FRG-DFT)

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)

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

Yokota and Naito. *In Progress*

2020 Superfluid system (See poster tomorrow by Kasuya)

Yokota, Kasuya, Yoshida, and Kunihiro. arXiv:2008.05919 [nucl-th]

2020 **$(3+1)$-D infinite homogeneous electron gas**

Yokota and Naito. *In Preparation*

Functional-Renormalization-Group Aided DFT (FRG-DFT)

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

1. Strength of interaction $\lambda \in [0, 1]$ is introduced: $U_\lambda = \lambda V_{\text{int}}$
2. Two-particle point-irreducible (2PPI) formalism is used for the effective action Γ
3. Flow equation $\partial_\lambda \Gamma_\lambda [\rho]$ is derived formally
4. Since flow equation is functional differential eq. (difficult to solve), some truncations are introduced
    - Second-order vertex expansion (Taylor expansion around $\rho_{\text{gs},\lambda}$)
    - A coefficient is fixed during the flow
      (The coeff. for non-interacting system is used)

Functional-Renormalization-Group Aided DFT (FRG-DFT)

Effective Action Γ

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

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

$$\rho(X) = \frac{\delta W\left[J_{\mathrm{sup}}[\rho]\right]}{\delta J(X)},$$

$$\Gamma[\rho] = \int J_{\mathrm{sup}}[\rho]\,\rho(X)\,dX - W\left[J_{\mathrm{sup}}[\rho]\right] \qquad \text{(Effective action)}$$

S: Action, $\rho_\psi = \psi^*\psi$: Density field J: External field, $X = (\tau, \boldsymbol{x})$: Imaginary time and space

Functional-Renormalization-Group Aided DFT (FRG-DFT)

Action for Homogeneous Electron Gas: Interaction is gradually turning on

Interaction U is gradually turning on with parameter λ:

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

Corresponding action is

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

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

$S_{\lambda=1}$ Real Fermi Gas

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

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

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

Functional-Renormalization-Group Aided DFT (FRG-DFT)

Partition function Z and Density Field ρ_ψ

$$Z_\lambda [J] = \int \exp\left[J(X)\,\rho_\psi(X) - S_\lambda[\psi^*,\psi]\right] \mathcal{D}\psi^*\,\mathcal{D}\psi$$

$$\rho_\psi(X) = \sum_s \psi_s^*(X_\varepsilon)\,\psi_s(X)$$

J: External field, s: spin index, $X_\varepsilon = (\tau + \varepsilon, \boldsymbol{x})$ to avoid ambiguity of time-ordered operator

Generating Function of Connected Density Correlation Function

$$W_\lambda[J] = \log Z_\lambda[J]$$

n-Point Correlation Function

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

Functional-Renormalization-Group Aided DFT (FRG-DFT)

Effective Action Γ in Two-Particle Point-Irreducible (2PPI) Formalism

$$\Gamma_\lambda[\rho] = \int J_{\mathrm{sup},\lambda}[\rho](X)\,\rho(X)\,dX - W_\lambda\left[J_{\mathrm{sup},\lambda}[\rho]\right],$$

$$\rho(X) = \left.\frac{\delta W_\lambda[J]}{\delta J(X)}\right|_{J=J_{\mathrm{sup},\lambda}[\rho]}$$

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

Chemical Potential μ_λ

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

To fix electron density as n, μ_λ has λ dependence,

where $\mu_{\lambda=0} = \left(3\pi^2 n\right)^{2/3}/2$

In spin-polarized systems, μ_λ also has s dependence

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

Functional-Renormalization-Group Aided DFT (FRG-DFT)

Change of Γ_λ: “Flow Equation”

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

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

Schwenk and Polonyi. 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.

Functional-Renormalization-Group Aided DFT (FRG-DFT)

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

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

Truncated Flow Equation

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

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

Functional-Renormalization-Group Aided DFT (FRG-DFT)

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

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

In Momentum Representation

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

Functional-Renormalization-Group Aided DFT (FRG-DFT)

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

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

n_{i}: Density for background charge

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

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

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

Functional-Renormalization-Group Aided DFT (FRG-DFT)

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

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

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

Functional-Renormalization-Group Aided DFT (FRG-DFT)

Final Result for E_{gs}

Preliminary Results

It will be shown in the workshop

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

Functional-Renormalization-Group Aided DFT (FRG-DFT)

Technique

Preliminary Results

It will be shown in the workshop

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)

Table of Contents

3D Homogeneous Electron Gas

Correlation Energy in 3D HEG (LDA Correlation Functional)

Preliminary Results

It will be shown in the workshop

3D Homogeneous Electron Gas

Calculation Results

- In $r_{\mathrm{s}} \to 0$, Gell-Mann-Brueckner limit is exactly reproduced
- QMC results are reproduced in the high-density region
- Since part of the correlation is still missing,
  in the low-density region, there is deviation from the QMC results
- However, the correlation in 3D is smaller than that in 2D
  → Results in 3D are better than those in 2D

Correlation Functional

Way to Construct Conventional LDA Correlation Functional

- Fitting to the VMC 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 $r_{\mathrm{s}} = 50\,\mathrm{Bohr}$ 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 (explained later)

LDA Correlation Functional

PZ81 Functional

$$\varepsilon_{\mathrm{c}}\left(r_{\mathrm{s}}\right) = \begin{cases} A \log r_{\mathrm{s}} + B + C r_{\mathrm{s}} \log r_{\mathrm{s}} + D r_{\mathrm{s}} & r_{\mathrm{s}} < 1, \\ \gamma / \left(1 + \beta_1 \sqrt{r_{\mathrm{s}}} + \beta_2 r_{\mathrm{s}}\right) & r_{\mathrm{s}} \geq 1 \end{cases}$$

- A and B are determined to reproduce Gell-mann-Brueckner limit ($A = 0.0311$, $B = -0.048$ in Hartree atomic unit)
- C, D, β_1, β_2, γ are determined to reproduce Ceperley-Alder data
- $\varepsilon_{\mathrm{c}}\left(1-0\right) = \varepsilon_{\mathrm{c}}\left(1+0\right)$ is satisfied
- $d\varepsilon_{\mathrm{c}}\left(1-0\right)/dr_{\mathrm{s}} = d\varepsilon_{\mathrm{c}}\left(1+0\right)/dr_{\mathrm{s}}$ is NOT satisfied

Perdew and Zunger. *Phys. Rev. B* **23**, 5048 (1981)

LDA Correlation Functional

PZ81-like Functional based on FRG-DFT (“PZ-FRG” Series)

Preliminary Results

It will be shown in the workshop

LDA Correlation Functional

Parameter Sets of PZ Series

Preliminary Results

It will be shown in the workshop

LDA Correlation Functional

Behaviour of Functionals (Error to PZ81 $\Delta E_{\mathrm{PZ}} = \left(E - E_{\mathrm{PZ}}\right) / E_{\mathrm{PZ}}$)

Preliminary Results

It will be shown in the workshop

LDA Correlation Functional

Calculation for Isolated Atoms

- Calculate total energies and densities of isolated atoms (noble gas are chosen)
- Since the PZ81 func. is chosen as “fitting functional” for FRG data, results are compared to PZ81 data
- Fitting-free method (direct method) is also tested

Fitting-free method

- ε_{c} and $d\varepsilon_{\mathrm{c}}/dr_{\mathrm{s}}$ for 65536 points in $0 < r_{\mathrm{s}} < 100\,\mathrm{a.u.}$ region is calculated by FRG-DFT
- Between two points, ε_{c} and $d\varepsilon_{\mathrm{c}}/dr_{\mathrm{s}}$ are calculated with linear interpolation
- In $r_{\mathrm{s}} > 100$, ε_{c} and $d\varepsilon_{\mathrm{c}}/dr_{\mathrm{s}}$ are calculated with extrapolation
  (to derive the extrapolation function, data for $95 < r_{\mathrm{s}} < 100\,\mathrm{a.u.}$ are used)

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

LDA Correlation Functional

Total Energies of Isolated Atoms (Compared with PZ81)

Preliminary Results

It will be shown in the workshop

LDA Correlation Functional

Density of Isolated Atoms

- Errors in YN series are larger than those in PW92/VWN
- Especially in large r-region: low-density region
- However, error is less than $5\,\%$

Total Energies of Isolated Atoms

- As Z increases, the error decreases ($E_{\mathrm{tot}}/E_{\mathrm{tot}}^{\mathrm{PZ}}$ converges to $100\,\%$)
  → It is related that TF approx. reaches to exact in $Z \to \infty$ limit
- Errors for YN series are a little bit larger than those for VWN & PW92, but almost comparable error (direction is opposite)
- Error for direct method is totally comparable to VWN & PW92 (direction is opposite)

What is the source of error?

LDA Correlation Functional

Error Sources

E	Exact functional	ρ	Exact density (derived by E)
$\tilde{E}$	Approximated functional	$\tilde{\rho}$	Approximated density (derived by $\tilde{E}$)

$$E[\rho] - \tilde{E}[\tilde{\rho}] = \left(E[\rho] - \tilde{E}[\rho]\right) + \Delta E_{\mathrm{D}}$$

First term	Functional-driven error
Second term	Density-driven error

Kim, Sim, and Burke. *Phys. Rev. Lett.* **117**, 073003 (2013)

In This Work

Since we compare from the PZ81, E is assumed to be PZ81 func., instead of the “exact” functional

LDA Correlation Functional

Functional-driven Error of Isolated Atoms (Compared with PZ81)

Preliminary Results

It will be shown in the workshop

LDA Correlation Functional

- Func.-driven errors are $25\,\%$ or less of the total error
- Func.-driven errors of VWN/PW92 are larger than those of YN series
- Func.-driven errors of PZ-FRG-1/PZ-FRG-2 are less than that of NumTable

LDA Correlation Functional

Preliminary Results

It will be shown in the workshop

LDA Correlation Functional

Preliminary Results

It will be shown in the workshop

Table of Contents

Conclusion

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- FRG-DFT was applied to 3D homogeneous electron gas
- The results are reasonable
- We made the PZ81-like functionals based on FRG-DFT results

Preliminary Results

It will be shown in the workshop

- Since numerical cost of FRG-DFT is low,
  “fitting-free” method can be applied with FRG-DFT data

Conclusion

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Thank you for attention!!