Density-based functional renormalization group for quantum many-body problems

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Collaborators

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TY, Yoshida, Kunihiro, PRC (2019)

TY, Yoshida, Kunihiro, PTEP (2019)

TY, Naito, PRB (2019)

TY, Naito, PRResearch (2021)

TY, Kasuya, Yoshida, Kunihiro PTEP (2021)

TY, Haruyama, Sugino, PRE (2021)

TY, Naito, PRB (2022)

Contents

- Density functional theory (DFT)
  - Introduction
  - Effective-action formalism for DFT
- Functional evolution equation
- Demonstration: electron system

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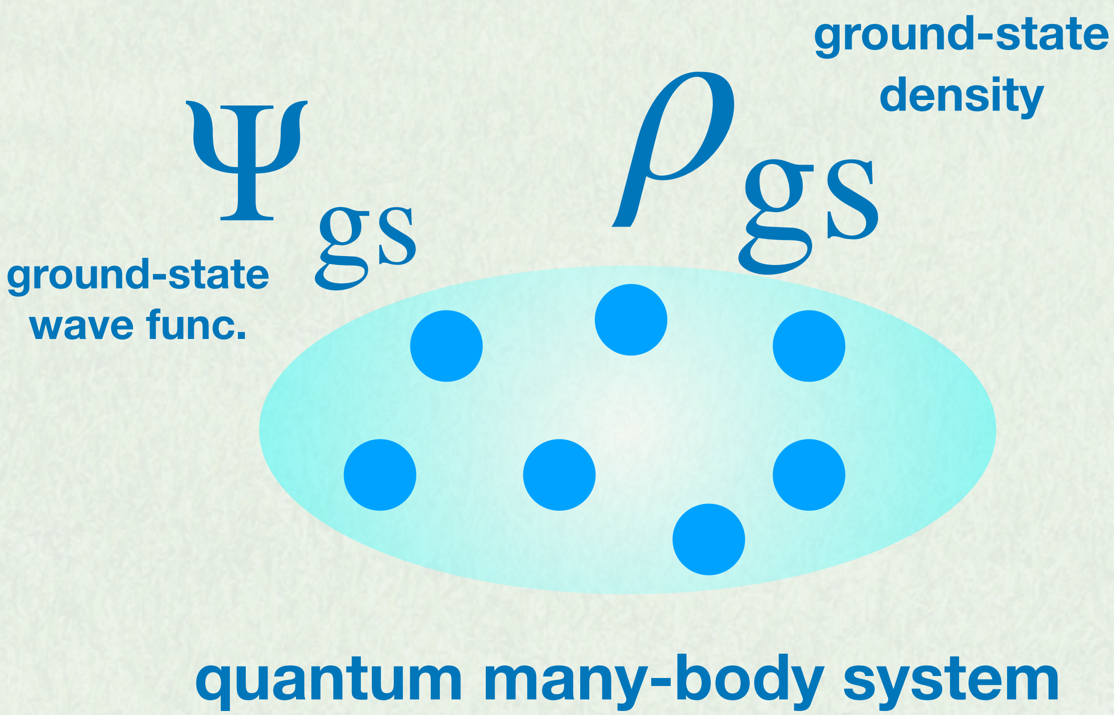
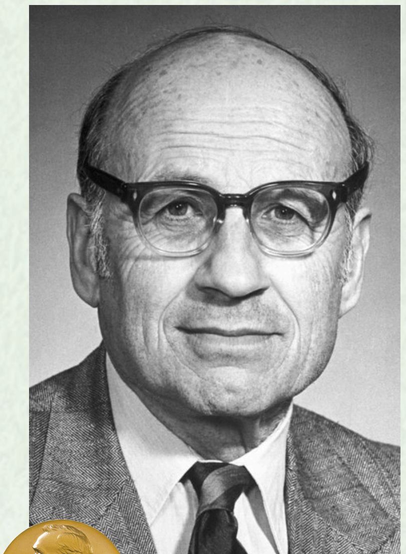
Density functional theory (DFT)



P. Hohenberg

W. Kohn



Chem. 1998

L. J. Sham

DFT: Exact many body theory based on ρ_{gs}

instead of Ψ_{gs}.

Why possible?

Hohenberg-Kohn theorem

Suppose a non-relativistic system whose Hamiltonian is given by $\hat{H} = \hat{T} + \hat{U} + \hat{V}$

kinetic interacting external potential

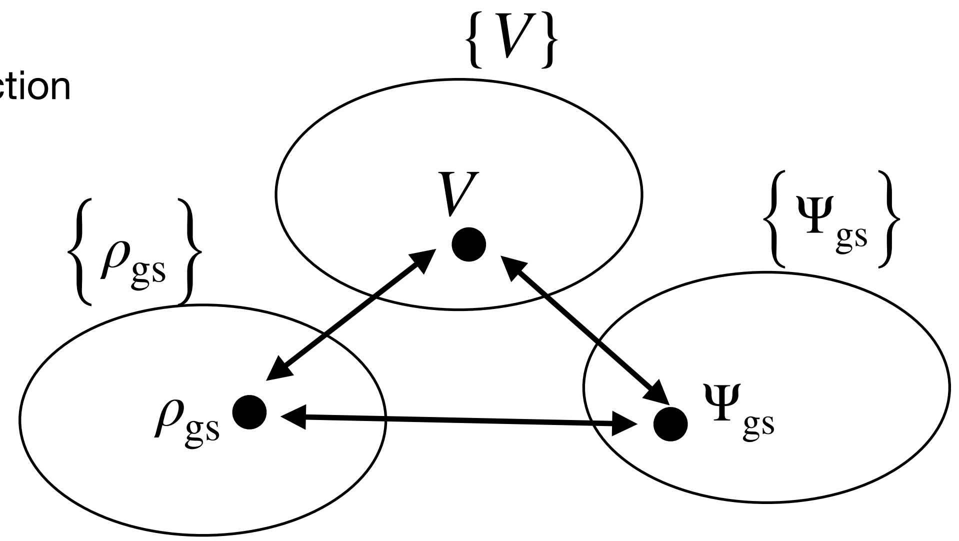
Hohenberg, Kohn, PR (1964)

$\hat{V} = \int d\boldsymbol{x} \hat{\rho}(\boldsymbol{x}) V(\boldsymbol{x})$

Statements (non-deregerate case)

1. Equivalence of density and wave func.

proved by contradiction



There exists 1-to-1 mapping b/w ρ_{gs}, Ψ_{gs}, V

➡ **Ψ_{gs} is a functional of ρ_{gs}: $\Psi_{gs} = \Psi_{gs}[\rho_{gs}]$**

2. Variational principle

There exists energy density functional (EDF), whose minimum point gives ρ_{gs}

EDF has the following form: $E[\rho] = \left\langle \Psi_{gs}[\rho] \middle| \hat{H} \middle| \Psi_{gs}[\rho] \right\rangle = F[\rho] + \int d\mathbf{x} \rho(\mathbf{x}) V(\mathbf{x})$

"Universal" part
(V-independent, dependent on particle mass, interaction)

Hohenberg-Kohn theorem

Suppose a non-relativistic system whose Hamiltonian is given by $\hat{H} = \hat{T} + \hat{U} + \hat{V}$

kinetic, interacting, external potential

Hohenberg, Kohn, PR (1964)

$\hat{V} = \int d\boldsymbol{x} \hat{\rho}(\boldsymbol{x}) V(\boldsymbol{x})$

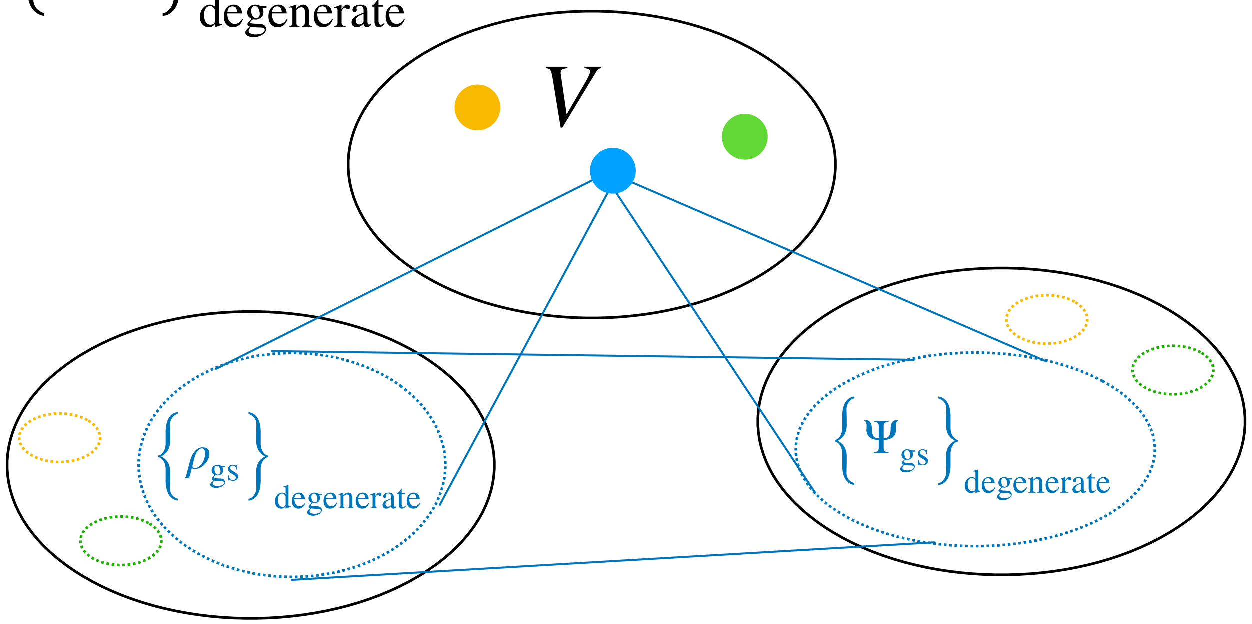
Degenerate case

- **1-to-1 mapping b/w sets:** $\left\{\rho_{\mathrm{gs}}\right\}_{\mathrm{degenerate}}, \left\{\Psi_{\mathrm{gs}}\right\}_{\mathrm{degenerate}}, V$

- **Well-defined EDF exists**

$$E[\rho] = \left\langle \Psi_{\mathrm{gs}}[\rho] \middle| \hat{H} \middle| \Psi_{\mathrm{gs}}[\rho] \right\rangle$$

↑ One of the degenerate wave functions



- Spontaneous symmetry breaking is in principle described, but calculation of the order parameter as a functional of ρ, $O[\rho] = \langle \Psi_{\mathrm{gs}}[\rho] | \hat{O} | \Psi_{\mathrm{gs}}[\rho] \rangle$ is usually infeasible in practice.
  - For practical analysis, additional density is introduced.

    e.g.) $E[\rho_\uparrow, \rho_\downarrow]$ to describe magnetism

Application to numerical analysis

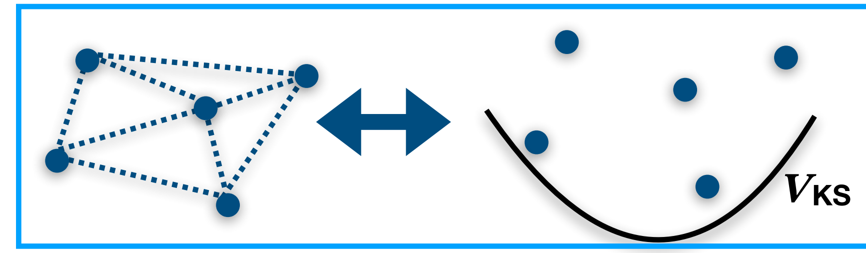
Kohn-Sham scheme

Kohn, Sham, PR (1965)

$$E[\rho] = T[\rho] + \Delta E[\rho]$$

free kinetic   residual

Var. eq. $$\frac{\delta T[\rho]}{\delta \rho(\boldsymbol{x})} + \frac{\delta \Delta E[\rho]}{\delta \rho(\boldsymbol{x})} = \mu$$



That for non-interacting system with ext. field $V_{\mathrm{KS}} = \delta \Delta E / \delta \rho$

Variational problem
= finding self-consistent solution for the non-int. Schrodinger eq.

$$\left(-\frac{\nabla^2}{2m} + V_{\mathrm{KS}}[\rho_{\mathrm{gs}}](x)\right)\phi_i(x) = \epsilon_i \phi_i(x) \text{ with } \rho_{\mathrm{gs}}(x) = \sum_{i=1}^{N} |\phi_i(x)|^2$$

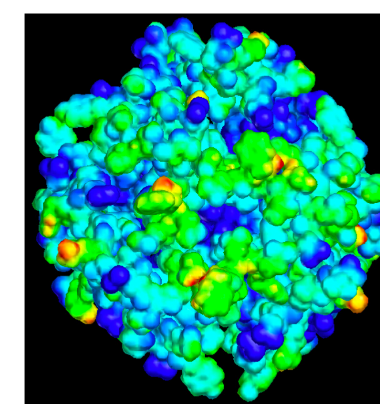
Computationally efficient!
$N \lesssim 10^4$ **(or $10^{5\sim6}$?)**

Application

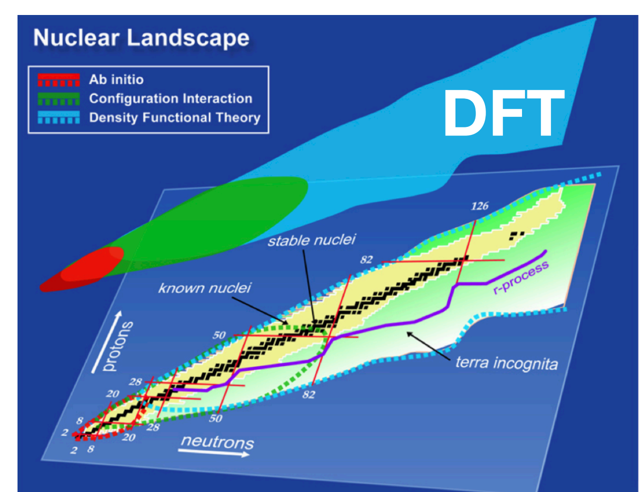
- **Electrons (crystal, molecule)**
- **Nucleus**
  - No external field. But DFT is a tool to describe nucleus with various particle number in a unified manner.

etc..

Proteins
($10^{3\sim4}$ atoms, electrons)



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



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

Energy density functional (EDF)

How can we obtain $E[\rho]$? **Most important but still open problem…**

Electron EDF

Microscopic int.: Coulomb

Jacob's ladder

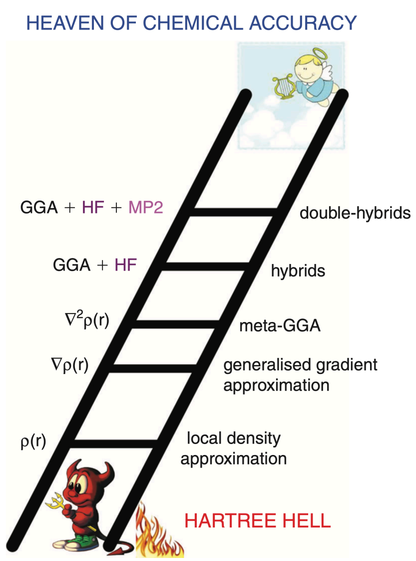


Figure from Goerigk, Mehta, Aust. J. Chem. (2019)

Many EDFs

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

Nuclear EDF

Microscopic int.: Nuclear force + Coulomb

Ambiguity in nuclear force

But determination of nuclear force is in progress: Scattering exp., lattice QCD, chiral EFT, …

So far, phenomenological EDFs obtained from fitting of experimental data have been usually used.

Construction of EDF

- Data-driven approach
  - Fitting data from Monte Carlo, few-body calc., experiments,…
- Many-body perturbation

…

Development of systematic bottom-up approach is still required

in order for…

- further improvement of accuracy
- making the relation to microscopic int. clear

DFT in effective action formalism

Density: composite field $\rho_\psi(\boldsymbol{x}) = \psi^*(\boldsymbol{x})\psi(\boldsymbol{x})$

Imaginary-time partition function for density correlation $\rho_\psi(\tau, \boldsymbol{x}) = \psi^*(\tau + 0, \boldsymbol{x})\psi(\tau, \boldsymbol{x})$

$$Z[J] = \int \mathscr{D}\psi\mathscr{D}\psi^* e^{-S[\psi,\psi^*]+\int_0^\beta d\tau \int d\boldsymbol{x} J(\tau,\boldsymbol{x})\rho_\psi(\tau,\boldsymbol{x})}$$

To extract the g.s. property, we replace $\rho(\tau, \boldsymbol{x}) \to \rho(\boldsymbol{x})$ **and take** $\beta \to \infty$ **at the end.**

Effective action for ρ (two-particle-point-irreducible effective action)

$$\Gamma[\rho] = \sup_J \left(\int_0^\beta d\tau \int d\boldsymbol{x} J(\tau, \boldsymbol{x})\rho(\tau, \boldsymbol{x}) - \ln Z[J] \right)$$

EDF

Fukuda, Kotani, Suzuki, Yokojima, PTP92 (1994)
Valiev, Fernando, arXiv:9702247 (1997)

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

for $\rho(\tau, \boldsymbol{x}) = \rho(\boldsymbol{x})$

$\because$ **Variational principle = quantum EOM** $\Gamma^{(1)}[\rho_{\mathrm{gs}}] = \mu$

$\Gamma[\rho_{\mathrm{gs}}] = \beta F_{\mathrm{Helm}}$

Approaches to DFT based on effective-action formalism

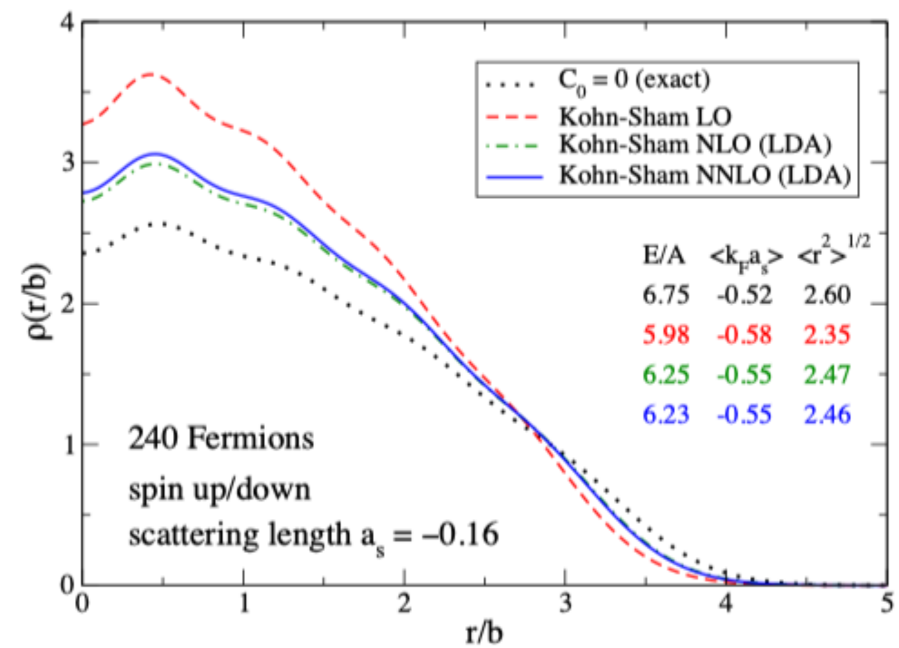
c.f.) Reviews by R.J. Furnstahl+

"EFT for DFT", Furnstahl (2007)

"Toward ab initio density functional theory for nuclei", Drut, Furnstahl, Platter (2009)

"Turning the nuclear energy density functional method into a proper effective field theory: reflections", Furnstahl (2019)

- **Expansion w.r.t. small parameter**
  - Power counting with fixing ρ is obtained.
  - e.g., Fermi-momentum expansion (dilute system)



Density profile of a dilute system of fermions in a trap

Puglia, Bhattacharyya, Furnstahl, NPA (2003)

- **FRG-like evolution eq.** This talk

Polonyi, Sailer (2002), Schwenk, Polonyi (2004)

Contents

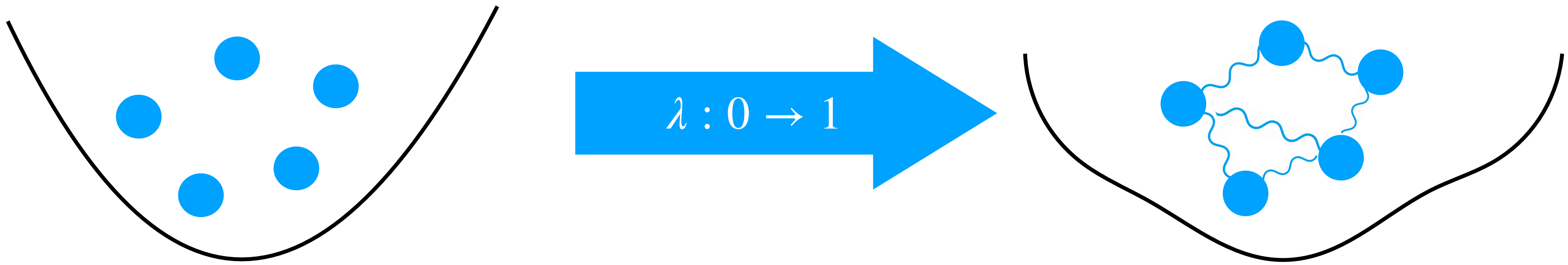
Adiabatic-connection fluctuation-dissipation theorem

Levy, Perdew (1985), Levy (1991), Gorling, Levy (1992)

Switching on of two-body int.

$$\hat{H} = \hat{T} + \lambda\hat{U} + \hat{V}_\lambda$$

Ext. field to fix ρ



$$E_{\rm xc}[\rho] = \frac{1}{2}\int_0^1 d\lambda \int d\boldsymbol{x} \int d\boldsymbol{x}' U(\boldsymbol{x}-\boldsymbol{x}')\left[S_\lambda(\boldsymbol{x},\boldsymbol{x}') - \rho(\boldsymbol{x})\delta(\boldsymbol{x}-\boldsymbol{x}')\right]$$

$$E[\rho] = T[\rho] + E_{\rm Hartree}[\rho] + E_{\rm xc}[\rho]$$

Density correlation $S_\lambda(\boldsymbol{x},\boldsymbol{x}') = \langle\hat{\rho}(\boldsymbol{x})\hat{\rho}(\boldsymbol{x}')\rangle_\lambda - \rho(\boldsymbol{x})\rho(\boldsymbol{x}')$
is needed as an input.

Evolution equation for effective action

Polonyi, Sailer (2002), Schwenk, Polonyi (2004)

$$\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{2}\int_0^\beta d\tau \int d\boldsymbol{x} \int_0^\beta d\tau' \int d\boldsymbol{x}' U(\boldsymbol{x}-\boldsymbol{x}')\delta(\tau-\tau'+0)$$
$$\times \left[\rho(\tau,\boldsymbol{x})\rho(\tau,'\boldsymbol{x}') + \left(\frac{\delta^2\Gamma_\lambda}{\delta\rho\delta\rho}\right)^{-1}[\rho](\tau,\boldsymbol{x},\tau',\boldsymbol{x}') - \rho(\tau,\boldsymbol{x})\delta(\boldsymbol{x}-\boldsymbol{x}') \right]$$

- **Closed equation for $\Gamma_\lambda[\rho]$**
  - Input from other calculation is not needed.
  - This in principle gives all the correlation functions.
- **Calculation techniques in FRG are possibly useful.**
  - Vertex expansion (VE), local potential approximation (LPA)
  - Real-time response function
    - Analytic continuation is easy.

e.g.) O(4), quark-meson model

Kamikado, Strodthoff, von Smekal, Wambach (2020)
Tripolt, Strodthoff, von Smekal, Wambach (2014)
TY, Kunihiro, Morita (2016), (2017)…

Studies of FRG-aided DFT

- **Classical & quantum anharmonic oscillators**

  Kemler, Braun, JPG (2013) **VE**

  Liang, Niu, Hatsuda, PLB (2018) **VE**

- **One-dim nuclear system**

  Kemler, Pospiech, Braun, JPG (2017) **VE**

  TY, Yoshida, Kunihiro, PRC (2019) **VE**

  TY, Yoshida, Kunihiro, PTEP (2019) **VE** — **Excited states (real-time correlation function)**

- **Electron systems**

  TY, Naito, PRB (2019) **VE**

  TY, Naito, PRResearch (2021) **VE**

  TY, Naito, PRB (2022) **VE**

- **Classical liquids**

  Lue, AIChE (2015) **LPA**

  TY, Haruyama, Sugino, PRE (2021) **VE**

- **Superfluid system**

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

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w/ T. Naito

TY, Naito, PRB (2019)
TY, Naito, PRResearch (2021)
TY, Naito, PRB (2022)

Local density approximation (LDA)

$$E[\rho] = F[\rho] + \int d\boldsymbol{x}\rho(\boldsymbol{x})V(\boldsymbol{x})$$

Hartree

$$F[\rho] = T[\rho] + \frac{1}{2}\int d\boldsymbol{x}\int d\boldsymbol{x}'U(\boldsymbol{x}-\boldsymbol{x}')\rho(\boldsymbol{x})\rho(\boldsymbol{x}') + E_{\mathrm{xc}}[\rho]$$

exchange-correlation (unknown)

LDA **Simple approx. for EDF**

small gradient limit $\nabla\rho(\boldsymbol{x})/\rho(\boldsymbol{x})^{4/3} \ll 1$

Proof: Lewin, Lieb, Seiringer (2020)

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

xc energy per particle of homogeneous gas

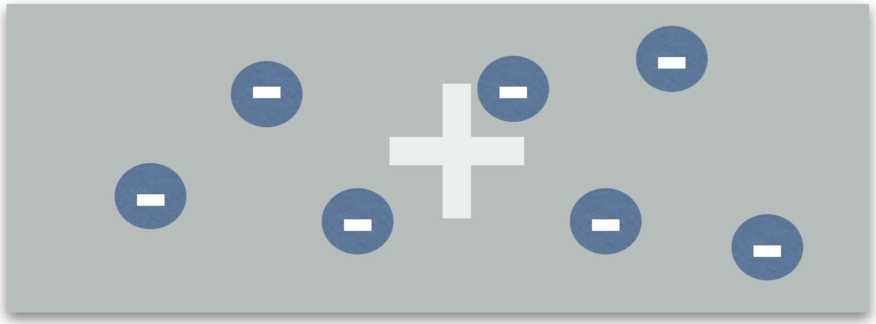
LSDA (local spin density approx.)

$$E_{\mathrm{xc}}[\rho_\uparrow,\rho_\downarrow] \approx \int d\boldsymbol{x}\epsilon_{\mathrm{xc}}\left(\rho_\uparrow(\boldsymbol{x}),\rho_\downarrow(\boldsymbol{x})\right)\sum_s \rho_s(\boldsymbol{x})$$

Let us derive E_{xc} with VE

Jellium model

Electron gas in homogeneous static background positive ion



$$S_\lambda[\psi, \psi^\dagger] = \int d\tau \int d\boldsymbol{x} \psi^\dagger(\tau+0, \boldsymbol{x}) \left(\partial_\tau - \frac{\Delta}{2} \right) \psi(\tau, \boldsymbol{x})$$
$$+ \frac{\lambda}{2} \int d\tau \int d\boldsymbol{x} \int d\boldsymbol{x}' U(\boldsymbol{x} - \boldsymbol{x}') \left(\rho_\psi(\tau, \boldsymbol{x}) - n \right) \left(\rho_\psi(\tau, \boldsymbol{x}') - n \right)$$

in Hartree atomic unit $a_{\mathrm{Bohr}} = m_{\mathrm{e}} = 1$

Electron field: $\psi = {}^{\mathrm{t}}(\psi_\uparrow, \psi_\downarrow)$

Coulomb force: $U(\boldsymbol{x} - \boldsymbol{x}') = |\boldsymbol{x} - \boldsymbol{x}'|^{-1}$

Electron density: $\rho_\psi(\tau, \boldsymbol{x}) = \psi^\dagger(\tau + 0, \boldsymbol{x}) \psi(\tau, \boldsymbol{x})$

Background-ion density: n

Vertex expansion

Expansion around $\rho_{\uparrow,\downarrow} = \rho_{gs\uparrow,\downarrow}$ of interest

$$\Gamma_\lambda[\rho_{\uparrow,\downarrow}] = \sum_{n=0}^{\infty} \frac{1}{n!} \int\!\!\!\!\!\!\sum_{X_1} \cdots \int\!\!\!\!\!\!\sum_{X_n} \Gamma_\lambda^{(n)}[\rho_{gs_{\uparrow,\downarrow}}](X_1 \ldots, X_n) \prod_{i=1}^{n} \left(\rho(X_i) - \rho_{gs,s_i} \right) \qquad X = (\tau, \boldsymbol{x}, s)$$

0th Energy	$\partial_\lambda \Gamma_\lambda[\rho_{gs,\uparrow\downarrow}] \left(= \partial_\lambda \beta E_{gs,\lambda} \right) = \mathrm{Flow}_\lambda^{(0)} \left[\rho_{gs,\uparrow\downarrow}, \Gamma_\lambda^{(2)}[\rho_{gs,\uparrow\downarrow}] \right]$
1st Chemical potential	$\partial_\lambda \Gamma_\lambda^{(1)}[\rho_{gs,\uparrow\downarrow}](X) \left(= \partial_\lambda \mu_\lambda \right) = \mathrm{Flow}_\lambda^{(1)} \left[X; \rho_{gs,\uparrow\downarrow}, \Gamma_\lambda^{(2)}[\rho_{gs,\uparrow\downarrow}], \Gamma_\lambda^{(3)}[\rho_{gs,\uparrow\downarrow}] \right]$
2nd Density correlation	$\partial_\lambda \Gamma_\lambda^{(2)}[\rho_{gs,\uparrow\downarrow}](X_1, X_2) \left(= \partial_\lambda G_\lambda^{(2)-1}(X_1, X_2) \right) = \mathrm{Flow}_\lambda^{(2)} \left[X_1, X_2; \rho_{gs,\uparrow\downarrow}, \Gamma_\lambda^{(2)}[\rho_{gs,\uparrow\downarrow}], \Gamma_\lambda^{(3)}[\rho_{gs,\uparrow\downarrow}], \Gamma_\lambda^{(4)}[\rho_{gs,\uparrow\downarrow}] \right]$
⋮	

Approximation for higher-order terms is needed

Flow equations for density correlations

Density correlation $$G_\lambda^{(n)}(X_1,\cdots,X_n)=\frac{\delta^n}{\delta J(X_1)\cdots\delta J(X_n)}\ln Z_\lambda[J]$$

Momentum space (homogeneous) $$(2\pi)^4\delta(P_1+\cdots+P_n)\tilde{G}^{(n)}_{\lambda,s_1,\ldots,s_n}(P_1,\cdots,P_{n-1})=\mathrm{F.T.}\left(G_\lambda^{(n)}\right)$$

$$P=(\omega,\boldsymbol{p})$$

Since $\tilde{G}_0^{(n)}$ is easier to calculate than $\Gamma_0^{(n)}$, we rewrite the flow eq. in terms of $\tilde{G}_\lambda^{(n)}$.

Flow eqs. (after spin summation)

$$\tilde{G}_\lambda^{(n)}=\sum_{s_1,\cdots,s_n}\tilde{G}^{(n)}_{\lambda,s_1,\ldots,s_n}$$

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

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

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

Truncation

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

$$= C_\lambda(P;\zeta,r_{\mathrm{s}})$$

Spin polarization: $\zeta = \dfrac{\rho_{\mathrm{gs},\uparrow} - \rho_{\mathrm{gs},\downarrow}}{\rho_{\mathrm{gs},\uparrow} + \rho_{\mathrm{gs},\downarrow}}$

Wigner-Seitz radius: $r_{\mathrm{s}} = \left[3/\left[4\pi\left(\rho_{\mathrm{gs},\uparrow} + \rho_{\mathrm{gs},\downarrow}\right)\right]\right]^{1/3}$

From the flow equation for $\tilde{G}^{(3,4)}_\lambda$, one can show

$$C_\lambda(P;\zeta,r_{\mathrm{s}}) = C_0(P;\zeta,r_{\mathrm{s}})\left(1 + \mathcal{O}\left(r_{\mathrm{s}} f(\overline{P},\zeta)\right)\right) \qquad \overline{P} = \left(r_{\mathrm{s}}^2\omega, r_{\mathrm{s}}\boldsymbol{p}\right)$$

We ignore this (high-density expansion)

Analytic solution can be obtained

$$\frac{E_{\mathrm{gs},\lambda=1}}{N} = \frac{E_{\mathrm{gs},\lambda=0}}{N}$$

Kinetic $\dfrac{3}{10r_{\mathrm{s}}^2}\left(\dfrac{9\pi}{4}\right)^{2/3}\dfrac{(1+\zeta)^{5/3}+(1-\zeta)^{5/3}}{2}$

$$+\frac{1}{2n}\int_{\mathbf{p}} \tilde{U}(\mathbf{p})\left(\int_\omega \tilde{G}^{(2)}_0(P) - n\right)$$

Exchange $-\dfrac{3}{4\pi}\left(\dfrac{9\pi}{4r_{\mathrm{s}}}\right)^{1/3}\dfrac{(1+\zeta)^{4/3}+(1-\zeta)^{4/3}}{2}$

$$+\frac{1}{2n}\int_P \left(\ln\left[\cosh\left(\sqrt{\tilde{U}(\mathbf{p})C_0(P)}\right) + \sqrt{\frac{\tilde{U}(\mathbf{p})}{C_0(P)}}\tilde{G}^{(2)}_0(P)\sinh\left(\sqrt{\tilde{U}(\mathbf{p})C_0(P)}\right)\right] - \tilde{U}(\mathbf{p})\tilde{G}^{(2)}_0(P)\right)$$

Correlation E_{corr}/N

Behavior at high density $(r_s \to 0)$

$$\frac{E_{\rm corr}}{N} = \frac{1}{2n}\int_P \left(\ln\left[\cosh\left(\sqrt{\tilde{U}(\mathbf{p})C_0(P)}\right) + \sqrt{\frac{\tilde{U}(\mathbf{p})}{C_0(P)}}\tilde{G}_0^{(2)}(P)\sinh\left(\sqrt{\tilde{U}(\mathbf{p})C_0(P)}\right)\right] - \tilde{U}(\mathbf{p})\tilde{G}_0^{(2)}(P)\right)$$

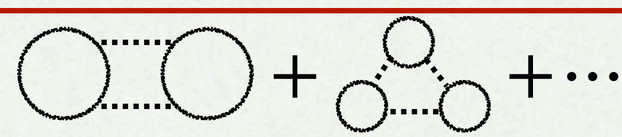
Scaling of C_0 and $\tilde{G}_0^{(2)}$ w.r.t. r_s:

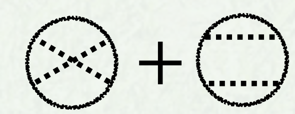
$$C_0(\omega, \mathbf{p}; r_s, \zeta) = C_0(r_s^2\omega, r_s\mathbf{p}; 1, \zeta)$$

$$\tilde{G}_0^{(2)}(\omega, \mathbf{p}; r_s, \zeta) = r_s^{-1}\tilde{G}_0^{(2)}(r_s^2\omega, r_s\mathbf{p}; 1, \zeta)$$

We have

$$\frac{E_{\rm corr}}{N} = \frac{1}{2n}\int_P \left(\ln\left[1 + \tilde{U}(\mathbf{p})\tilde{G}_0^{(2)}(\omega, \mathbf{p})\right] - \tilde{U}(\mathbf{p})\tilde{G}_0^{(2)}(\omega, \mathbf{p})\right) + \frac{1}{4n}\int_P \tilde{U}(\mathbf{p})C_0(\omega, \mathbf{p}) + \mathcal{O}(r_s)$$





RPA **2nd-order ex.**

Gell-Mann-Brueckner (GB) resum.!! Gell-Mann, Brueckner, PR (1957)

- Exact behavior at high density ($r_s \to 0$) given by GB resum. is reproduced.
- Higher-order contribution is resumed with solving flow eq.

→ **Our approximation seems to be good at low and moderate r_s**

Reduction of integrals (e.g. $\zeta = 0$)

$$\frac{E_{\rm corr}}{N} = \frac{1}{2n}\int\frac{d\omega}{2\pi}\int\frac{d^3\mathbf{p}}{(2\pi)^3}\left(\ln\left[\cosh\left(\sqrt{\tilde{U}(\mathbf{p})C_0(P)}\right)+\sqrt{\frac{\tilde{U}(\mathbf{p})}{C_0(P)}}\tilde{G}_0^{(2)}(P)\sinh\left(\sqrt{\tilde{U}(\mathbf{p})C_0(P)}\right)\right]-\tilde{U}(\mathbf{p})\tilde{G}_0^{(2)}(P)\right)$$

quadruple integral

$$C_{\lambda=0}(P) = 2N_{\rm s}\int\frac{d^3\mathbf{p}'}{(2\pi)^3}\int\frac{d^3\mathbf{p}''}{(2\pi)^3}U(\mathbf{p}')\,\theta\left(-\xi(\mathbf{p}'')\right)\left(\theta\left(-\xi(\mathbf{p}+\mathbf{p}'+\mathbf{p}'')\right)-\theta\left(-\xi(\mathbf{p}'+\mathbf{p}'')\right)\right)$$

$$\times\left[\frac{\left(\xi(\mathbf{p}''+\mathbf{p})-\xi(\mathbf{p}'')\right)^2-\omega^2}{\left(\omega^2+\left(\xi(\mathbf{p}''+\mathbf{p})-\xi(\mathbf{p}'')\right)^2\right)^2}-\frac{\left(\xi(\mathbf{p}''+\mathbf{p}+\mathbf{p}')-\xi(\mathbf{p}''+\mathbf{p}')\right)\left(\xi(\mathbf{p}''+\mathbf{p})-\xi(\mathbf{p}'')\right)-\omega^2}{\left(\omega^2+\left(\xi(\mathbf{p}''+\mathbf{p}+\mathbf{p}')-\xi(\mathbf{p}''+\mathbf{p}')\right)^2\right)\left(\omega^2+\left(\xi(\mathbf{p}''+\mathbf{p})-\xi(\mathbf{p}'')\right)^2\right)}\right]$$

$(\xi(\mathbf{p}) = \mathbf{p}^2/2 - \mu_0)$

sextuple integral

$\tilde{G}_0^{(2)}(P)$ is obtained analytically

Reduction of integrals (e.g. $\zeta = 0$)

$$\frac{E_{\rm corr}}{N} = \frac{1}{2n}\int \frac{d\omega}{2\pi}\int \frac{d^3\mathbf{p}}{(2\pi)^3}\left(\ln\left[\cosh\left(\sqrt{\tilde U(\mathbf{p})C_0(P)}\right) + \sqrt{\frac{\tilde U(\mathbf{p})}{C_0(P)}}\tilde G_0^{(2)}(P)\sinh\left(\sqrt{\tilde U(\mathbf{p})C_0(P)}\right)\right] - \tilde U(\mathbf{p})\tilde G_0^{(2)}(P)\right)$$

quadruple integral

$$C_{\lambda=0}(P) = 2N_{\rm s}\int \frac{d^3\mathbf{p}'}{(2\pi)^3}\int \frac{d^3\mathbf{p}''}{(2\pi)^3} U(\mathbf{p}')\,\theta\left(-\xi(\mathbf{p}'')\right)\left(\theta\left(-\xi(\mathbf{p}+\mathbf{p}'+\mathbf{p}'')\right) - \theta\left(-\xi(\mathbf{p}'+\mathbf{p}'')\right)\right)$$

$$\times\left[\frac{\left(\xi(\mathbf{p}''+\mathbf{p}) - \xi(\mathbf{p}'')\right)^2 - \omega^2}{\left(\omega^2 + \left(\xi(\mathbf{p}''+\mathbf{p}) - \xi(\mathbf{p}'')\right)^2\right)^2} - \frac{\left(\xi(\mathbf{p}''+\mathbf{p}+\mathbf{p}') - \xi(\mathbf{p}''+\mathbf{p}')\right)\left(\xi(\mathbf{p}''+\mathbf{p}) - \xi(\mathbf{p}'')\right) - \omega^2}{\left(\omega^2 + \left(\xi(\mathbf{p}''+\mathbf{p}+\mathbf{p}') - \xi(\mathbf{p}''+\mathbf{p}')\right)^2\right)\left(\omega^2 + \left(\xi(\mathbf{p}''+\mathbf{p}) - \xi(\mathbf{p}'')\right)^2\right)}\right]$$

$(\xi(\mathbf{p}) = \mathbf{p}^2/2 - \mu_0)$

sextuple integral

$\tilde G_0^{(2)}(P)$ is obtained analytically

$$\frac{E_{\rm corr}}{N} = \frac{1}{(2\pi)^2 n}\int \frac{d\omega}{2\pi}\int_0^\infty dp\, p^2\left(\ln\left[\cosh\left(\sqrt{\tilde U(\mathbf{p})C_0(P)}\right) + \sqrt{\frac{\tilde U(\mathbf{p})}{C_0(P)}}\tilde G_0^{(2)}(P)\sinh\left(\sqrt{\tilde U(\mathbf{p})C_0(P)}\right)\right] - \tilde U(\mathbf{p})\tilde G_0^{(2)}(P)\right)$$

double integral

$$C_{\lambda=0}(P) = -\frac{N_{\rm s}}{2}\int_{\mathbf{p}',\mathbf{p}''}\int_{\mathbf{x}} U(\mathbf{x})\mathbf{e}^{-\mathbf{i}(\mathbf{p}'-\mathbf{p}'')\cdot\mathbf{x}}\left[\theta\left(-\xi(\mathbf{p}''+\mathbf{p})\right) - \theta\left(-\xi(\mathbf{p}'')\right)\right]\left[\theta\left(-\xi(\mathbf{p}+\mathbf{p}')\right) - \theta\left(-\xi(\mathbf{p}')\right)\right]\left(\frac{\mathbf{1}}{\mathbf{i}\omega + \xi(\mathbf{p}''+\mathbf{p}) - \xi(\mathbf{p}'')} - \frac{\mathbf{1}}{\mathbf{i}\omega + \xi(\mathbf{p}'+\mathbf{p}) - \xi(\mathbf{p}')}\right)^{\mathbf{2}}$$

$$= -\frac{N_{\rm s}}{(2\pi)^6}\int_{-p_{\rm F}}^{p_{\rm F}} dp_z'\int_0^{\sqrt{p_{\rm F}^2 - p_z'^2}} dp_r'\int_0^{2\pi} d\phi'\,p_r'\int_{-p_{\rm F}}^{p_{\rm F}} dp_z''\int_0^{\sqrt{p_{\rm F}^2 - p_z''^2}} dp_r''\int_0^{2\pi} d\phi''\,p_r''\,{\rm Re}\left(\frac{1}{i\omega + pp_z' + p^2/2} - \frac{1}{i\omega + pp_z'' + p^2/2}\right)^2\int_{-\infty}^\infty dz\int_0^\infty dr\int_0^{2\pi} d\theta\, r\, U(\sqrt{r^2+z^2})e^{-ip_z' r\cos(\phi'-\theta) + ip_z'' r\cos(\phi''-\theta)}e^{-ip_z' z + ip_z'' z}$$

$$+\frac{N_{\rm s}}{(2\pi)^6}\int_{-p_{\rm F}}^{p_{\rm F}} dp_z'\int_0^{\sqrt{p_{\rm F}^2 - p_z'^2}} dp_r'\int_0^{2\pi} d\phi'\,p_r'\int_{-p_{\rm F}}^{p_{\rm F}} dp_z''\int_0^{\sqrt{p_{\rm F}^2 - p_z''^2}} dp_r''\int_0^{2\pi} d\phi''\,p_r''\,{\rm Re}\left(\frac{1}{i\omega + pp_z' + p^2/2} + \frac{1}{-i\omega + pp_z'' + p^2/2}\right)^2\int_{-\infty}^\infty dz\int_0^\infty dr\int_0^{2\pi} d\theta\, r\, U(\sqrt{r^2+z^2})e^{-ip_z' r\cos(\phi'-\theta) - ip_z'' r\cos(\phi''-\theta)}e^{-i(p_z' + p_z'' + p)z}$$

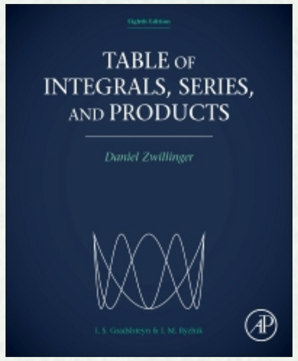
$$= -\frac{2N_{\rm s}}{(2\pi)^3}\int_{-p_{\rm F}}^{p_{\rm F}} dp_z'\int_{-p_{\rm F}}^{p_{\rm F}} dp_z''\sqrt{p_{\rm F}^2 - p_z'^2}\sqrt{p_{\rm F}^2 - p_z''^2}\,{\rm Re}\left(\frac{1}{i\omega + pp_z' + p^2/2} - \frac{1}{i\omega + pp_z'' + p^2/2}\right)^2\int_0^\infty dr\frac{1}{r}J_1\left(r\sqrt{p_{\rm F}^2 - p_z'^2}\right)J_1\left(r\sqrt{p_{\rm F}^2 - p_z''^2}\right)K_0(r|p_z' - p_z''|)$$

$$+\frac{2N_{\rm s}}{(2\pi)^3}\int_{-p_{\rm F}}^{p_{\rm F}} dp_z'\int_{-p_{\rm F}}^{p_{\rm F}} dp_z''\sqrt{p_{\rm F}^2 - p_z'^2}\sqrt{p_{\rm F}^2 - p_z''^2}\,{\rm Re}\left(\frac{1}{i\omega + pp_z' + p^2/2} + \frac{1}{-i\omega + pp_z'' + p^2/2}\right)^2\int_0^\infty dr\frac{1}{r}J_1\left(r\sqrt{p_{\rm F}^2 - p_z'^2}\right)J_1\left(r\sqrt{p_{\rm F}^2 - p_z''^2}\right)K_0(r|p_z' + p_z'' + p|)$$

double integral!!

analytic integral is possible!

[Zwillinger, "Table of integrals, series, and products"]



Drastically reduces the dimension of integrals

→ **Fast numerical calculation!!**

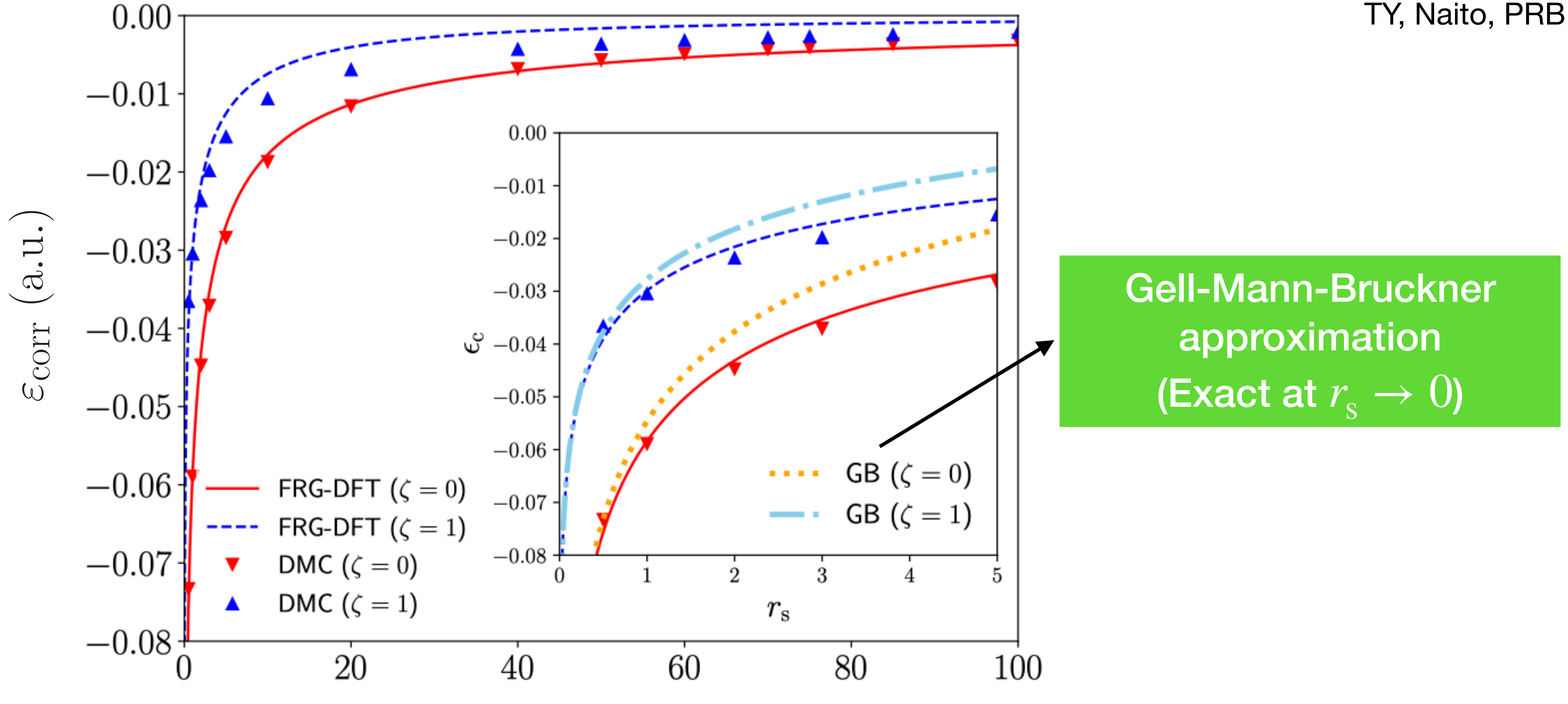
(only a few minutes to obtain $E_{\rm corr}$ with laptops)

Correlation energy per particle

$$\epsilon_{\rm xc} = \epsilon_{\rm x} + \epsilon_{\rm corr} \qquad \epsilon_{\rm x} = -\frac{3}{4\pi}\left(\frac{9\pi}{4r_{\rm s}}\right)^{1/3}\frac{(1+\zeta)^{4/3}+(1-\zeta)^{4/3}}{2}$$

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.)

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

Construction of EDF without empirical parameters ($\zeta = 0$ case)

Correlation part of LDA EDF $E_{\rm corr}^{\rm LDA}[\rho] = \int d\mathbf{x}\epsilon_{\rm corr}(\rho(\mathbf{x}))\rho(\mathbf{x})$

Many of conventional EDFs (PZ81, VWN, PW92…):
The form of $\epsilon_{\rm corr}(\rho)$ is assumed empirically and free parameters are fit to few DMC data…

e.g.) PZ81 — Perdew, Zunger, PRB (1981)

$$\epsilon_{\rm corr}(r_s) = \begin{cases} A \ln r_s + B + C r_s \ln r_s + D r_s & r_s < 1\,\mathrm{a.u.} \\ \gamma/\left(1 + \beta_1\sqrt{r_s} + \beta_2 r_s\right) & r_s \geq 1\,\mathrm{a.u.} \end{cases}$$

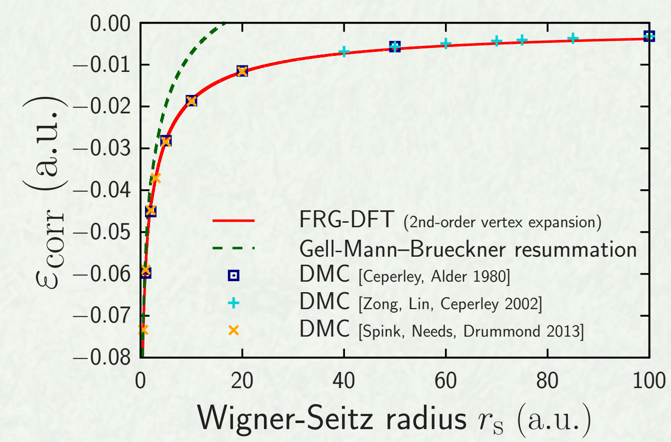
Many-data point obtained by FRG-DFT

→ **Numerical-table method**

Non-empirical parameter in $10^{-6} \leq r_s < 10^2$ (physically relevant region)

Details
- Linear interpolation between data
- Replaced by Gell-Mann-Brueckner resum in $r_s < 10^{-6}\mathrm{a.u.}$
- Extrapolation to $r_s \geq 10^2\mathrm{a.u.}$ by PZ81-type function (parameters are determined from data in $95\mathrm{a.u.} < r_s < 100\mathrm{a.u.}$)

But the results hardly depend on these choices.



65536 points in logarithmic mesh

Derivative of $\epsilon_{\rm corr}$ are also obtained **analytically.**

Need for Kohn-Sham calculation

$$\left(-\frac{\Delta}{2} + \int dx' \frac{\rho(x')}{|x - x'|} + \frac{\delta E_{\rm ex}^{\rm LDA}[\rho]}{\delta\rho(x)} + \frac{\delta E_{\rm corr}^{\rm LDA}[\rho]}{\delta\rho(x)}\right)\phi_i(x) = \epsilon_i\phi_i(x)$$

$$\frac{\delta E_{\rm corr}^{\rm LDA}[\rho]}{\delta\rho(\mathbf{x})} = \epsilon_{\rm corr}(\rho(\mathbf{x})) + \epsilon'_{\rm corr}(\rho(\mathbf{x}))\rho(\mathbf{x})$$

$$\epsilon'_{\rm corr}(r_s) = \frac{1}{2n r_s}\int_P \cdots$$

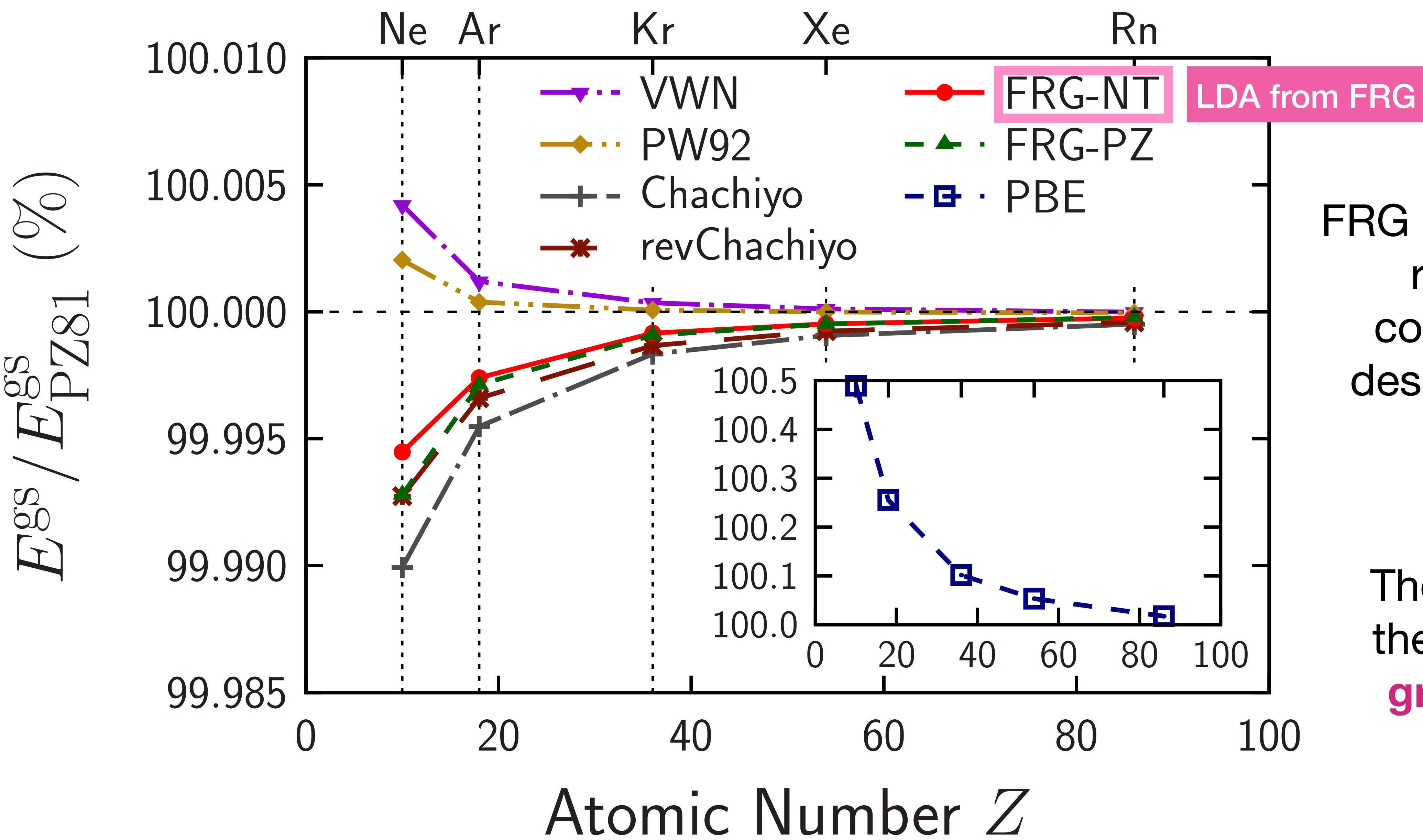
see arXiv:2010.07172

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.**

Summary

Density functional theory (DFT)

Efficient method to analyze electrons, nuclei, …

How to derive energy density functional (EDF)?

Key quantity in DFT

Effective-action formalism will provide a new way to construct EDF

Functional evolution equation in a closed form for effective action

FRG techniques are useful

Application: vertex expansion (electrons, …)

Other direction: spectral function TY, Yoshida, Kunihiro, PTEP (2019)

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

Outlook

Inclusion of gradient effect (LPA? Neural-net ansatz?)

Application to realistic nuclear matter, nuclei

Numerical study of superfluid systems

Appendix

Calculation of excited states

Analytic continuation to real time

FRG technique to obtain real-time spectral function via **analytic continuation of flow eq. for correlation function** has been developed.

e.g.) meson spectral function in O(4), quark-meson model

Kamikado, Strodthoff, von Smekal, Wambach (2020)
Tripolt, Strodthoff, von Smekal, Wambach (2014)
TY, Kunihiro, Morita (2016), (2017)…

This technique can be used to calculate spectral function of density fluctuation in FRG-DFT!

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

↓ Analytic continuation **for flow eq.**

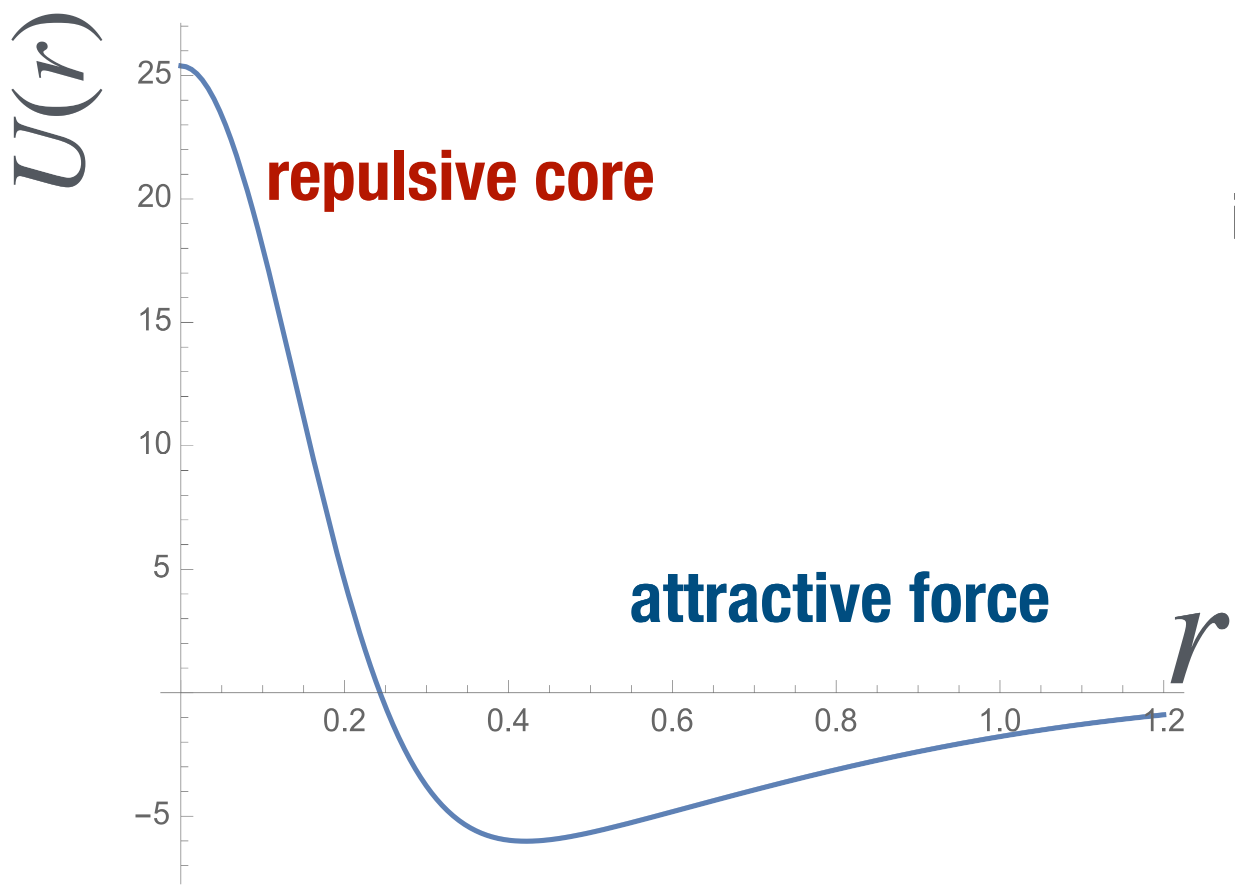
Flow eq. for real-time correlation $\tilde{G}^{(2)}_{{\rm R},\lambda}(\omega, p)$

↓ **Solution**

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

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

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

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

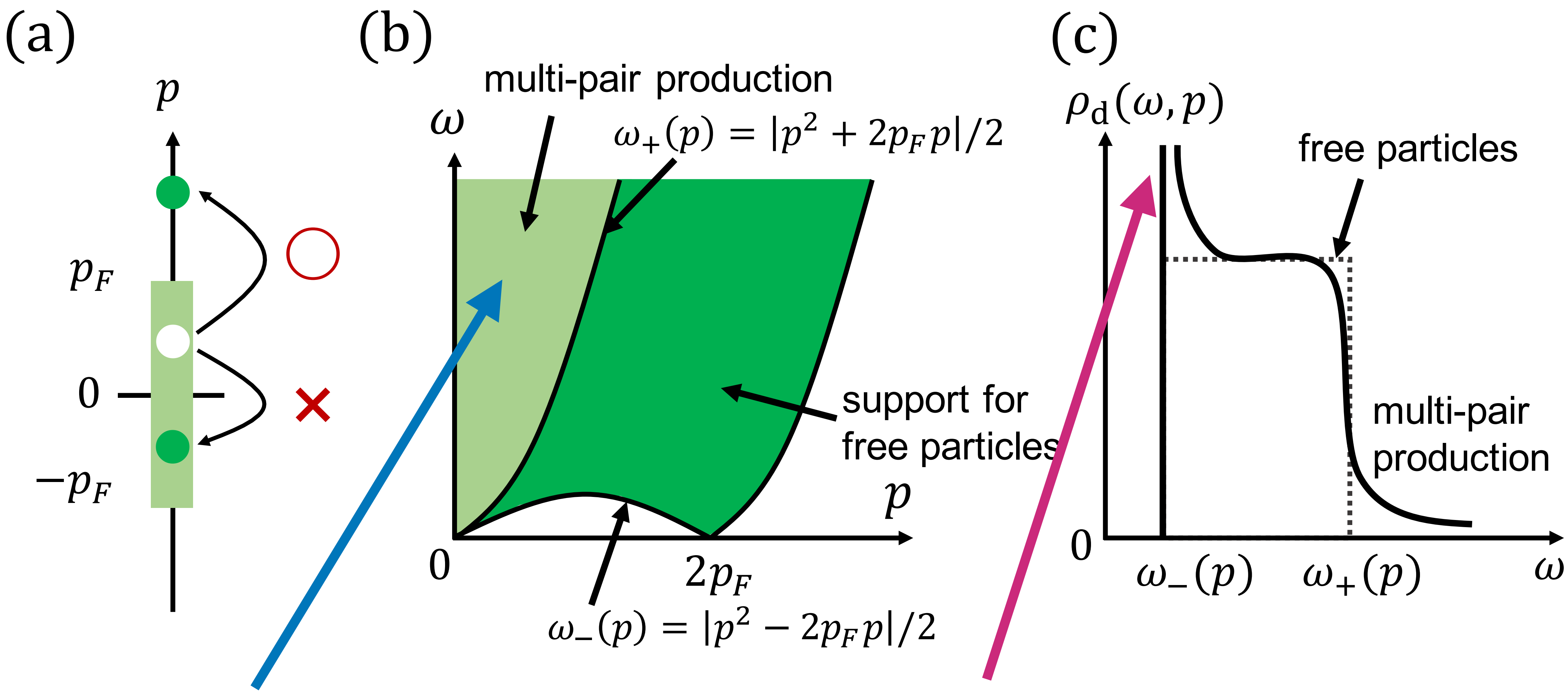
fermion mass=1 unit

Alexandro, Myczkowski, Negele, PRC (1989)

Excitation in Tomonaga-Luttinger liquid

Previous results
(such as bosonization)

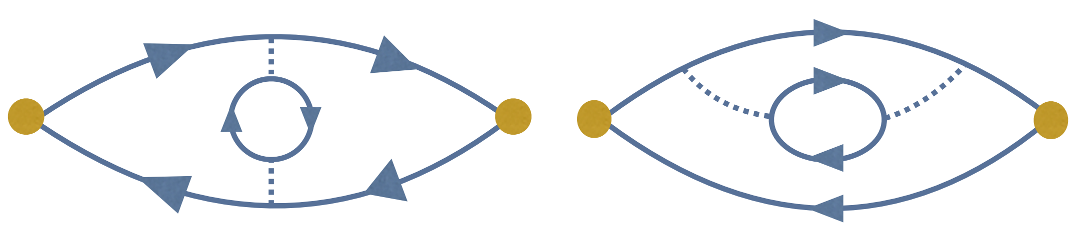
Pustilnik, Khodas, Kamenev, Glazman, PRL (2006)
Teber, PRB (2007)
Imambekov, Schmidt, Glazman, RMP (2012)



Multi-pair production

Mahan (X-ray edge) singularity

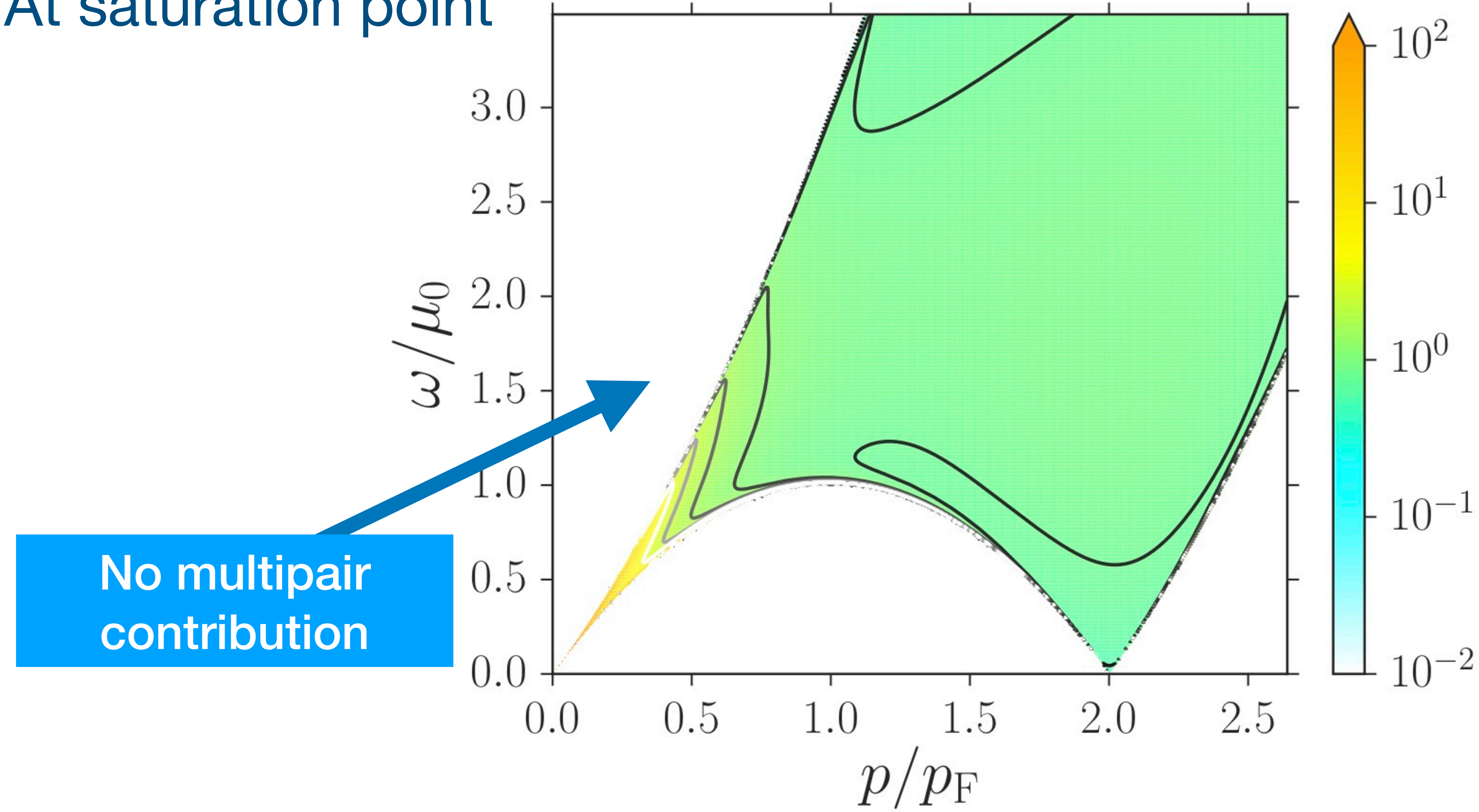
Nozieres, De Dominicis, PR178 (1969); Mahan (1981)



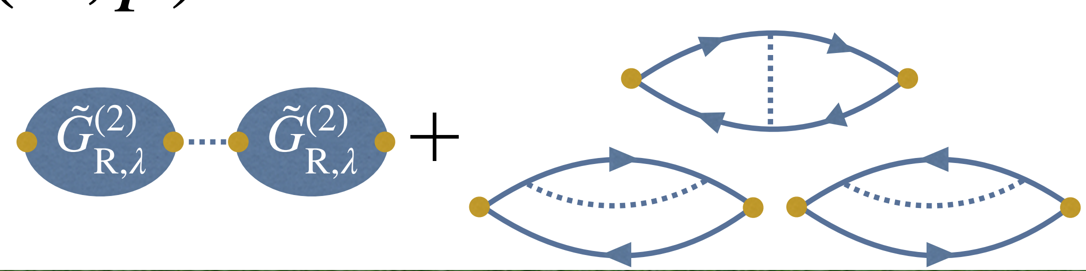
FRG-DFT result of $\rho_{\mathrm{d}}(\omega, p)$

TY, Yoshida, Kunihiro, PTEP (2019)

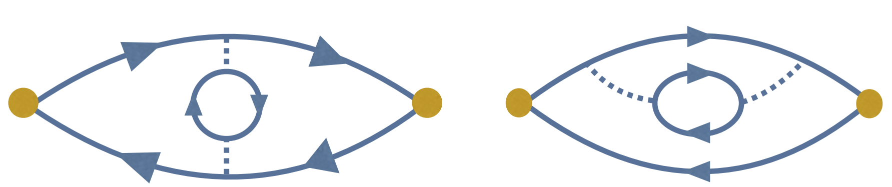
At saturation point



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

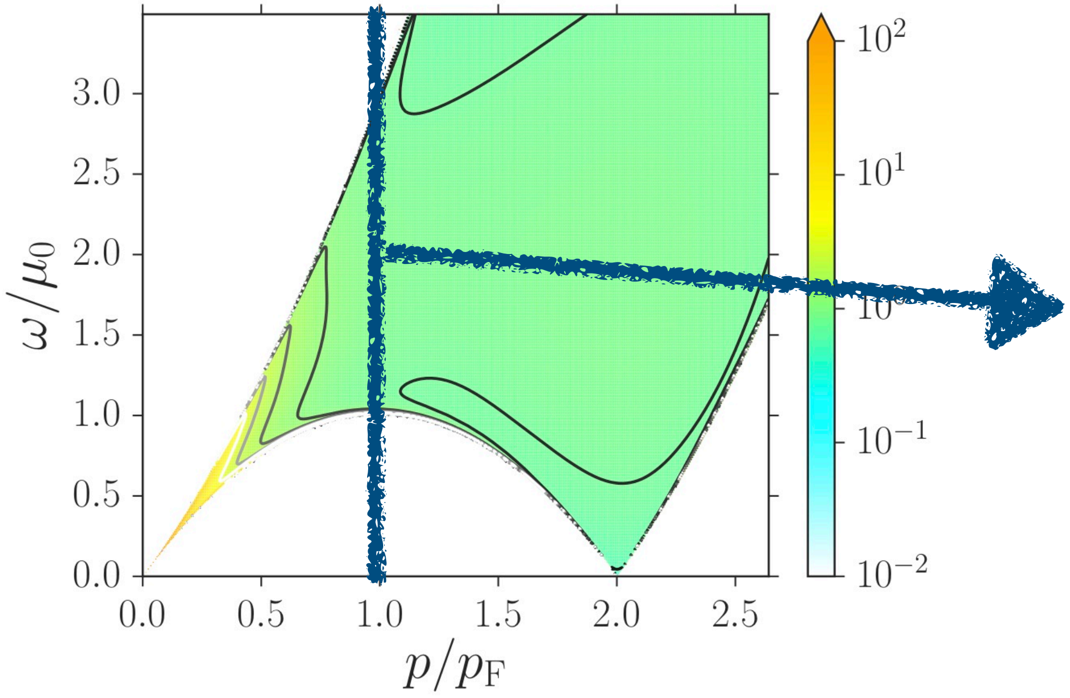


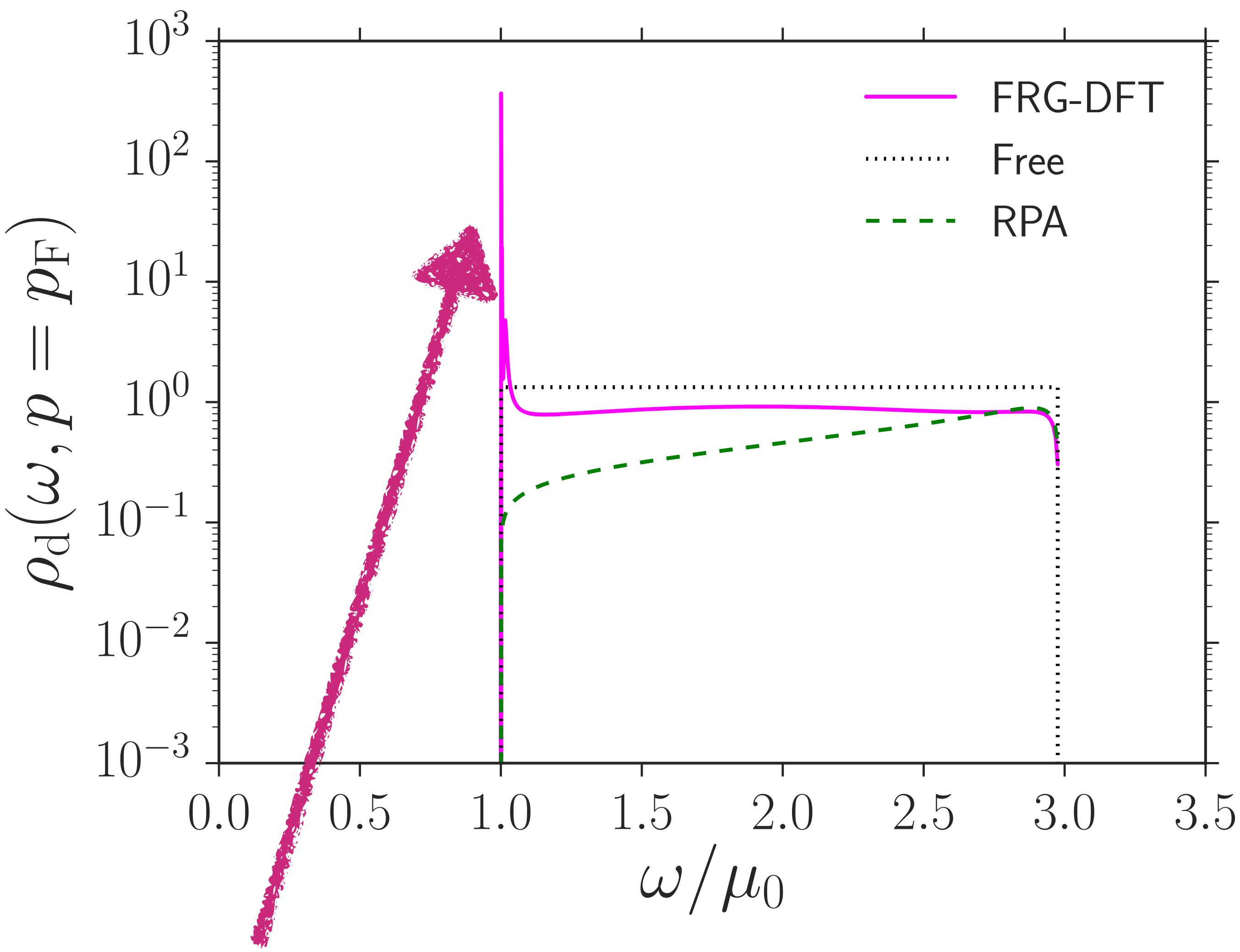
No multi-pair diagrams



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

TY, Yoshida, Kunihiro, PTEP (2019)





Reproduced in FRG-DFT!

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