Towards an ab-initio DFT via functional formalism

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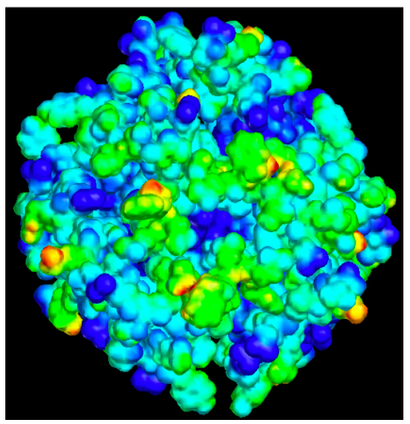
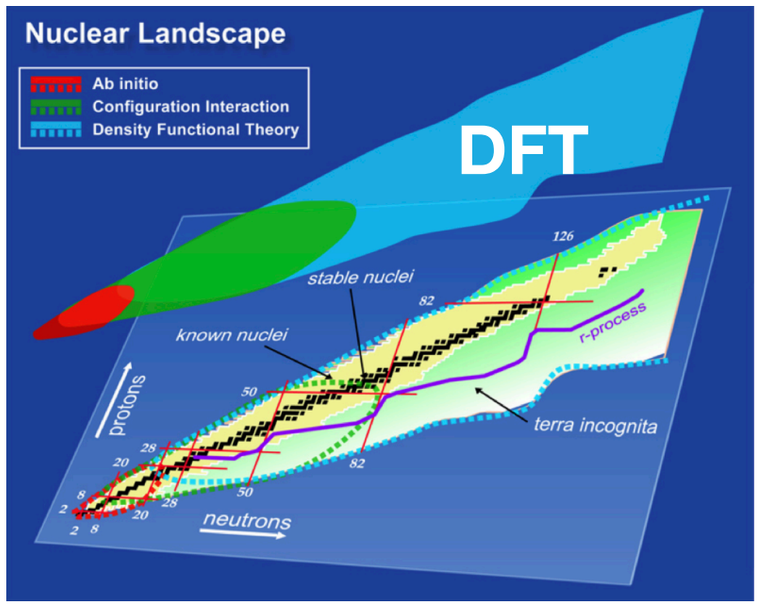
Density functional theory

- **Nuclear physics**
- **Condensed matter physics**
- **Classical liquids**



Proteins

http://www.slis.tsukuba.ac.jp/cicsj27/cicsj27/J13.pdf



Bertsch, Dean, Nazarewicz (2007), SciDAC Review, (6):42

Energy density functional (EDF)

$$E[\rho] = F_{\mathrm{HK}}[\rho] + \int dx \rho(x) V(x) \quad (V\text{: external field})$$

$$F_{\mathrm{HK}}[\rho] = \langle \psi[\rho] \,|\, \hat{H}_{V-\mathrm{indep}} \,|\, \psi[\rho] \rangle$$

Ground state ψ is a functional of density ρ (Hohenberg-Kohn thm.)

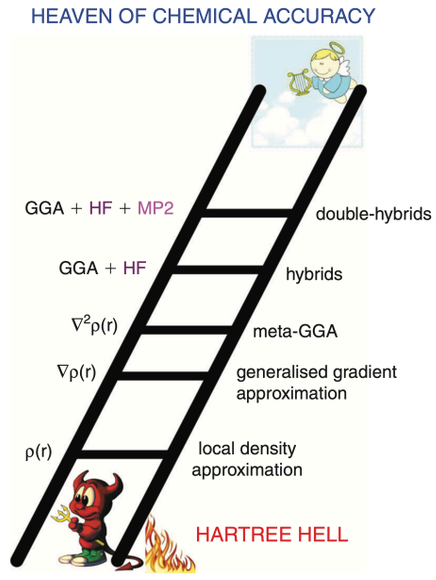


Figure from Goerigk, Mehta, Aust. J. Chem. (2019)

How can we derive EDF? (problem known as “Jacob’s ladder”)

[Perdew, Schmidt (2001)]

Construction of EDF

Phenomenological, data-driven approaches

- Parameter fitting for physical data (nuclei, electrons)
    - Advanced one: Machine learning (electrons) [Talk by Dr. Akashi]
- Fundamental-measure theory (classical liquids) [Rosenfeld (1989)]

Bottom-up approaches

- Monte Carlo based approach (LDA functional for electrons)
- Many-body perturbation (inclusion of phonon)
- Density matrix expansion (nuclei from chiral effective field theory)

  [Carlsson, Dobaczewski, Kortelainen (2008), Stoitsov+ (2010), Kaiser, Weise (2010), Holt, Kaiser, Weise (2011)]
- **Functional-renormalization-group (FRG) approach**

Contents

- Basic idea of FRG aided DFT

  EDF as effective action

  Evolution equation for EDF

- Case studies

  Low dim. models

  Electrons

  Classical liquids

- Towards superfulid systems

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Functional renormalization group (FRG)

Wilsonian exact renormalization group eq.

[Wilson (1971), Wilson, Kogut (1974)]

- Evolution of Wilsonian effective action (coarse-graining in momentum space)

$$S_\Lambda^W\left[\phi_{|q|<\Lambda}\right] = -\ln\left(\int D\phi_{|q|>\Lambda}\, e^{-S[\phi]}\right)$$

Wegner-Houghton eq.

[Wegner, Houghton (1973)]

- Continuum RG transform
- Sharp cutoff

Polchinski eq.

[Polchinski (1984)]

- Flow eq. for Schwinger functional ($\ln Z$)

Legendre trans. w.r.t. one-particle source $\int J\phi$

Wetterich eq.

[Wetterich (1991, 1993)]

$$\partial_\Lambda \Gamma_\Lambda[\phi] = \frac{1}{2}\mathrm{Tr}\left[\partial_\Lambda R_\Lambda \frac{1}{\Gamma^{(2)}[\phi] + R_\Lambda}\right]$$

Effective action $\Gamma_\Lambda[\phi] = \sup_J\left(\int J\phi - \ln Z_\Lambda[J]\right) - \frac{1}{2}\int \phi R_\Lambda \phi$

$$Z_\Lambda[J] = \int D\phi \exp\left(-S[\phi] - \frac{1}{2}\int \phi R_\Lambda \phi + \int J\phi\right)$$

👍 **Relation between $\Gamma_\Lambda[\phi]$ and correlation functions is clear. (generating functional for 1-particle irreducible diagrams)**

👍 **Relation between $\Gamma_\Lambda[\phi]$ and classical action $S_{\Lambda_{\mathrm{UV}}}[\phi]$ is clear: $\Gamma_{\Lambda\to\Lambda_{\mathrm{UV}}}[\phi] = S_{\Lambda_{\mathrm{UV}}}[\phi]$**

Effective Action for density

Effective action for composite fields

[Luttinger (1960), Baym (1962), Cornwall, Jackiw, Tomboulis (1974)]

Effective action for density

[Fukuda, Kotani, Suzuki, Yokojima (1994), Valiev, Fernando (1997)]

Progress of Theoretical Physics, Vol. 92, No. 4, October 1994

Density Functional Theory through Legendre Transformation

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(Received May 16, 1994)

Theoretical foundation of density functional theory in terms of field theoretical Legendre transformation is presented. The ground state energy is first written as a functional of local probe coupled to the density operator. The density functional is then defined by the functional Legendre transformation, which leads to a systematic formulation of density functional theory. Excitation spectrum is also determined within the same formalism in a unified way. The diagrammatic evaluation is most conveniently done by using auxiliary field method. Several generalizations of the formalism and extension to the case other than the density operator are also discussed.

Effective Action for Density (Definition)

Partition function (imaginary-time formalism)

$$Z = \int D\psi D\overline{\psi} e^{-S[\psi,\overline{\psi}]}$$

$$Z[V] = \int D\psi D\overline{\psi} e^{-S[\psi,\overline{\psi}]+\int d\tau dx V(\tau,x)\overline{\psi}(\tau,x)\psi(\tau,x)}$$

$$\Gamma[\rho] = \sup_J \left(\int d\tau dx V(x)\rho(x) - \ln Z[V] \right)$$

EDF as Effective Action

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

$$\Gamma[\rho] = \sup_V \left(\int_0^\beta d\tau \int dx V(\tau, x)\rho(\tau, x) - \ln Z[V] \right)$$

Inverse temperature β is
introduced to regulate τ integral

$\Gamma[\rho]$ and requirement by Hohenberg-Kohn theorem

Variational principle (quantum EOM)

$$\frac{\delta\Gamma[\rho]}{\delta\rho(\tau, x)} = \mu \quad \Rightarrow \quad \rho(X) = \frac{1}{Z[\mu]} \int D\psi D\psi^\dagger \rho_\psi(\tau, x) e^{-S[\psi^\dagger,\psi]+\mu\int d\tau' dx \rho_\psi(\tau',x)} = \rho_{\mathrm{gs}}(\tau, x)$$

$$\Gamma[\rho_{\mathrm{gs}}] = \mu \int d\tau dx \rho_{\mathrm{gs}}(\tau, x) - \ln Z[\mu] = \beta F_{\mathrm{Helm}} \quad \Rightarrow \quad E_{\mathrm{gs}} = \lim_{\beta\to\infty} \Gamma[\rho_{\mathrm{gs}}]/\beta$$

Linear dependence on external potential

Shift of external potential
⇔ Shift of V

$$\Rightarrow \quad \Gamma[\rho] = \int d\tau \int dx \int_X V_{\mathrm{ext}}(x)\rho(\tau, x) + (V_{\mathrm{ext}}\textbf{-independent terms})$$

RG description

Polonyi & Sailer's work

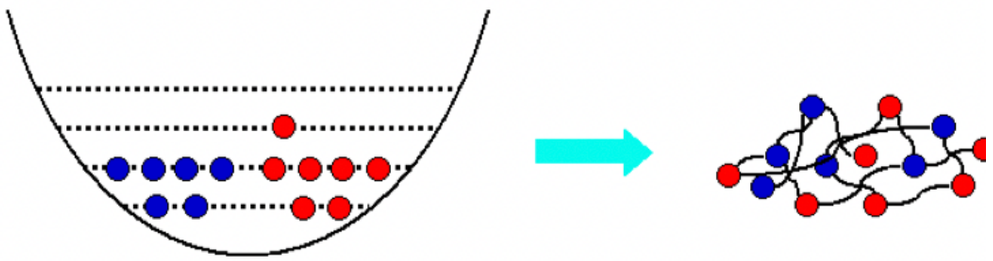
[Polonyi, Sailer (2002)]

- Electron-photon system (QED)
- Regulator for photons (photon fluctuations are gradually taken in RG)
- Flow equation for EDF

Schwenk & Polonyi's work

[Schwenk, Polonyi (2004)]

- Fermions with a two-body interaction
- Regulator for the two-body coupling
  - Equivalent to RG of QED case after integrating photons out
- Description of self-bound system by introducing atrificial background



RG param. $\lambda : 0 \to 1$

Coupling $U_\lambda : 0 \to U$

Background $V_\lambda : V \to 0$

Regulated effective action

Fermions with a two-body interaction

$$S_\lambda[\psi,\overline{\psi}] = \int d\tau dx \overline{\psi}(\tau,x)\left(-\frac{\Delta}{2m}\right)\psi(\tau,x) + \frac{1}{2}\int d\tau dx dx' \overline{\psi}(\tau,x)\overline{\psi}(\tau,x')U_\lambda(x-x')\psi(\tau,x')\psi(\tau,x)$$

Regulated two-body interaction

Partition function in background

Density field

$$Z_\lambda[V] = \int D\psi D\overline{\psi}\exp\left(-S_\lambda[\psi,\overline{\psi}] + \int dx d\tau V(x,\tau)\overline{\psi}(\tau,x)\psi(\tau,x)\right)$$

Background potential (it also plays a role of chemical potential)

Legendre transform

$$\Gamma_\lambda[\rho] = \sup_V\left(\int dx d\tau V(x,\tau)\rho(x,\tau) - \ln Z_\lambda[V]\right) = \int dx d\tau V_\lambda[\rho](x,\tau)\rho(x,\tau) - \ln Z_\lambda\left[V_\lambda[\rho]\right]$$

Background realizing density ρ

Derivation of flow equation (illustration)

$$\partial_\lambda \Gamma_\lambda[\rho] = -\left(\partial_\lambda \ln Z_\lambda\right)[V_\lambda[\rho]] + \int d\tau dx\, \partial_\lambda V_\lambda[\rho](\tau, x) \frac{\delta}{\delta V(\tau, x)} \left(\int_X V(X)\rho(X) - \ln Z_\lambda[V] \right) \Bigg|_{V=V_\lambda[\rho]}$$

$$= -\frac{1}{Z_\lambda}\left(\partial_\lambda Z_\lambda\right)[V_\lambda[\rho]]$$

$$= \frac{1}{2}\int d\tau dx dx' \partial_\lambda U_\lambda(x-x') \langle \overline{\psi}(\tau, x)\overline{\psi}(\tau, x')\psi(\tau, x')\psi(\tau, x)\rangle_{\lambda, V_\lambda[\rho]}$$

$$= \frac{1}{2}\int dx dx' d\tau \partial_\lambda U_\lambda(x-x') \Bigg(\underbrace{\rho(\tau, x)\rho(\tau, x')}_{\text{Direct term}} + \underbrace{\left(\frac{\delta^2 \Gamma_\lambda[\rho]}{\delta\rho\delta\rho}\right)^{-1}(\tau, x, \tau, x')}_{\text{Density correlation}} - \underbrace{\rho(\tau, x')\delta(x-x')}_{\text{From normal order}} \Bigg)$$

Flow Equation

$$\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{2}\int dx dx' d\tau \partial_\lambda U_\lambda(x-x')\left(\underbrace{\rho(\tau,x)\rho(\tau,x')}_{\text{Hartree}} + \underbrace{\left(\frac{\delta^2\Gamma_\lambda[\rho]}{\delta\rho\delta\rho}\right)^{-1}(\tau,x,\tau,x') - \rho(\tau,x')\delta(x-x')}_{\text{Ex.+Corr.}}\right)$$

- **Right-hand side: Hartree+exchange-correlation terms**
- **Exact equation for $\Gamma_\lambda[\rho]$, but it is computationally too tough to treat functionals w/o approximation…**

Approximation

- Vertex expansion

  Taylor expansion around a density of interest

  Hierarchy of flow eqs for density correlation functions

- Derivative expansion

  Expansion w.r.t. ∇

  Local potential approximation, … e.g.) Classical liquid [Lue (2015)]

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Computational studies for FRG-DFT

- **Zero-dim classical anharmonic oscillators**

  Kemler, Braun, JPG (2013)

  Liang, Niu, Hatsuda, PLB (2018)

- **Zero-dim quantum anharmonic oscillators**

  Kemler, Braun, JPG (2013)

- **One-dim nuclear system**

  Kemler, Pospiech, Braun, JPG (2017)

  TY, Yoshida, Kunihiro, PRC (2019)

  TY, Yoshida, Kunihiro, PTEP (2019)

- **Electron systems**

  TY, Naito, PRB (2019)

  TY, Naito, PRResearch (2021)

  TY, Naito, PRB (2022)

- **Classical liquids**

  Lue, AIChE (2015)

  TY, Haruyama, Sugino, PRE (2021)

Vertex expansion

- **Canonical formalism**
- **Grand-canonical formalism**

  Flow of chemical potential

[Kemler, Braun (2013)]

[TY, Yoshida, Kunihiro (2019)]

$$\Gamma_\lambda[\rho] = \sum_{n=0}^{\infty} \frac{1}{n!} \int d\tau_1 \int d\mathbf{x}_1 \cdots \int d\tau_n \int d\mathbf{x}_n \Gamma_\lambda^{(n)}[\rho_{\mathrm{gs}}](\tau_1, \mathbf{x}_1, \ldots, \tau_n, \mathbf{x}_n) \prod_{i=1}^{n} (\rho(\tau_i, \mathbf{x}_i) - \rho_{\mathrm{gs}})$$

0th Energy

$$\partial_\lambda \Gamma_\lambda[\rho_{\mathrm{gs}}] \left(= \partial_\lambda \beta E_{\mathrm{gs},\lambda} \right) = \mathrm{Flow}_\lambda^{(0)} \left[\rho_{\mathrm{gs}}, \Gamma_\lambda^{(2)}[\rho_{\mathrm{gs}}] \right]$$

1st Chemical potential

$$\partial_\lambda \Gamma_\lambda^{(1)}[\rho_{\mathrm{gs}}](\tau, \mathbf{x}) \left(= \partial_\lambda \mu_\lambda \right) = \mathrm{Flow}_\lambda^{(1)} \left[\tau, \mathbf{x}; \rho_{\mathrm{gs}}, \Gamma_\lambda^{(2)}[\rho_{\mathrm{gs}}], \Gamma_\lambda^{(3)}[\rho_{\mathrm{gs}}] \right]$$

2nd Density correlation

$$\partial_\lambda \Gamma_\lambda^{(2)}[\rho_{\mathrm{gs}}](\tau_1, \mathbf{x}_1, \tau_2, \mathbf{x}_2) \left(= \partial_\lambda G_\lambda^{(2)-1}(\tau_1, \mathbf{x}_1, \tau_2, \mathbf{x}_2) \right)$$
$$= \mathrm{Flow}_\lambda^{(2)} \left[\tau_1, \mathbf{x}_1, \tau_2, \mathbf{x}_2; \rho_{\mathrm{gs}}, \Gamma_\lambda^{(2)}[\rho_{\mathrm{gs}}], \Gamma_\lambda^{(3)}[\rho_{\mathrm{gs}}], \Gamma_\lambda^{(4)}[\rho_{\mathrm{gs}}] \right]$$

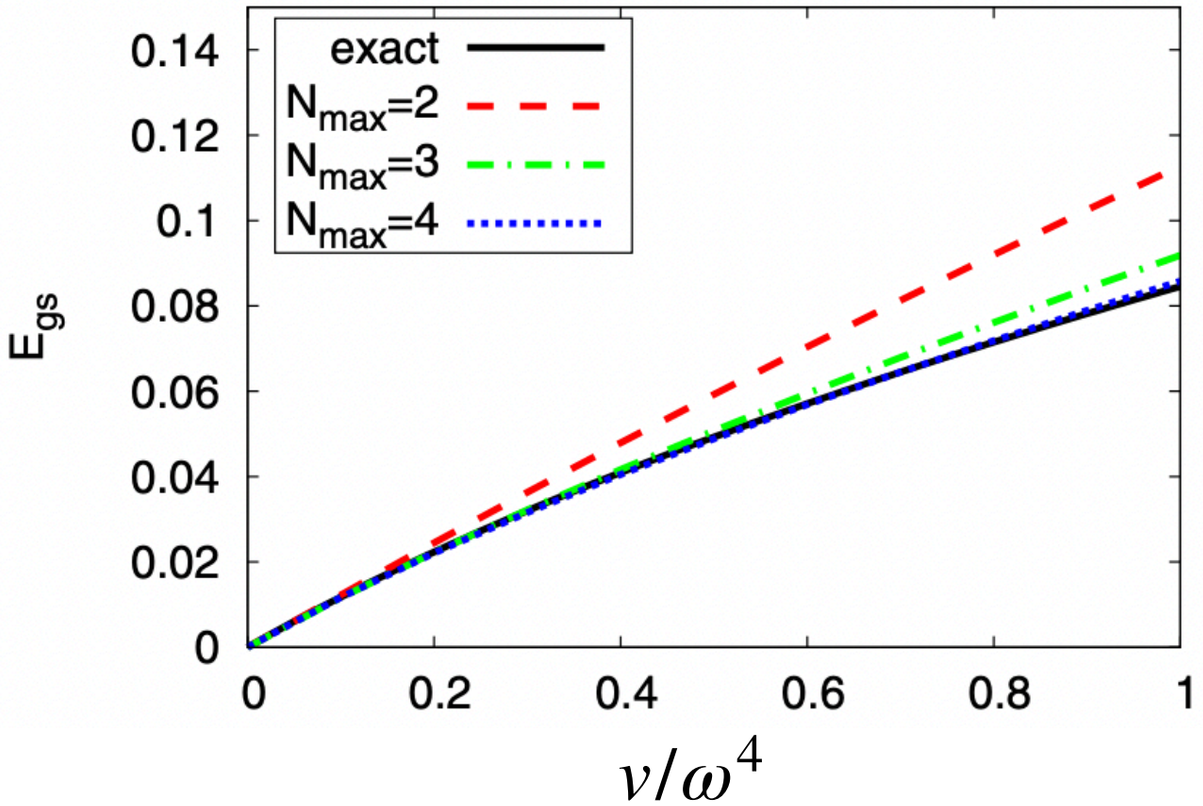
⋮

Higher-order terms are approximated
(e.g. $\Gamma_\lambda^{(3,4)} \approx \Gamma_0^{(3,4)}$)

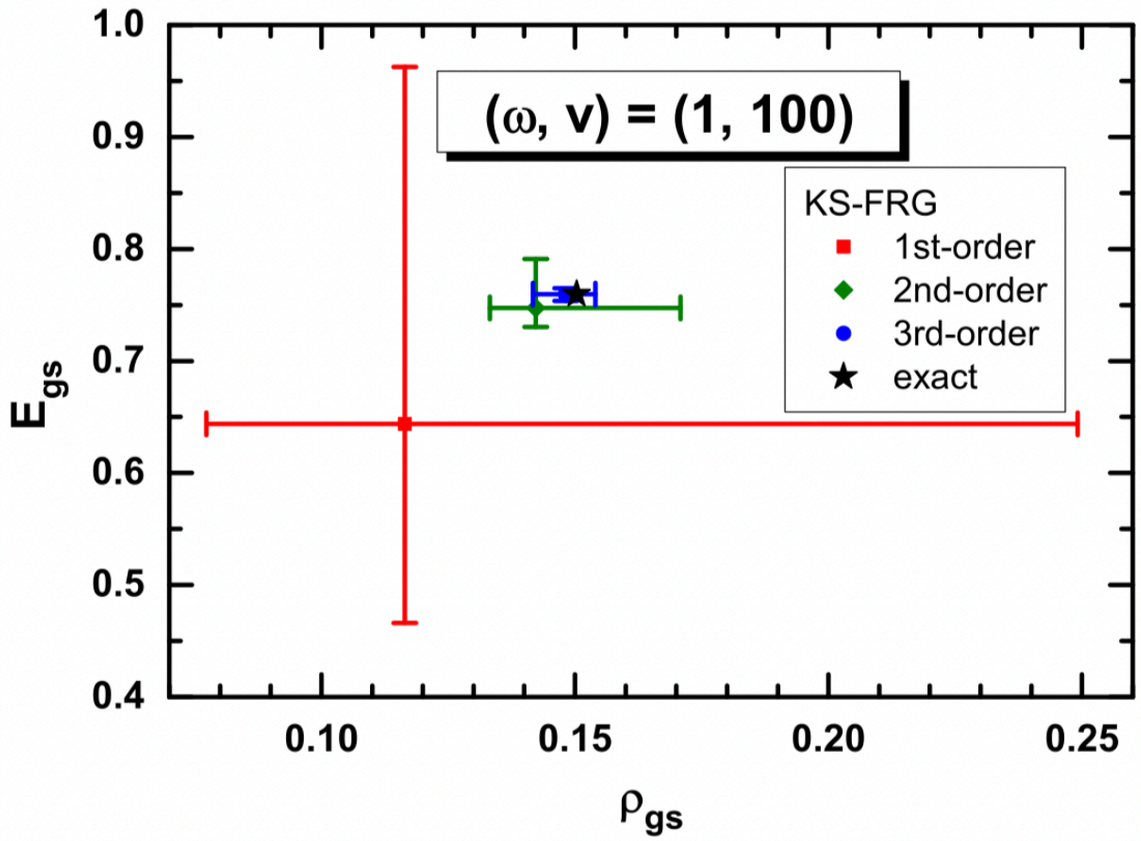
Zero-dim anharmonic oscillators

$$S(\phi) = \frac{1}{2}\omega^2\phi^2 + \frac{1}{4!}v\varphi^4$$

Kemler, Braun, JPG (2013)



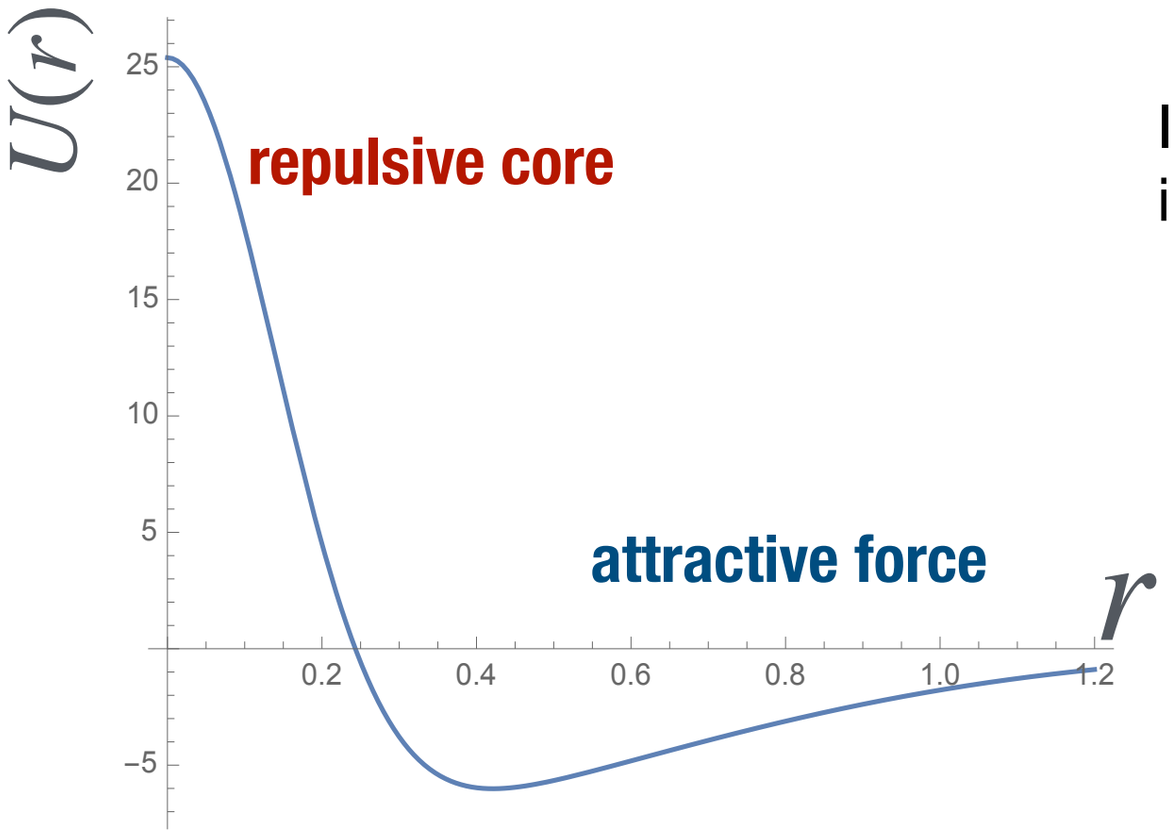
Liang, Niu, Hatsuda, PLB (2018)



Formalism based on flow of Kohn-Sham potential

One-dim. nuclear matter

- **Finite particle number in finite volume** Kemler, Pospiech, Braun, JPG (2017)
- **Infinite matter** TY, Yoshida, Kunihiro, PRC (2019)



Identical fermions (e.g. spin polarized system) interacting via very-simplified nuclear-like force

$$U(r) = \frac{g}{\sigma_1\sqrt{\pi}} e^{-\frac{r^2}{\sigma_1^2}} - \frac{g}{\sigma_2\sqrt{\pi}} e^{-\frac{r^2}{\sigma_2^2}}$$

$g = 12,\ \sigma_1 = 0.2,\ \sigma_2 = 0.8$

fermion mass=1 unit

Alexandro, Myczkowski, Negele, PRC (1989)

Bench mark: Monte Carlo result near the saturation point

extrapolation from finite systems with 2~12 particles.

Expansion around homogeneous density

generating functional for connected density correlators

$$\Gamma_\lambda^{(1)}[\rho](\tau,x) = V_\lambda[\rho](\tau,x), \qquad \Gamma_\lambda^{(2)}[\rho](\tau,x,\tau',x') = \left(\frac{\delta^2 \ln Z_\lambda}{\delta V \delta V}[V_\lambda[\rho]]\right)^{-1}(\tau,x,\tau',x')$$

Derivatives of $\Gamma_\lambda[\rho]$ are related to chemical potential μ_λ and imaginary-time density correlators $\tilde{G}_\lambda^{(n)}$

2nd-order expansion around homogeneous density ρ in terms of density correlators

0th
$$\partial_\lambda \frac{E_{\mathrm{gs},\lambda}}{N} = \frac{1}{2\rho}\int_p \partial_\lambda \tilde{U}_\lambda(p)\left(\int_\omega \tilde{G}_\lambda^{(2)}(P) - \rho\right)$$

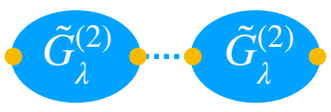
$$P = (\omega, p)$$

1st
$$\partial_\lambda \mu_\lambda = \frac{1}{2\tilde{G}_\lambda^{(2)}(0)}\int_P \partial_\lambda \tilde{U}_\lambda(p)\tilde{G}_\lambda^{(3)}(P,-P) - \frac{1}{2}\partial_\lambda U_\lambda(0)$$

2nd
$$\partial_\lambda \tilde{G}_\lambda^{(2)}(P) = -\partial_\lambda \tilde{U}_\lambda(p)\tilde{G}_\lambda^{(2)}(P)^2 - \frac{1}{2}\int_{P'} \partial_\lambda \tilde{U}_\lambda(p)\left(\tilde{G}_\lambda^{(4)}(P',-P',P) - \frac{\tilde{G}_\lambda^{(3)}(P,-P)\tilde{G}_\lambda^{(3)}(P',-P')}{\tilde{G}_\lambda^{(2)}(0)}\right)$$

⋮

Direct terms



Exchange-correlation (Higher-order) terms

Approximation

$$\partial_\lambda \tilde{G}^{(2)}_\lambda(P) = -\partial_\lambda \tilde{U}_\lambda(p)\tilde{G}^{(2)}_\lambda(P)^2 - \frac{1}{2}\int_{P'} \partial_\lambda \tilde{U}_\lambda(p')\left(\tilde{G}^{(4)}_\lambda(P',-P',P) - \frac{\tilde{G}^{(3)}_\lambda(P',-P')\tilde{G}^{(3)}_\lambda(P,-P)}{\tilde{G}^{(2)}_\lambda(0)}\right)$$

$$=: C_\lambda(P)$$

Approximation 1: $C_\lambda(P) \approx C_{\lambda=0}(P)$

👍 **If we choose $U_\lambda(x) = \lambda U(x)$, the flow eqation can be analytically solved (Riccaci equation)**

TY, Naito, PRB (2019)

Approximation 2: $C_\lambda(P) \approx c_\lambda C_{\lambda=0}(P)$

Kemler, Pospiech, Braun, JPG (2017)

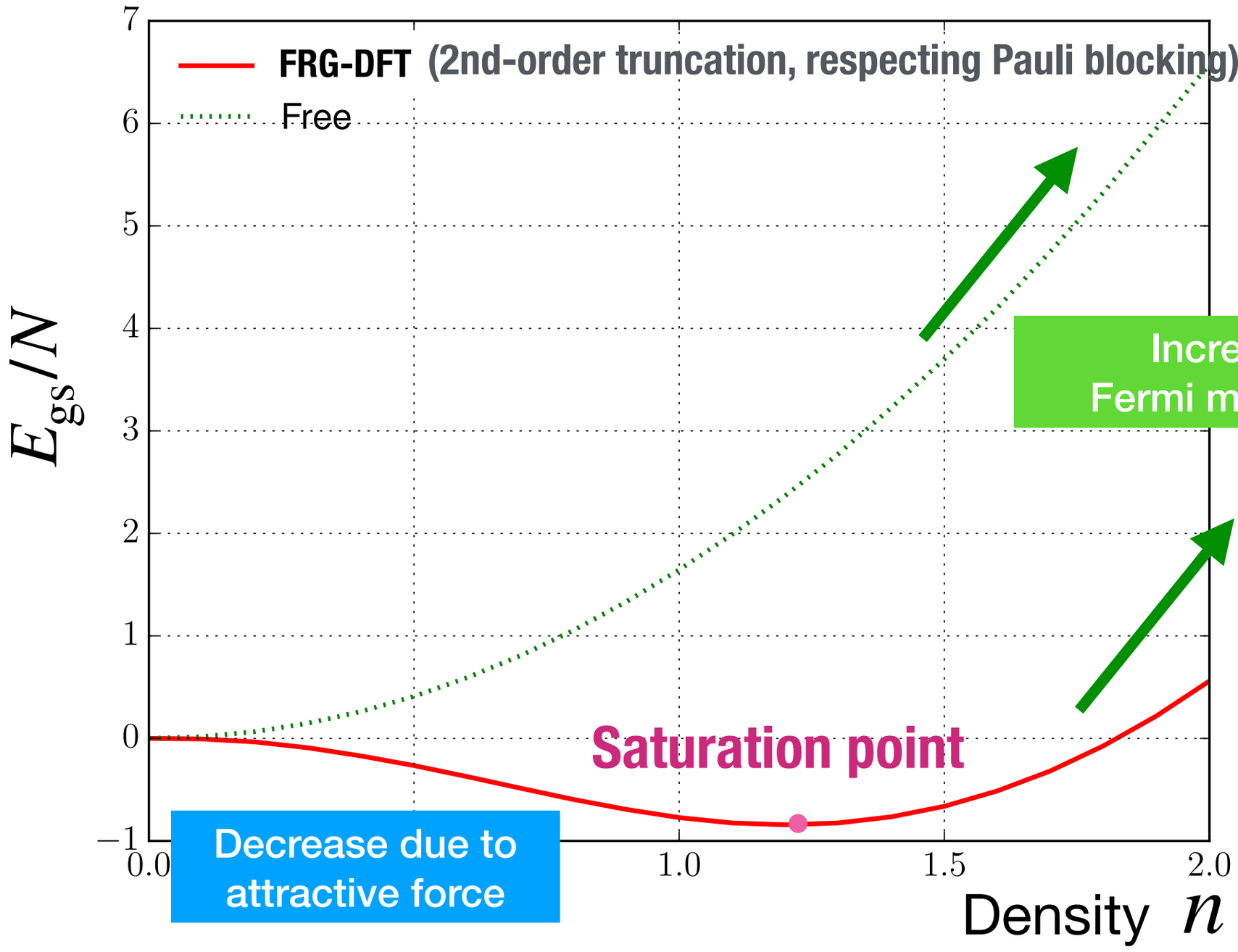
c_λ is a coefficient to recover a Pauli-blocking condition

$$0 = \lim_{x\to x'} f^{(2)}_\lambda(x,x') = \lim_{x\to x'}\left[G^{(2)}_\lambda(\tau,x,\tau,x') - \rho\delta(x-x')\right] = \int_P \left[\tilde{G}^{(2)}_\lambda(P) - \rho\delta(\omega)\right]$$

two-particle distribution

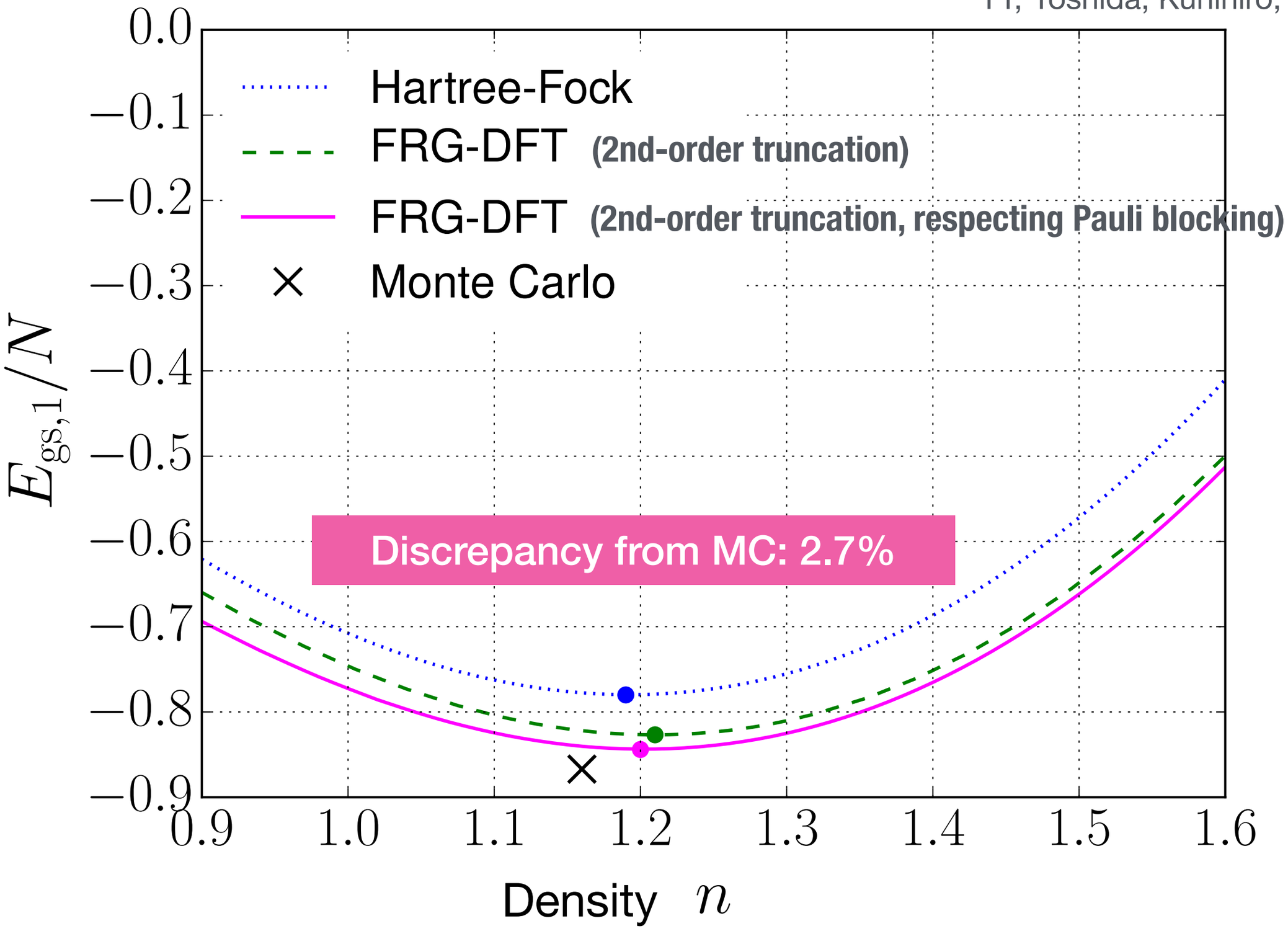
Result: Equation of State of infinite matter

TY, Yoshida, Kunihiro, PRC (2019)



Near the saturation point

TY, Yoshida, Kunihiro, PRC (2019)



Spectral function

Flow eq. for correlation with Matsubara freq. $\tilde{G}^{(2)}_{\lambda}(\omega_{\mathrm{i}}, p)$

↓ Analytic continuation **for flow eq.**

Flow eq. for real-time correlation $\tilde{G}^{(2)}_{\mathrm{R},\lambda}(\omega, p)$

↓ **Solution**

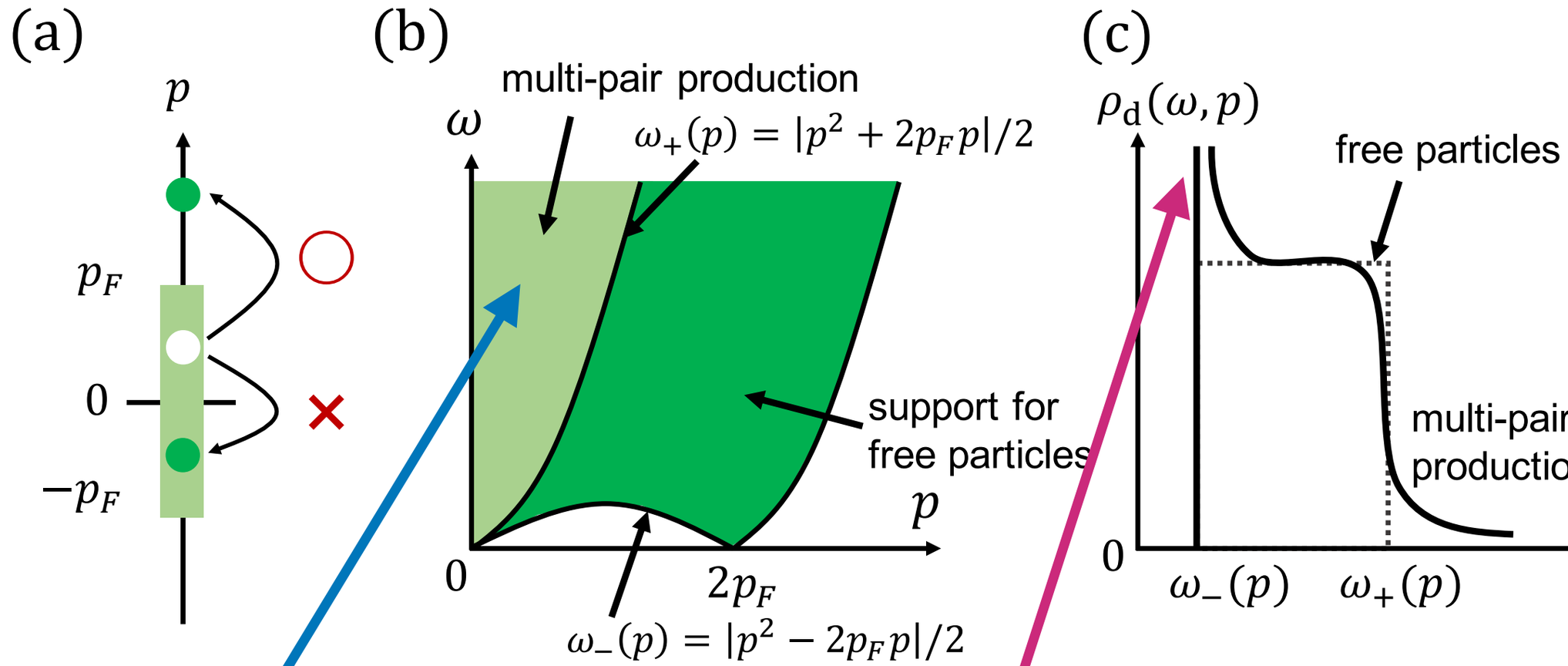
Spectral function in density channel: $\rho_{\mathrm{d}}(\omega, p) = -2\mathrm{Im}\tilde{G}^{(2)}_{\mathrm{R},\lambda=1}(\omega, p)$

- **c.f.) FRG studies on 1PI formalism** [Kamikado+ (2014), Tripolt+ (2014)]
- **Elaborate numetical analytic contination from imaginary-frequency data (e.g. Padé approx.) is not needed!**

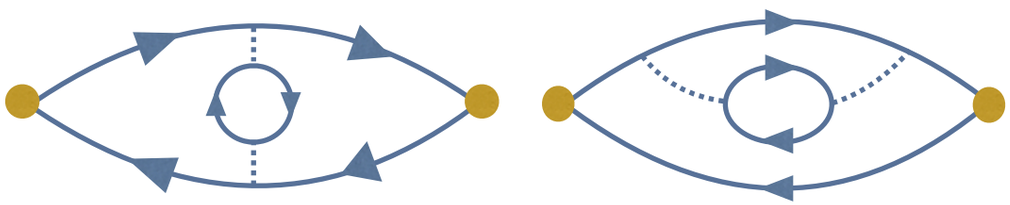
Excitation in Tomonaga-Luttinger liquid

Previous results
(such as bosonization)

Pustilnik, Khodas, Kamenev, Glazman, PRL (2006)
Teber, PRB (2007)
Imambekov, Schmidt, Glazman, RMP (2012)



Multi-pair production



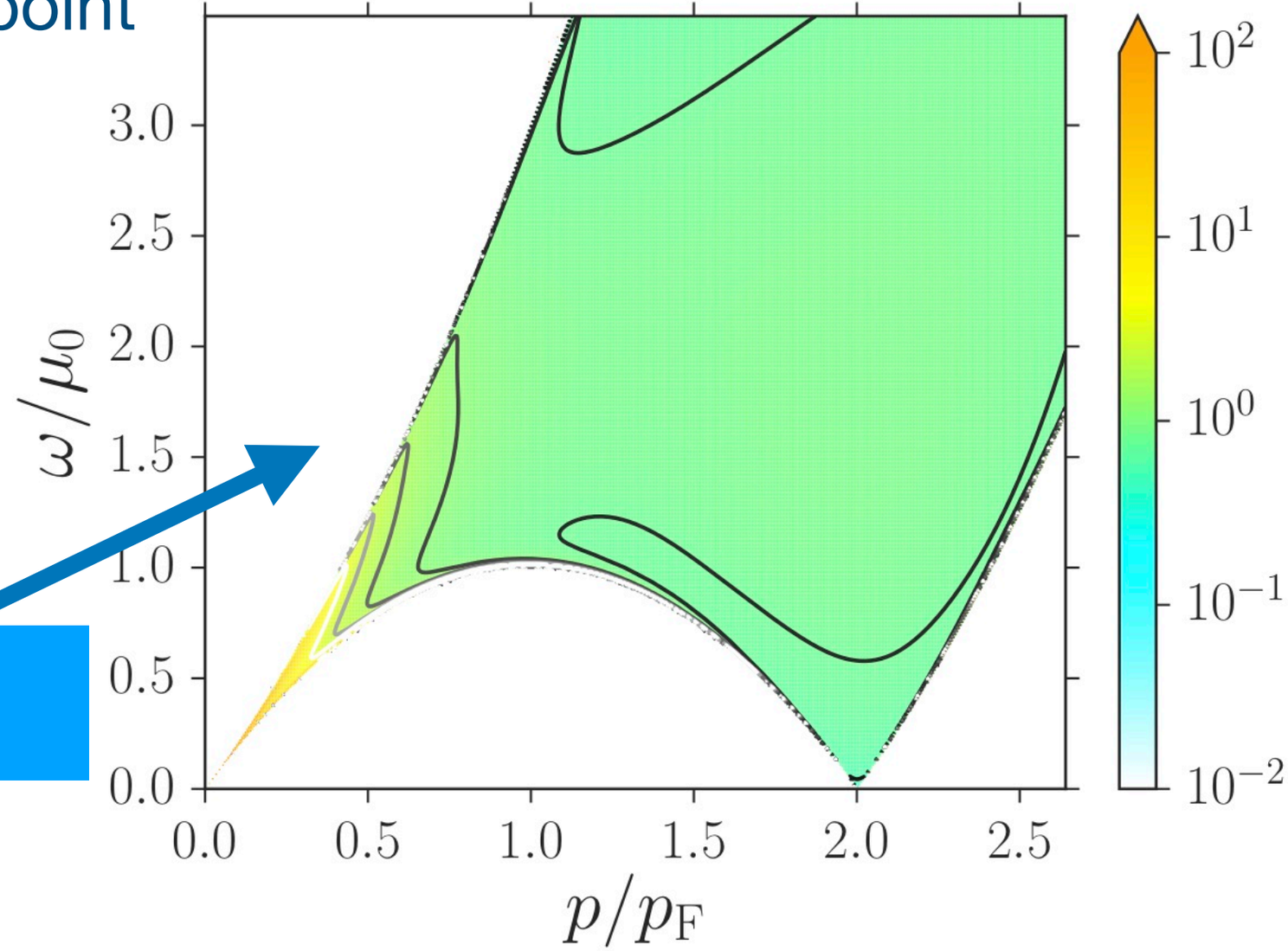
Mahan (X-ray edge) singularity

Nozieres, De Dominicis, PR178 (1969); Mahan (1981)

FRG-DFT result of $\rho_{\mathrm{d}}(\omega, p)$

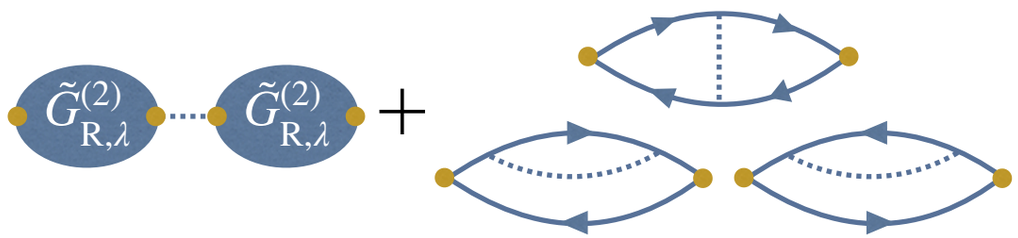
TY, Yoshida, Kunihiro, PTEP (2019)

At saturation point

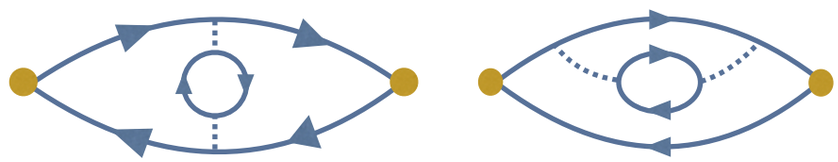


No multipair contribution

$$\partial_\lambda \tilde{G}^{(2)}_{\mathrm{R},\lambda}(\omega, p) =$$

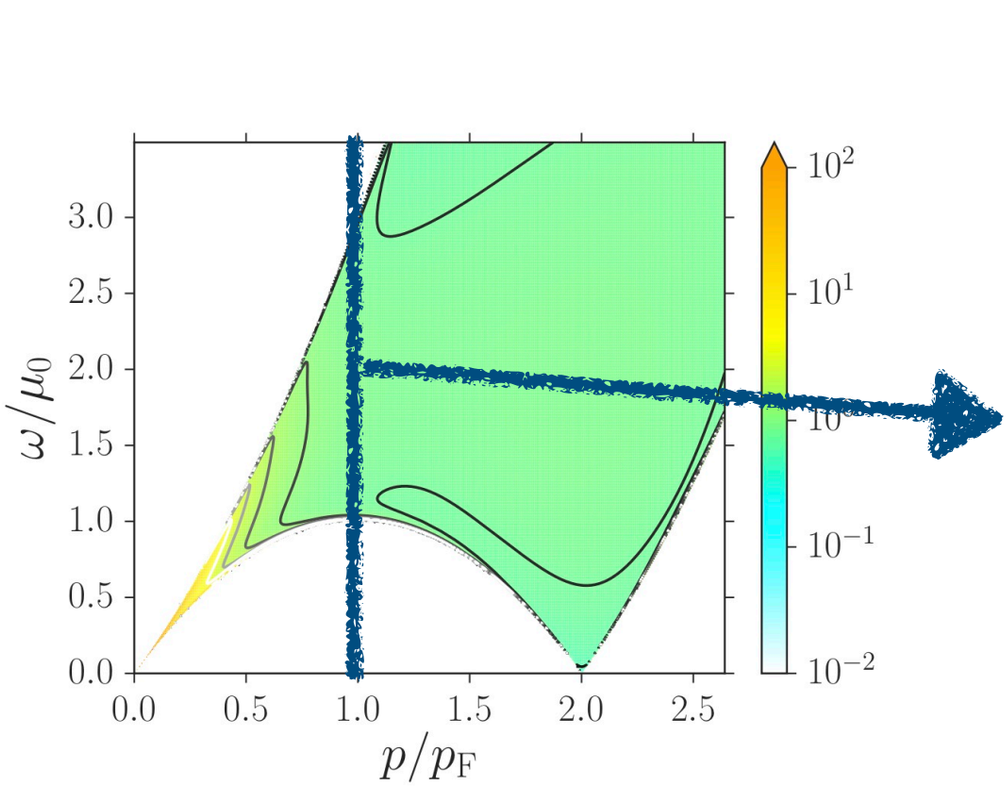


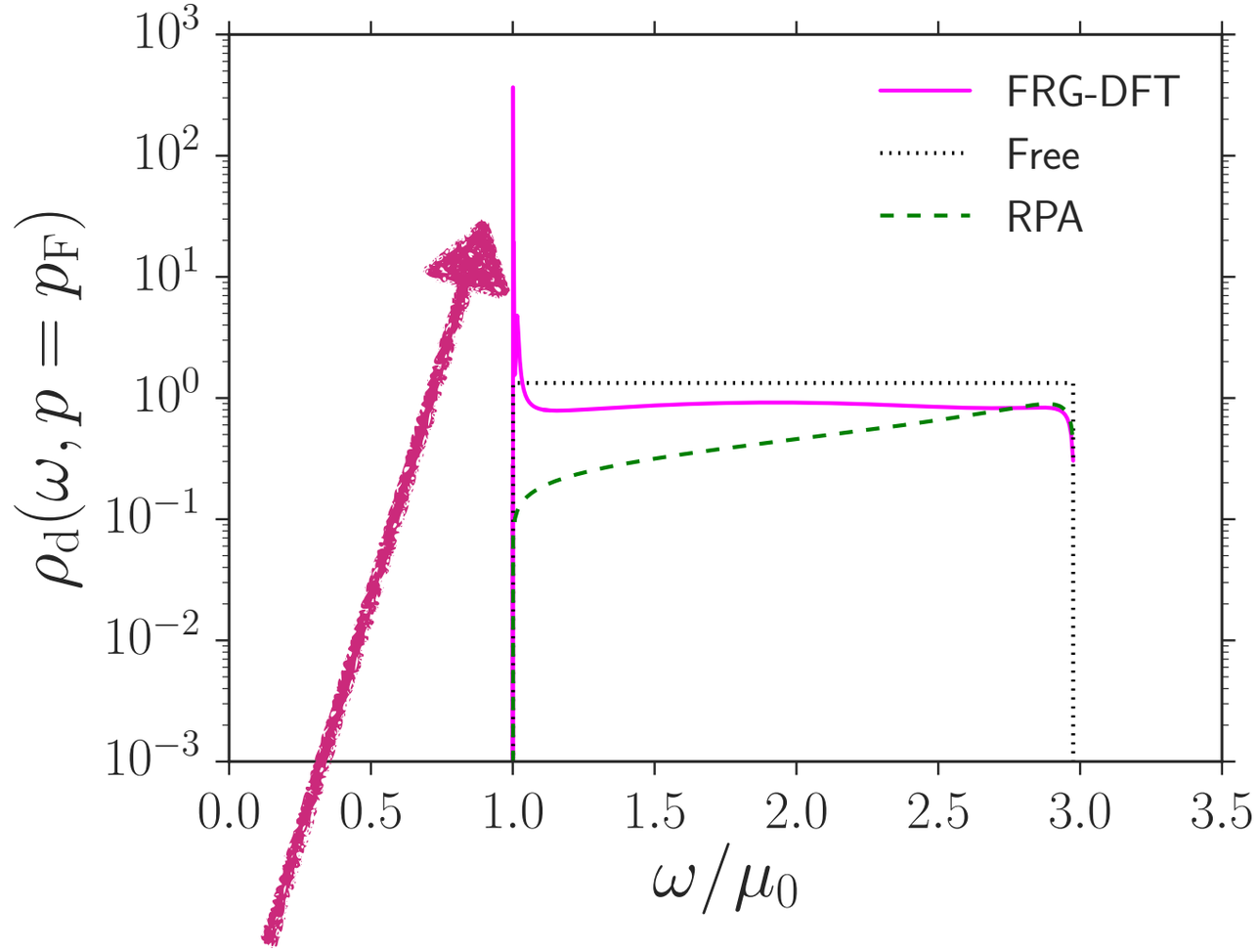
No multi-pair diagrams



$\rho_{\mathrm{d}}(\omega, p)$ at fixed momentum

TY, Yoshida, Kunihiro, PTEP (2019)

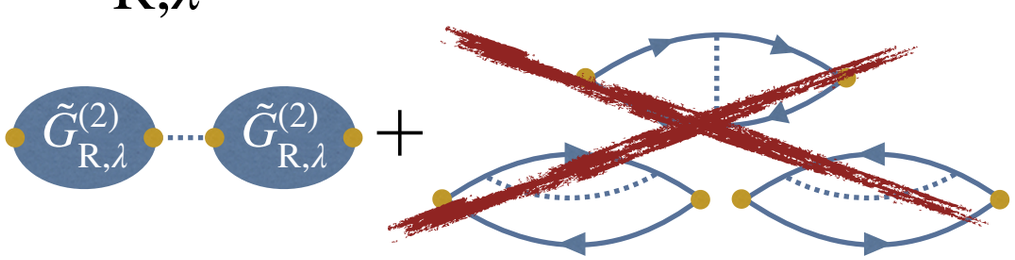




Reproduced in FRG-DFT!

$$\partial_\lambda \tilde{G}^{(2)}_{\mathrm{R},\lambda}(\omega, p) =$$

RPA



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Construction of EDF for electrons

$$E[\rho] = T_{\text{kin}}[\rho] + E_{\text{Hartree}}[\rho] + E_{\text{xc}}[\rho] + \int dx \rho(x) V(x)$$

Zoo of $E_{\text{xc}}[\rho]$

Many empirical EDFs!

Figure from Burke, J. Chem. Phys. (2012)

Local density approximation

When the gradient $\nabla\rho(\mathbf{x})$ is small,

$$E_{\text{xc}}[\rho] \approx \int d\mathbf{x} \epsilon_{\text{xc}}\left(\rho(\mathbf{x})\right)\rho(\mathbf{x})$$

$\epsilon_{\text{xc}}(\rho)$: exchange-correlation energy per particle of **homogeneous gas**

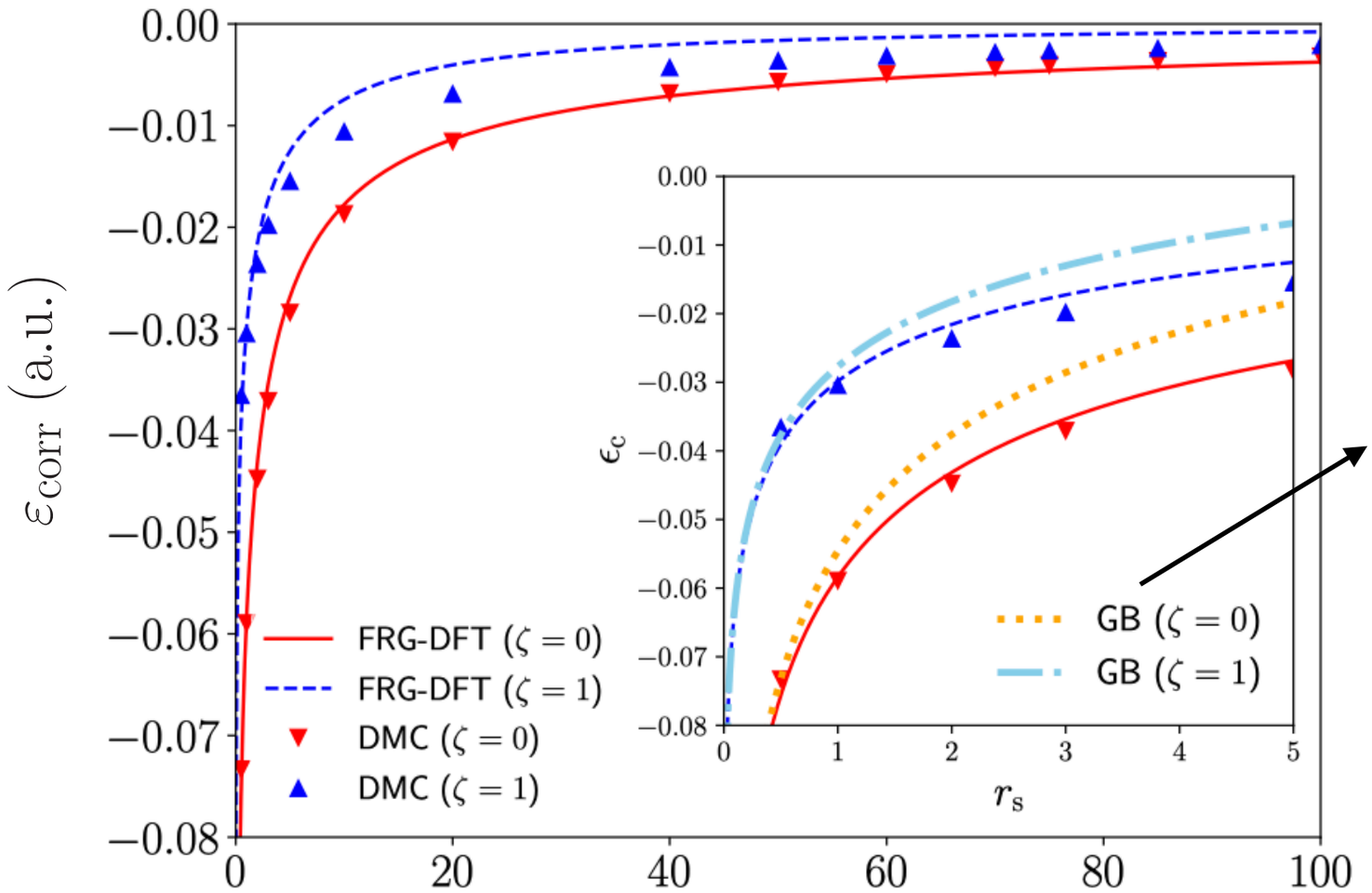
Mathematical proof: Lewin, Lieb, Seiringer, Pure and Applied Analysis 2 (2020), …

Homogeneous electron gas

Coulomb interaction: $U_\lambda(r) = \lambda/r$ $\quad \epsilon_{\rm xc}(\rho) = \epsilon_{\rm x}(\rho) + \epsilon_{\rm corr}(\rho)$ $\quad \epsilon_{\rm x}(\rho) = -\frac{3}{4\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_{\rm s}}$

Correlation energy in spin polarized ($\zeta = 0$) and unpolarized ($\zeta = 1$) cases

TY, Naito, PRResearch (2021)
TY, Naito, PRB (2022)



Wigner-Seitz radius $r_{\rm s}$ (a.u.)

Gell-Mann-Bruckner approximation
(Exact at $r_{\rm s} \to 0$)

$r_{\rm s} = \left(3\rho/4\pi\right)^{1/3}$

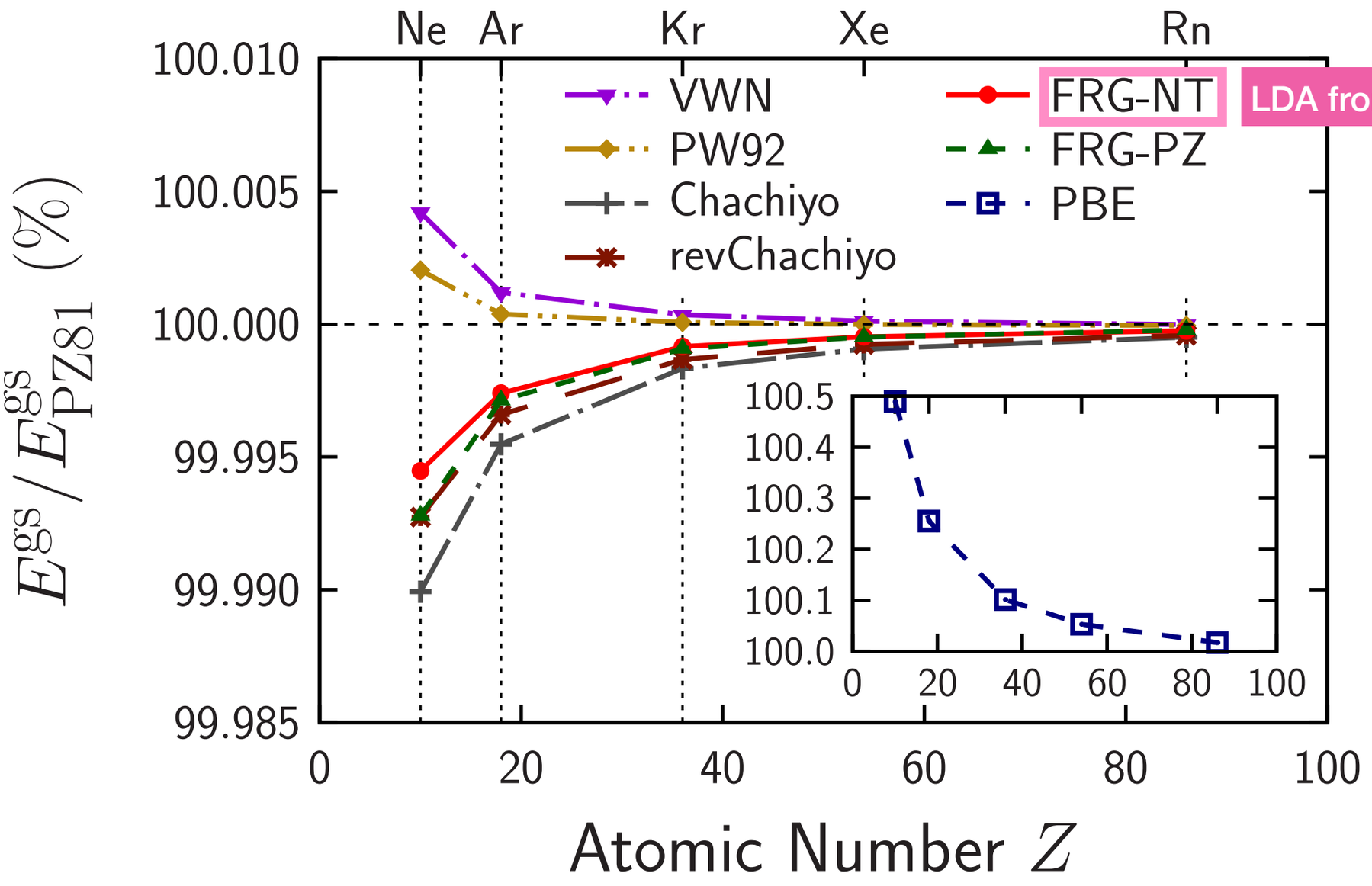
FRG-DFT results agree with Monte-Carlo (MC) results without any empirical parameter!
FRG-DFT gives many data points than MC! ⇒ LDA functional without fitting

Kohn-Sham calc. for noble gas atoms

TY, Naito, PRResearch (2021)

Comparison to other conventional functionals

VWN, PW92 (LDA obtained by fitting of MC data)
PBE (generalized gradient approximation)



FRG shows comparable results to other conventional LDAs despite **no empirical parameter.**

The key to improve the accuracy is the **gradient effects.**

Contents

- Basic idea of FRG aided DFT
  - EDF as effective action
  - Evolution equation for EDF
- Case studies
  - Low dim. models
  - Electrons
  - Classical liquids
- Towards superfulid systems

EDF for superfluid

In principle, the ground-state number density ρ is enough to determine the properties of the system **even if the ground state is degenerate** (HK theorem)

In other words, the order parameters (pairing density, energy gap) are functionals of ρ.

😣 **BUT the concrete forms are difficult to obtain.**

Practical way: Extension of EDF

Oliveira, Gross, Kohn, PRL (1988)
Dobaczewski, Flocard, Treiner, NPA (1984)

$$E[\rho] \xrightarrow{\text{Extension}} E[\rho, \kappa, \kappa^*]$$

EDF

pairing density

How to treat this EDF with FRG-DFT?

TY, Kasuya, Yoshida, Kunihiro, PTEP (2021)

***Not only local pairings $\langle\psi(x)\psi(x)\rangle$,**
but also non-local pairings $\langle\psi(x)\psi(x')\rangle$ are discussed.

FRG-DFT for superfluid systems

Effective action

For simplicity, coordinates and internal degrees of freedom are abbreviated (see [TY+, PTEP (2021)] for explicit forms with non-local parings)

$$Z_\lambda\left[\overrightarrow{J}\right] = \int D\psi D\overline{\psi} \exp\left(-S_\lambda[\psi,\overline{\psi}] + \int J_\rho \cdot \overline{\psi}\psi + \int J_\kappa \cdot \psi\psi + \int J_{\kappa^*} \cdot \overline{\psi}\overline{\psi}\right)$$

$$\overrightarrow{J} = (J_\rho, J_\kappa, J_{\kappa^*})$$

$$\Gamma_\lambda[\overrightarrow{\rho}] = \sup_{\overrightarrow{J}}\left(\int \overrightarrow{J}\cdot\overrightarrow{\rho} - \ln Z_\lambda\left[\overrightarrow{J}\right]\right)$$

$$\overrightarrow{\rho} = (\rho, \kappa, \kappa^*)$$

Flow eq.

$$\partial_\lambda\Gamma_\lambda[\overrightarrow{\rho}] = \frac{1}{2}\int dx dx' d\tau \partial_\lambda U_\lambda(x-x')\left(\rho(\tau,x)\rho(\tau,x') + \left(\frac{\delta^2\Gamma_\lambda[\overrightarrow{\rho}]}{\delta\overrightarrow{\rho}\delta\overrightarrow{\rho}}\right)^{-1}_{\rho\rho}(\tau,x,\tau,x') - \rho(\tau,x')\delta(x-x')\right)$$

Hartree-Fock-Bogoliubov (HFB) theory, quasi-RPA (QRPA)

$$\partial_\lambda \Gamma_\lambda[\overrightarrow{\rho}] = \frac{1}{2}\int dx dx' d\tau \partial_\lambda U_\lambda(x-x')\left(\rho(\tau,x)\rho(\tau,x') + \left(\frac{\delta^2\Gamma_\lambda[\overrightarrow{\rho}]}{\delta\overrightarrow{\rho}\delta\overrightarrow{\rho}}\right)^{-1}_{\rho\rho}(\tau,x,\tau,x') - \rho(\tau,x')\delta(x-x')\right)$$

density correlator

Wick's theorem

$$\langle\overline{\psi}_x\psi_x\overline{\psi}_{x'}\psi_{x'}\rangle - \langle\overline{\psi}_x\psi_x\rangle\langle\overline{\psi}_{x'}\psi_{x'}\rangle - \rho_x\delta(x-x') = \kappa(x,x')\kappa^*(x,x') + \langle\overline{\psi}_x\psi_{x'}\rangle\langle\psi_x\overline{\psi}_{x'}\rangle + O(\lambda)$$

Pairing — Exchange — Correlation

HFB theory

$$\left(\frac{\delta^2\Gamma_\lambda[\overrightarrow{\rho}]}{\delta\overrightarrow{\rho}\delta\overrightarrow{\rho}}\right)^{-1}_{\rho\rho} \approx \left(\frac{\delta^2\Gamma_{\lambda=0}[\overrightarrow{\rho}]}{\delta\overrightarrow{\rho}\delta\overrightarrow{\rho}}\right)^{-1}_{\rho\rho}$$

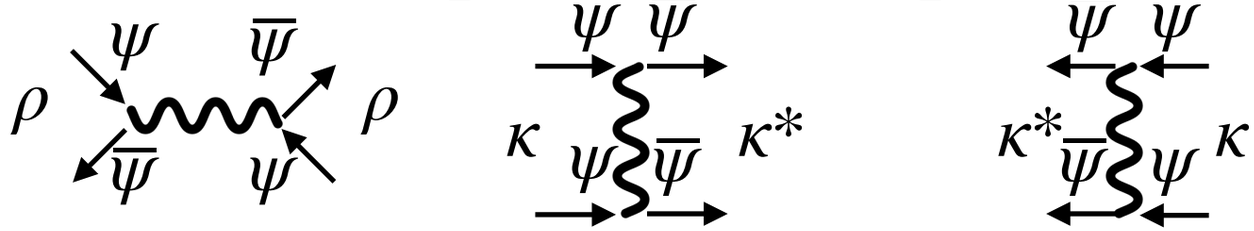
$$E_{\rm gs} = \frac{1}{2}\int dx dx' U(x-x')\left(\rho_{\rm gs}(x)\rho_{\rm gs}(x') + |\kappa_{\rm gs}(x,x')|^2 + \langle\overline{\psi}_x\psi_{x'}\rangle\langle\psi_x\overline{\psi}_{x'}\rangle\right)$$

QRPA — **Ignorance of exchange-correlation in the second derivative of flow eq.**

Inverse two-point correlator between ρ, $\kappa^{(*)}$

ph term — **pp term** — **hh term** — **Equivalent to Dyson eq. for QRPA**

$$\partial_\lambda G^{-1}_{\lambda,ij} = \delta_{i\rho}\delta_{j\rho}\partial_\lambda U_\lambda(x-x') + \frac{1}{2}\delta_{i\kappa}\delta_{j\kappa^*}\partial_\lambda U_\lambda(x-x') + \frac{1}{2}\delta_{i\kappa^*}\delta_{j\kappa}\partial_\lambda U_\lambda(x-x') + (\text{exchange, correlation})$$



Beyond QRPA: Inclusion of exchange-correlation term (on-going)

Summary

- **How to construct EDF?**
- **Functional renormalization group**

  EDF ⇔ effective action

  Evolution of two-body interaction
- **Case studies**

  Low-dim. models, excited states, electrons, classical liquids

  Extension to superfuld systems

Outlook

Inclusion of gradient (average density approximation? machine learning?)

Description of self-bound systems

Numerical study of superfluid systems