Functional flow approach in classical liquids

Kiyoharu Kawana (KIAS)

Based on PTEP 2019, 1, 013A01 (arXiv:1808.08133) and arXiv: 2309.10496

2024/1/7-8@FRG at Niigata

Who am I ?

- Ph.D. (Science) in 2017; Supervised by Prof. Hikaru Kawai

Title of thesis: “The problems of the Standard Model and their relations to Planck scale Physics”

- First postdoc in KEK as JSPS fellow hosted by Prof. Satoshi Iso (~2018)

One of the collaborations: “Density Renormalization Group (DRG) for classical liquids”

→ I will explain this below

- Postdoc in Standard University and Seoul National University (~ 2022)
- Now → Research fellow in Korean institute for Advanced Study (KIAS)
- My primary research field is particle physics and cosmology

Why did we get interested in liquid systems ?

- Originally, we were interested in the analogy between statistical mechanics and quantum field theory (QFT)

QFT

$$Z(\{\lambda_l\}) = \int \mathscr{D}\phi \ \exp\left(i \sum_l \lambda_l S_l[\phi] \right)$$

Partition function in QFT

Statistical mechanics

$$Z(T,\mu) = \mathrm{Tr}\left(e^{-\hat{H}/T+\mu\hat{N}/T} \right) = \int \mathscr{D}\phi e^{-S_E[\phi]+\mu N[\phi]}$$

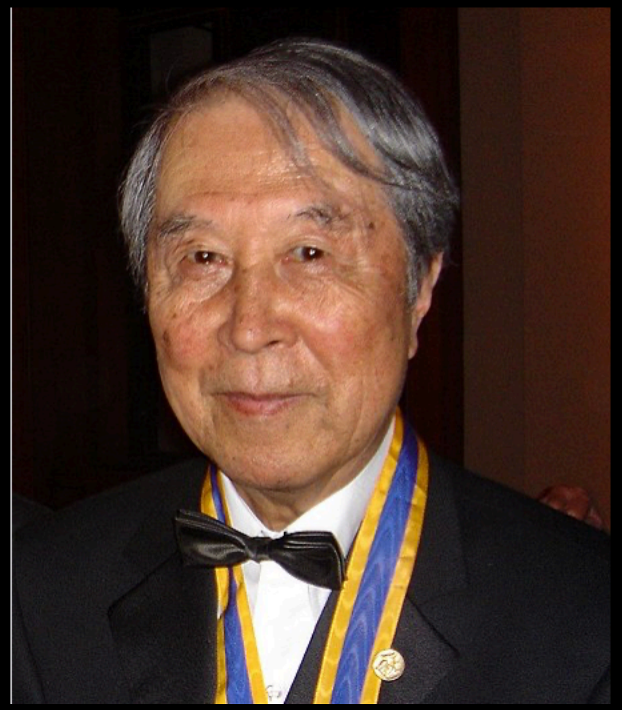
(Grand) canonical partition function

Renormalization Group (RG) $\dfrac{dG^{(n)}(\{x_i\};M)}{dM} = 0$ ↔ ?

Observables do not depend on the renormalization scale M
=artificial parameter to regularize the system

Classical liquid system is a good nontrivial system
to seek for this question

Nambu's unpublished paper ('87)



THERMODYNAMIC ANALOGY IN QUANTUM FIELD THEORY*

Y. Nambu†
The University of Chicago, Enrico Fermi Institute
Chicago, Illinois, 60637 USA

The thermodynamics analogy is now clear in any of such interpretations. In a system of infinite degrees of freedom, as in quantum field theory, the action exponential is usually assumed to have a sharp Gaussian maximum at the classical "on shell" value, and the tangent space around it spans the Hilbert space of physical states. The partition function then assumes the form

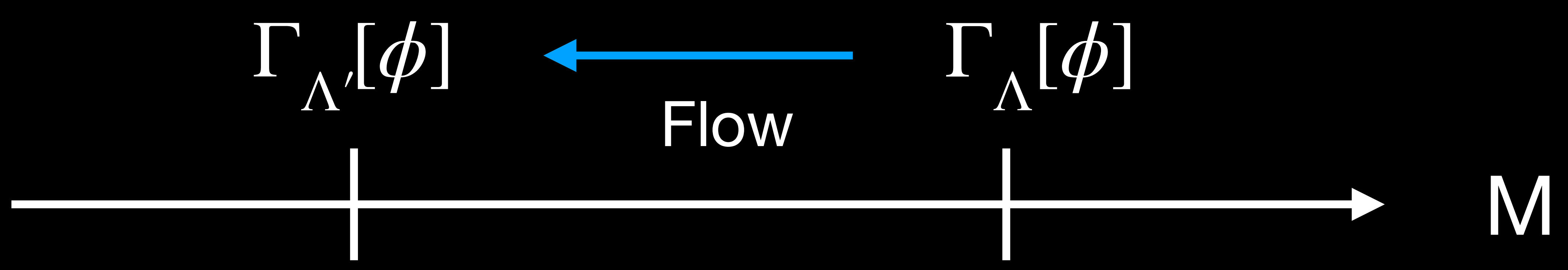
$$Z = \exp[-\bar{F}/T],\ \bar{F} = \bar{L}_c - T\bar{S} \tag{5}$$

All these arguments are formal ones, and ignores the fact that there are intrinsic divergences which have to be controlled by renormalization. What is the thermodynamic interpretation of the renormalization process?

＊ In this paper, he argued that the RGE of (gauge) coupling in QFT can be interpreted as the thermodynamic relation of ideal gas system

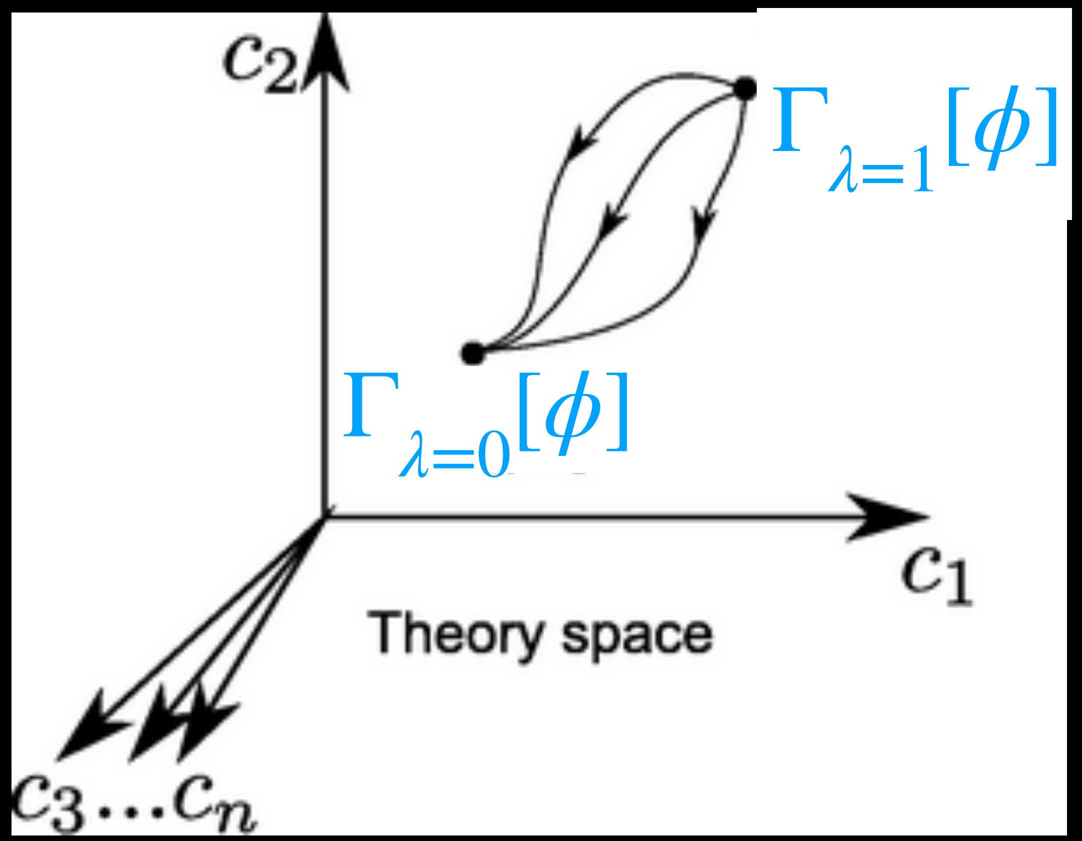
Q: How can we formulate RG in general equilibrium systems ?

→ Roughly speaking, RG in QFT sees the response of a system according to the change of renormalization scale M (or cut off Λ)



→ Why not consider a general response of general (artificial) parameters λ ?

→ General functional flow !



Brief summary of this talk

1. It is possible to construct a variety of exact functional flow equations in equilibrium systems

$$\frac{d(-\beta\Gamma[\{\lambda_a\};\phi])}{d\lambda_a} = -\beta\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n} d^d x_i\right)\frac{\partial v_n}{\partial\lambda_a}\times G^{(n)}(\{x_i\};J_\phi)$$

2. For a given system, what we have to do is (i) to pick up/introduce a good parameter and (ii) to find a good approximation/truncation in order to solve the flow equation

3. In classical liquid system, a Wilsonian-type RG called Hierarchical reference theory (HRT) has been well studied so far

4. We discuss another functional flow approach, i.e. Density Renormalization Group (DRG) , which describes the response of correlation functions (1PI vertices) against the change of density.

$$\frac{dc_l(x_1,\cdots,x_l)}{d\log n} = \cdots$$

Plan of Talk

1. General functional flow in statistical mechanics
2. Classical liquid systems (HRT and DRG)
3. Optimized cut-off and critical phenomena in HRT (in progress) ← If we have time
4. Summary

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Set up (equilibrium systems)

d = space dimension

$\beta = 1/T$

e.g. $\phi(x)$ = density in classical liquid system

- For simplicity, we consider a real scalar system

$$H[\{\lambda_l\};J] = \sum_{n=1}^{\infty} \int \left(\prod_{i=1}^{n} d^d x_i \right) \frac{1}{n!} v_n(\{x_i\};\{\lambda_l\}) \times \prod_{i=1}^{n} \phi(x_i) - \beta^{-1} \int d^d x J(x) \phi(x)$$

$v_n(\{x_i\};\{\lambda_k\})$ = n-body microscopic potential (interaction)

$J(x)$ = external source (e.g. chemical potential)

$\{\lambda_l\}$ denotes general parameters (coupling constants)

It can be an artificial parameter

e.g. $v_n = v_{n,R} + t \times v_{n,A} \ , \quad t \in [0,1]$

Set up (equilibrium systems)

cont'd

d = space dimension

$\beta = 1/T$

$$H[\phi; J] = \sum_{n=1}^{\infty} \int \left(\prod_{i=1}^{n} dx_i^d \right) \frac{1}{n!} v_n(\{x_i\}; \{\lambda_l\}) \times \prod_{i=1}^{n} \phi(x_i) - \beta^{-1} \int d^d x J(x) \phi(x)$$

- Partition function

$$Z[\{\lambda_k\}; J] = \exp(-\beta W[\{\lambda_k\}; J]) = \int \mathcal{D}\phi e^{-\beta H[\phi; J]}$$

$W[\{\lambda_k\}; J]$ is grand-canonical potential = generating functional of connected correlation functions

$$F^{(n)}(\{x_i\}; J) = \frac{\delta(-\beta W[\{\lambda_k\}; J])}{\delta J(x_1) \cdots \delta J(x_n)} \longleftrightarrow G^{(n)}(\{x_i\}; J) = \frac{1}{Z} \frac{\delta(-\beta Z[\{\lambda_k\}; J])}{\delta J(x_1) \cdots \delta J(x_n)}$$

Connected ones

Non-connected ones

Functional flow theory

[KK, arXiv: 2309.10496]

- Consider a small variation of a parameter: $\lambda_a \to \lambda_a + \delta\lambda_a$
- Correspondingly, the microscopic potential varies as $\delta v_n(\{x_i\}, \{\lambda_l\}) := \delta\lambda_a \times \frac{\partial v_n}{\partial \lambda_a}$
- Then, the variation of grand-canonical potential is

$$\delta(-\beta W[\{\lambda_l\}; J]) = -\delta\lambda_a \times \beta \sum_{n=1}^{\infty} \frac{1}{n!} \int \left(\prod_{i=1}^{n} d^d x_i \right) \frac{\partial v_n}{\partial \lambda_a} \times G^{(n)}(\{x_i\}; J)$$

$$\therefore \frac{d(-\beta W[\{\lambda_l\}; J])}{d\lambda_a} = -\beta \sum_{n=1}^{\infty} \frac{1}{n!} \int \left(\prod_{i=1}^{n} d^d x_i \right) \frac{\partial v_n(\{x_i\})}{\partial \lambda_a} \times G^{(n)}(\{x_i\}; J)$$

General flow equation in grand-canonical formulation

non-connected correlation functions

Parameter response theory

cont'd

$$\frac{d(-\beta W[\{\lambda_l\};J])}{d\lambda_a} = -\beta\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n}d^dx_i\right)\frac{\partial v_n}{\partial\lambda_a}\times G^{(n)}(\{x_i\};J)$$ (General flow equation)

- By taking the functional derivatives, we can obtain hierarchical equations for correlation functions
- By definition, n-th functional derivatives of the L.H.S gives $\frac{d}{d\lambda_a}F^{(n)}(\{x_i\};J)$
- Once we know the relations between $G^{(n)}$ and $F^{(m)}$, we can also calculate the R.H.S

e.g. When only $n=2$ contributes in the R.H.S $\quad G^{(2)}(x,y) = F^{(2)}(x,y) + F^{(1)}(x)F^{(1)}(y)$

$$\frac{d(-\beta W[\{\lambda_l\};J])}{d\lambda_a} = -\frac{\beta}{2}\int d^dx\int d^dy\frac{\partial v_2(x,y)}{\partial\lambda_a}\left[F^{(2)}(x,y;J) + F^{(1)}(x;J)F^{(1)}(y;J)\right]$$

Cont'd

When only $n=2$ contributes in the R.H.S

$$\frac{d(-\beta W[\{\lambda_l\};J])}{d\lambda_a} = -\frac{\beta}{2}\int d^dx\int d^dy\frac{\partial v_2(x,y)}{\partial\lambda_a}\left[F^{(2)}(x,y;J)+F^{(1)}(x;J)F^{(1)}(y;J)\right]$$

Functional derivative $\delta/\delta J(x_1)$

$$\frac{dF^{(1)}(x_1;J)}{d\lambda_a} = -\frac{\beta}{2}\int d^dx\int d^dy\frac{\partial v_2(x,y)}{\partial\lambda_a}\left[F^{(3)}(x,y,x_1;J)+2F^{(2)}(x,x_1;J)F^{(1)}(y;J)\right]$$

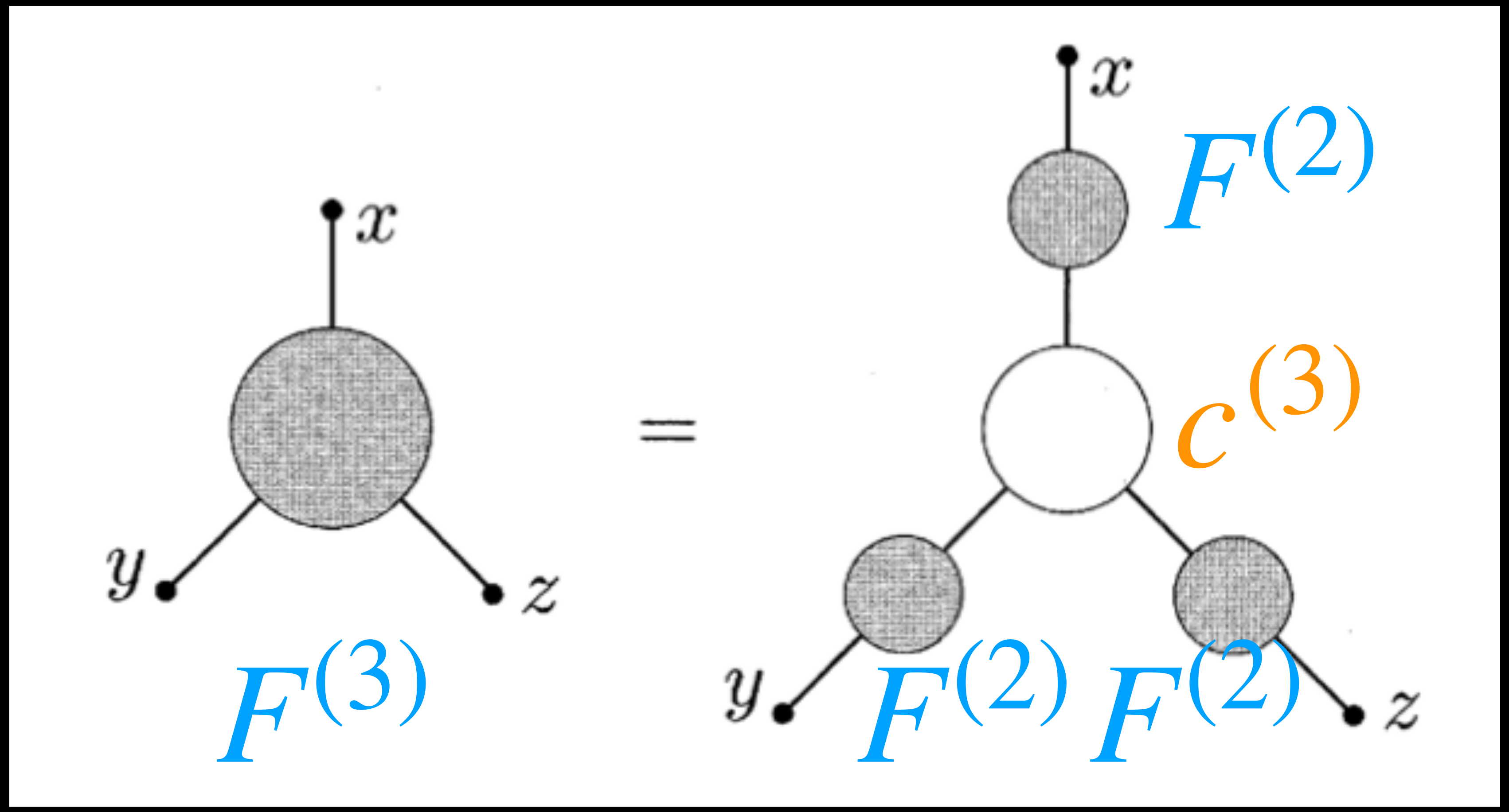
Functional derivative $\delta/\delta J(x_2)$

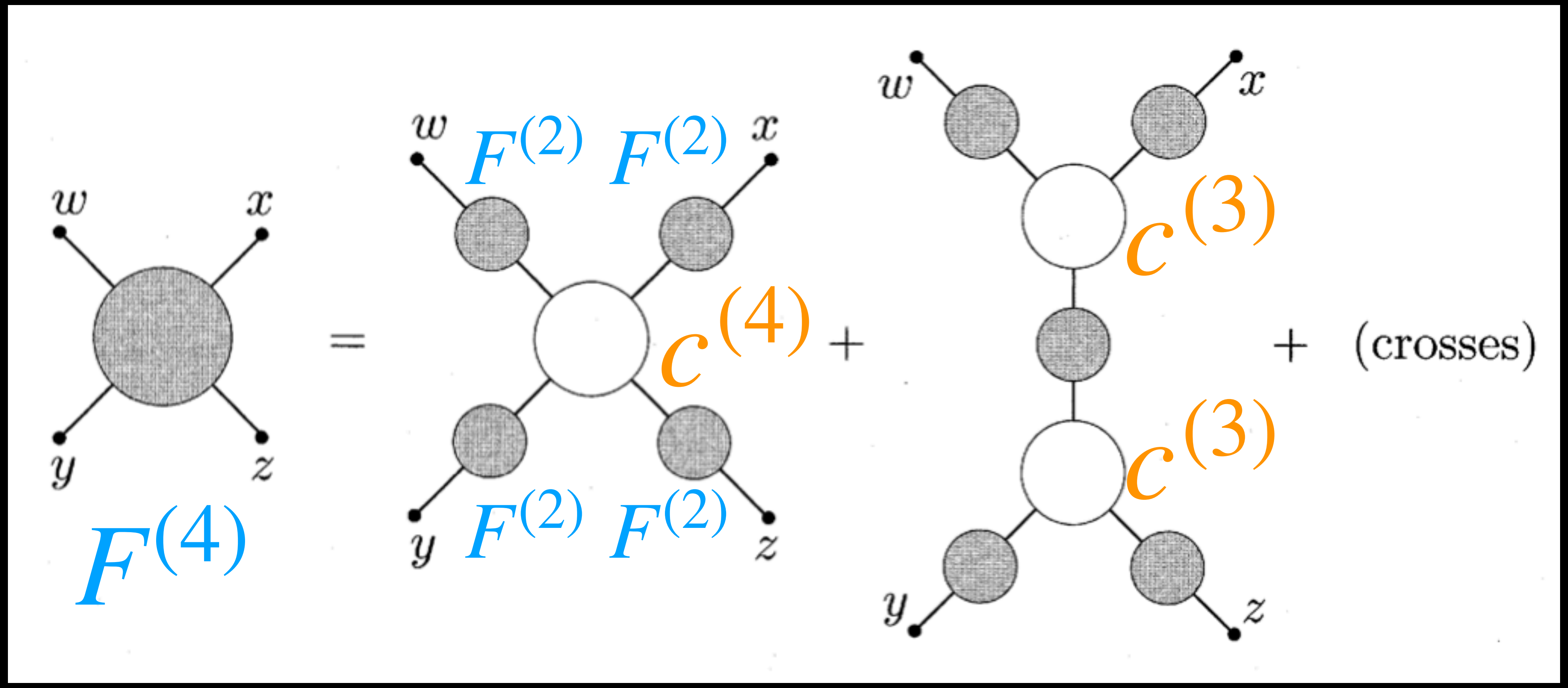
$$\frac{dF^{(2)}(x_1,x_2;J)}{d\lambda_a} = -\frac{\beta}{2}\int d^dx\int d^dy\frac{\partial v_2(x,y)}{\partial\lambda_a}\left[F^{(4)}(x,y,x_1,x_2;J)+2F^{(3)}(x,x_1,x_2;J)F^{(1)}(y;J)+2F^{(2)}(x,x_1;J)F^{(2)}(y,x_2;J)\right]$$

Flow equations for higher-order correlation functions can be obtained straightforwardly !

- However, $W[\{\lambda_l\};J]$ is not the most fundamental generating functional because

Figures from Peskin's textbook





$c^{(l)}(\{x_i\})$ = one-particle irreducible (1PI) l-point vertex

∴ Generating functional of 1PI vertices = canonical potential is more fundamental

Canonical formulation

- Canonical potential: $\Gamma[\{\lambda_l\};\phi]$ = Generating functional of 1PI vertices

Defined by Legendre transformation → $$-\beta\Gamma[\{\lambda_k\};\phi] = \min_J \left[-\beta W[\{\lambda_k\};J] - \int d^d x J(x)\phi(x)\right]$$

The extremum solution is represented by $J(x) = J_\phi(x)$

- Important property: Parameter derivative of $\Gamma[\{\lambda_l\};\phi]$ is the same as that of $W[\{\lambda_l\};J]$

$$\frac{d(-\beta\Gamma[\{\lambda_k\};\phi])}{d\lambda_l} = \left.\frac{d(-\beta W[\{\lambda_k\};J])}{d\lambda_l}\right|_{J=J_\phi} - \underbrace{\int \frac{d\delta J_\phi(x)}{d\lambda_l}\frac{\delta}{\delta J_\phi(x)}\left(-\beta W[\{\lambda_l\};J_\phi] - \int d^d x J_\phi(x)\phi(x)\right)}_{=0}$$

$$= \left.\frac{d(-\beta W[\{\lambda_k\};J])}{d\lambda_l}\right|_{J=J_\phi}$$

Parameter dependence via $J_\phi(x)$

Canonical formulation

Cont'd

$$\therefore \quad \frac{d(-\beta\Gamma[\{\lambda_a\};\phi])}{d\lambda_a} = -\beta\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n}d^dx_i\right)\frac{\partial v_n}{\partial\lambda_a}\times G^{(n)}(\{x_i\};J_\phi)$$

General flow equation in canonical formulation

- By taking the functional derivatives, we can obtain hierarchical equations for 1PI vertices

$$c^{(n)}(\{x_i\};\phi) := \frac{\delta^n(-\beta\Gamma[\{\lambda_l\};\phi])}{\delta\phi(x_1)\cdots\delta\phi(x_n)}$$

← definition of 1PI vertex

- For calculating the flow of vertices, we need to express $G^{(n)}$ ($F^{(m)}$) by $c^{(n)}$

e.g. When only $n=2$ contributes in the R.H.S

$$G^{(2)} = F^{(2)} + F^{(1)}F^{(1)} = -c^{(2)^{-1}} + \phi\phi$$

by Legendre transformation

$$\frac{d(-\beta\Gamma[\{\lambda_l\};J])}{d\lambda_a} = -\frac{\beta}{2}\int d^dx\int d^dy\frac{\partial v_2(x,y)}{\partial\lambda_a}\left[-c^{(2)^{-1}}(x,y)+\phi(x)\phi(y)\right]$$

Cont'd

When only $n = 2$ contributes in the R.H.S

$$\frac{d(-\beta\Gamma[\{\lambda_l\};\phi])}{d\lambda_a} = -\frac{\beta}{2}\int d^dx \int d^dy \frac{\partial v_2(x,y)}{\partial \lambda_a}\left[F^{(2)}(x,y;J_\phi) + \phi(x)\phi(y)\right]$$

Functional derivative $\delta/\delta\phi(x_1)$

$$\frac{dc^{(1)}(x_1;\phi)}{d\lambda_a} = -\frac{\beta}{2}\int d^dx \int d^dy \frac{\partial v_2(x,y)}{\partial \lambda_a}\left[F^{(2)} \cdot c^{(3)}(x_1) \cdot F^{(2)} + 2\delta^{(d)}(x_1 - x)\phi(y)\right]$$

Functional derivative $\delta/\delta\phi(x_2)$

$$\frac{dc^{(2)}(x_1,x_2;\phi)}{d\lambda_a} = -\frac{\beta}{2}\int d^dx \int d^dy \frac{\partial v_2(x,y)}{\partial \lambda_a}\left[F^{(2)} \cdot c^{(4)}(x,y) \cdot F^{(2)} + 2F^{(2)} \cdot c^{(3)}(x_1) \cdot F^{(2)} \cdot c^{(3)}(x_2) \cdot F^{(2)} + 2\delta^{(d)}(x_1 - x)\delta^{(d)}(x_2 - y)\right]$$

Calculations of higher-order vertex flows are also straightforward !

A few important remarks

$$\frac{d(-\beta\Gamma[\{\lambda_a\};\phi])}{d\lambda_a} = -\beta\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n}d^d x_i\right)\frac{\partial v_n}{\partial\lambda_a}\times G^{(n)}(\{x_i\};J_\phi)$$

- This is a quite general flow equation. We can apply this to various equilibrium systems. But, we solve nothing yet.
- For practical calculations, some reasonable approximations (truncations) are necessary

e.g. Derivative expansion, Local potential approximation, Kirkwood approximations, etc

$$\Gamma[\phi] = \int d^d x\left(\frac{Z}{2}(\partial\phi)^2 + U(\phi) + \cdots\right)$$

Leading derivative   Local potential

- When partition function has some symmetry (= invariance under some changes of parameters), we can obtain another exact relation among correlation functions (Schwinger Dyson equations)

See my paper 2309.10496 for more details

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Classical Liquid Systems

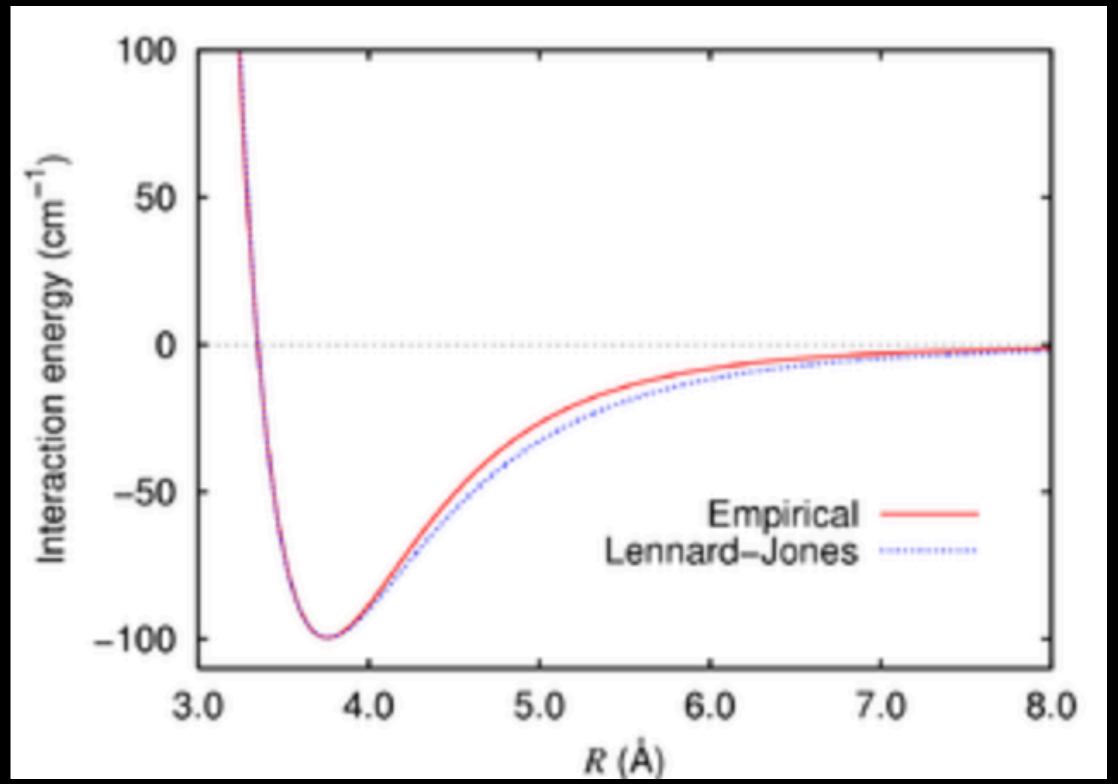
- Hamiltonian:

$$H_N = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V_N(\{x_i\})$$

← General N-body potential

$$V_N(\{x_i\}) = \sum_{i<j} v(x_i, x_j) + \sum_{i<j<k} v_3(x_i, x_j, x_k) + \cdots$$

2-body 3-body



Typical two-body potential

- In the following, we consider simple liquids

$$v(x, y) = v(|x - y|)\ , \quad v_n(\{x_i\}) = 0 \quad n \geq 3$$

depends only on the relative distance

Classical Liquid Systems

Cont'd

- Grand-canonical partition function

$$Z[\beta U] = \exp(-\beta W[\beta U]) = \mathrm{Tr}\left[e^{-\beta H_N + \beta \int d^d x U(x)\rho(x)}\right]$$

$$\rho(x) = \sum_{i=1}^{N} \delta^{(d)}(x - x_i)$$ (Density operator)

- The potential can be written as

$$\sum_{i<j} v(x_i, x_j) = \frac{1}{2}\int d^d x \int d^d y \rho(y) v(x, y) \rho(x) + \int d^d x \rho(x) \left(-\frac{1}{2} v(x, x)\right)$$

Only v_1 and v_2 exist !

cf. general Hamiltonian $H[\{\lambda_l\}; J] = \sum_{n=1}^{\infty} \int \left(\prod_{i=1}^{n} dx_i^d\right) \frac{1}{n!} v_n(\{x_i\}; \{\lambda_l\}) \times \prod_{i=1}^{n} \phi(x_i)$

Classical Liquid Systems

Cont'd

- We already know a general flow equation

$$\frac{d(-\beta\Gamma[\{\lambda_a\};\phi])}{d\lambda_a} = -\beta\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n}d^d x_i\right)\frac{\partial v_n}{\partial \lambda_a}\times G^{(n)}(\{x_i\};J_\phi)$$

Simple liquid →

$$\frac{d(-\beta\Gamma[\rho])}{d\lambda_a} = -\frac{\beta}{2}\int d^d x\int d^d y\frac{\partial v(x,y)}{\partial \lambda_a}\times\left[G^{(2)}(x,y)-\delta^{(d)}(x-y)\rho(x)\right]$$

$$= -\frac{\beta}{2}\int d^d x\int d^d y\frac{\partial v(x,y)}{\partial \lambda_a}\times\left[F^{(2)}(x,y)+\rho(x)\rho(y)-\delta^{(d)}(x-y)\rho(x)\right]$$

Note

$$F^{(1)}(x) = \rho(x)$$

$$G^{(2)} = F^{(2)} + F^{(1)}F^{(1)}$$

A general flow equation in simple liquid !

Question: what parameter should we choose/introduce ?

Hierarchical Reference Theory (HRT)

[Parola, Reatto ('84)]

- Introduce an IR cut off k in the (some part of) two-body potential:

$$\tilde{v}(q) \;\rightarrow\; \tilde{v}_k(q) \sim \begin{cases} \tilde{v}(q) & \text{for } q \gg k \\ 0 & \text{for } q \ll k \end{cases}$$

Fourier mode

Low momentum modes are suppressed

- Why is this called "Reference" theory ? → Initial ($k = \infty$) system = Reference system

$$\lim_{k=\infty} \tilde{v}_k(q) = \tilde{v}_R(q) = \quad \text{Potential of reference system}$$

As a reference system, the short-range repulsive part is usually chosen.

e.g. $v_k(x) = v_R(x) + v_{A,k}(x)$ such that $v_{A,k=\infty}(x) = 0$

Hierarchical Reference Theory (HRT)

[Parola, Reatto ('84)]

Cont'd

- The flow equation in HRT (Just putting $\lambda_a = k$)

$$\frac{d(-\beta\Gamma_k[\rho])}{dk} = -\frac{\beta}{2}\int d^dx \int d^dy \frac{\partial v_k(x,y)}{\partial k} \times \left[F_k^{(2)}(x,y) + \underline{\rho(x)\rho(y) - \delta^{(d)}(x-y)\rho(x)}\right]$$

Trivial terms (mean field contributions)

- To eliminate these terms, it is convenient to define a new canonical generating potential

$$-\beta\mathscr{A}_k[\rho] = -\beta\Gamma_k[\rho] - \frac{\beta}{2}\int d^dx \int d^dy \left(v_k(x,y) - v(x,y)\right)\{\rho(x)\rho(y) - \delta^{(d)}(x-y)\rho(x)\}$$

$$\therefore \quad \frac{d(-\beta\mathscr{A}_k[\rho])}{dk} = -\frac{\beta}{2}\int d^dx \int d^dy \frac{\partial v_k(x,y)}{\partial k} \times F_k^{(2)}(x,y) = -\frac{\beta}{2}\mathrm{Tr}\left[(\partial_k v_k)F_k^{(2)}\right]$$

Only $F_k^{(2)}$ appears

Cont'd

Hierarchical Reference Theory (HRT)

[Parola, Reatto ('84)]

- By using the two-point vertex $\dfrac{\delta^2(\beta\mathscr{A}_k[\rho])}{\delta\rho(x)\delta(y)} := C_k^{(2)}(x,y)$

$$\frac{d(\beta\mathscr{A}_k[\rho])}{dk} = \frac{1}{2}\mathrm{Tr}\left[(\partial_k R_k)\left(C_k^{(2)} + R_k\right)^{-1}\right]$$

with

$$R_k(x,y) = \beta\left[v_k(x,y) - v(x,y)\right]$$

- This flow equation is well-known as Wetterich's equation in QFT

$$\frac{d(\hbar^{-1}\Gamma_k[\phi])}{dk} = \frac{1}{2}\mathrm{Tr}\left[(\partial_k R_k)\left(\Gamma^{(2)} + R_k\right)^{-1}\right]$$

$\Gamma_k[\phi] =$ Effective action in QFT

[Wetterich ('91)]

$R_k(x)$ = regulator function which suppresses low energy modes

$$\tilde{R}_k(q) \sim \begin{cases} 0 & \text{for } q \gg k \\ \mathcal{O}(k^2) & \text{for } q \ll k \end{cases}$$

HRT=Functional Renormalization Group in QFT

Cont'd

They are completely same !

HRT

$$\frac{d(\beta \mathscr{A}_k[\rho])}{dk} = \frac{1}{2}\mathrm{Tr}\left[(\partial_k R_k)\left(C_k^{(2)} + R_k\right)^{-1}\right]$$

QFT (Euclidean)

$$\frac{d(\hbar^{-1}\Gamma_k[\phi])}{dk} = \frac{1}{2}\mathrm{Tr}\left[(\partial_k R_k)\left(\Gamma_k^{(2)} + R_k\right)^{-1}\right]$$

What are the differences ? → Choice of initial system !

$$\mathscr{A}_{k=\infty}[\rho] = \Gamma_R[\rho]$$

Some reference system

Non-local in general

$$\Gamma_{k=\Lambda}[\phi] = S_\Lambda[\phi]$$

Some bare action

which is usually local

∴ We can apply many functional techniques developed in QFT to HRT ! (Part 3 when time is allowed)

Density renormalization group

[KK, S.Iso ('18)]

- The scale transformation, $x \to \lambda x$, corresponds to the change of density, $\rho \to \lambda^{-d}\rho$

$\therefore$ Variation of λ should be somehow related to that of ρ

$$\frac{d(-\beta\Gamma[\rho])}{d\lambda} = \cdots \quad \overset{?}{\longleftrightarrow} \quad \frac{d(-\beta\Gamma[\rho])}{d\rho} = \cdots$$

- In the following, we consider a general N-body potential

$$H_N = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V_N(\{x_i\})$$

- Replace the potential $V_N(\{x_i\}) \to V_N(\{\lambda x_i\})$, and correspondingly we denote

$$\Gamma[V,\rho] \;\to\; \Gamma_\lambda[V,\rho] \;, \qquad G^{(n)}(\{x_i\}) \;\to\; G^{(n)}_\lambda(\{x_i\}) \;,$$

$\lambda = 1$corresponds to the original system

V=Volume

Cont’d

Density renormalization group

[KK, S.Iso (’18)]

- We already know the flow equation of $\Gamma_\lambda[\phi]$

$$\frac{d(-\beta\Gamma_\lambda[V,\rho])}{d\lambda} = -\beta\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n}d^dx_i\right)\frac{\partial v_n(\lambda x_i)}{\partial\lambda}\times G_\lambda^{(n)}(\{x_i\};J_\phi)$$

$$= -\lambda\times\beta\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n}d^dx_i\right)\sum_{i=1}^{n}\sum_{\mu=1}^{d}x_i^\mu\frac{\partial v_n(\{x_i\})}{\partial x_i^\mu}\Bigg|_{x=\lambda x}\times G_\lambda^{(n)}(\{x_i\};J_\phi)$$

How can we relate this to density response ?

→ Use the symmetry (redundancy) of the system !

$$-\beta\Gamma_{1+\epsilon}[V,\rho(x)] = -\beta\Gamma[V+\delta_\epsilon V,\rho(x)+\delta_\epsilon\rho(x)] - d\epsilon\int d^dx\rho(x) + \mathcal{O}(\epsilon^2)$$

Transformed Γ Original Γ

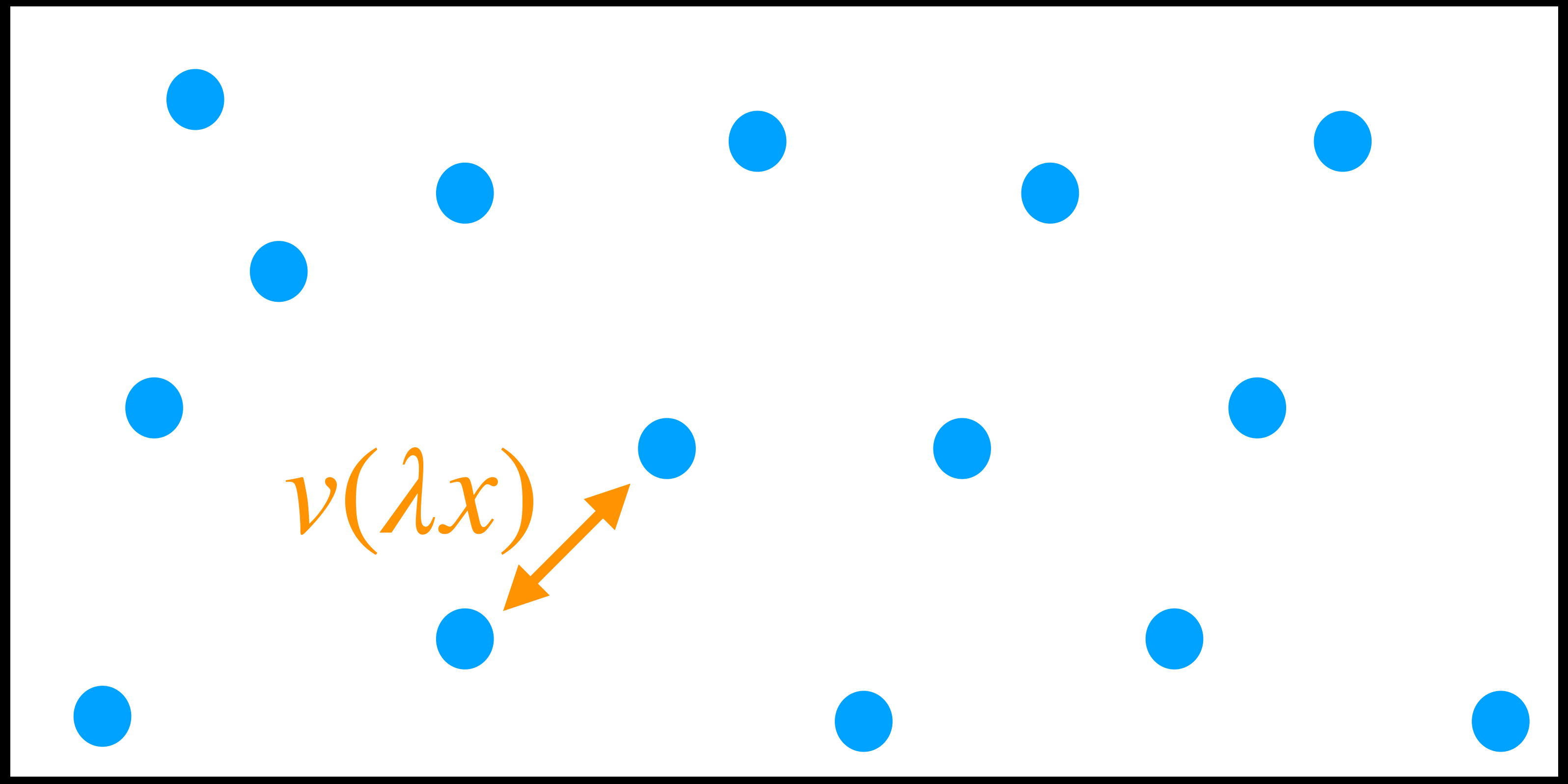
See our paper for the detailed derivation

Intuitive understanding

Cont'd

Scale-transformed system

$$\Gamma_{\lambda=1+\epsilon}[V, \rho(x)]$$



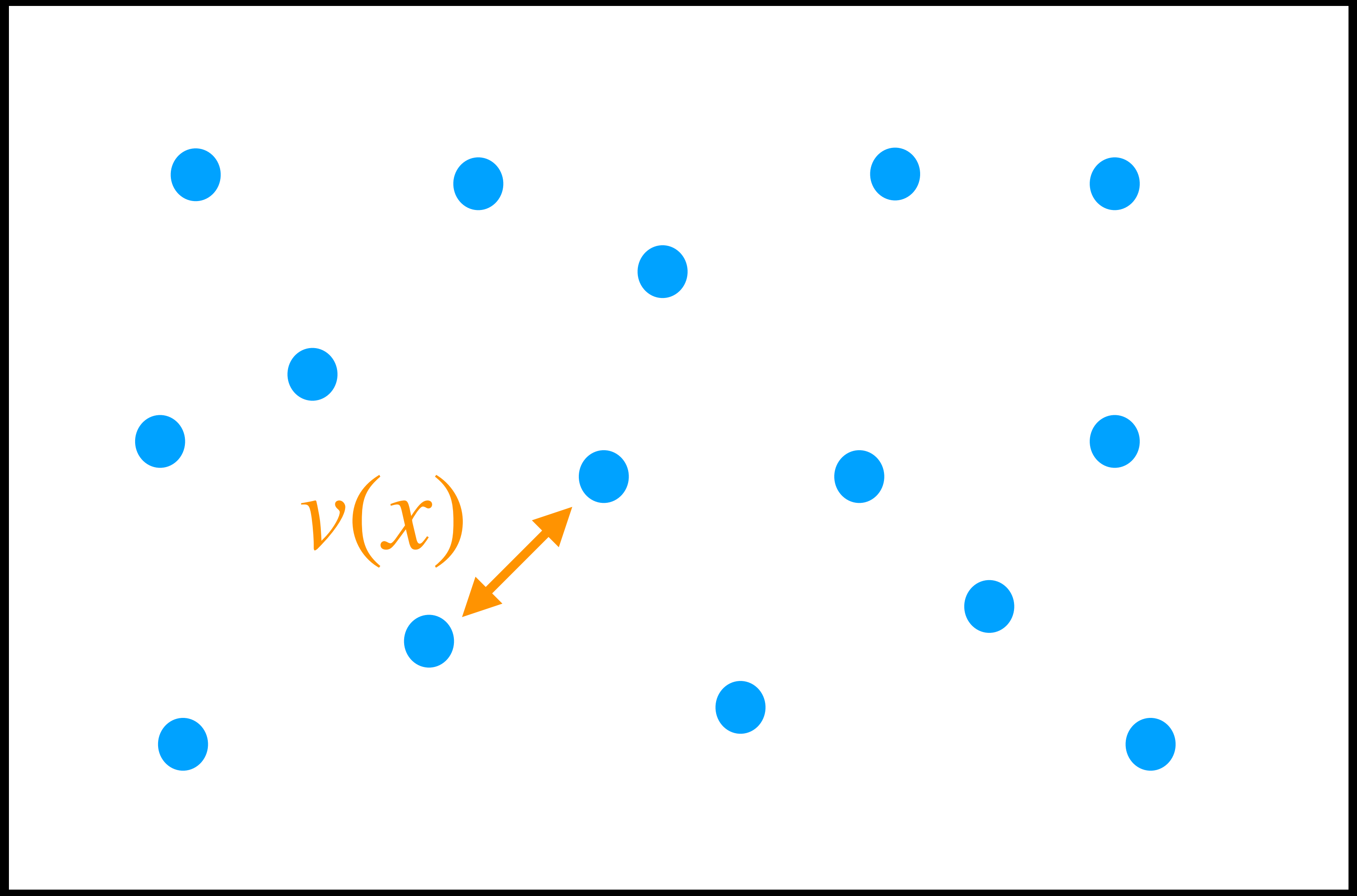
Volume = V

Density field = $\rho(x)$

$$\lambda x \rightarrow x$$

Original system but with different variables

$$\Gamma[V+\delta_\epsilon V, \rho(x)+\delta_\epsilon \rho(x)]$$



Volume = $\lambda^d V$,

Density field= $\rho(x/\lambda)$

$$\therefore -\beta\Gamma_{1+\epsilon}[V, \rho(x)] = -\beta\Gamma[V+\delta_\epsilon V, \rho(x)+\delta_\epsilon \rho(x)] - d\epsilon \int d^d x \rho(x) + \mathcal{O}(\epsilon^2)$$

Additional term is coming from Legendre transformation

Cont'd

$$-\beta\Gamma_{1+\epsilon}[V,\rho(x)] = -\beta\Gamma[V+\delta_\epsilon V,\rho(x)+\delta_\epsilon\rho(x)] - d\epsilon\int d^dx\rho(x) + \mathcal{O}(\epsilon^2)$$

In particular, when we put $\rho(x) = \rho = N/V =$ constant, we only have volume dependence

$$\left.\frac{d(-\beta\Gamma_{1+\epsilon}[V])}{d\epsilon}\right|_{\epsilon=0} = d\left.\frac{\partial}{\partial\log V}\right|_{T,N}(-\beta\Gamma[V]) - d\int d^dx\rho$$

$\because$ By using the flow equation in the L.H.S and putting $\epsilon = 0$ $(\lambda = 1)$

$$\left.\frac{\partial}{\partial\log V}\right|_{T,N}(-\beta\Gamma[V]) - \int d^dx\rho = -\frac{\beta}{d}\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n}d^dx_i\right)\sum_{i=1}^{n}\sum_{\mu=1}^{d}x_i^\mu\frac{\partial v_n(\{x_i\})}{\partial x_i^\mu}\times G^{(n)}(\{x_i\})$$

Density renormalization group for canonical potential = Zero-th order equation

However…

$$\frac{\partial}{\partial \log V}\bigg|_{T,N}(-\beta\Gamma[V]) - \int d^d x\rho = -\frac{\beta}{d}\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n}d^d x_i\right)\sum_{i=1}^{n}\sum_{\mu=1}^{d}x_i^\mu\frac{\partial v_n(\{x_i\})}{\partial x_i^\mu}\times G^{(n)}(\{x_i\})$$

- This equation itself is not new. This is well-known as pressure equation in liquid theory

In fact, by using $\frac{\partial\Gamma[\rho]}{\partial V} = -p$

$$\longrightarrow \quad \frac{p}{T} - \rho = -\frac{\beta}{d}\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n}d^d x_i\right)\sum_{i=1}^{n}\sum_{\mu=1}^{d}x_i^\mu\frac{\partial v_n(\{x_i\})}{\partial x_i^\mu}\times G^{(n)}(\{x_i\})$$

(Pressure equation)

- On the other hand, the flow equations for higher-order vertices are new !

Step 1: Take the functional derivative of $-\beta\Gamma_{1+\epsilon}[V,\rho(x)] = -\beta\Gamma[V+\delta_\epsilon V, \rho(x)+\delta_\epsilon\rho(x)] - d\epsilon\int d^d x\rho(x) + \mathcal{O}(\epsilon^2)$

Step 2: and use the flow equation in the L.H.S $\frac{dc^{(n)}(\{x_i\})}{d\epsilon} = \cdots$

DRGE for n-point 1PI vertex

[KK, S.Iso ('18), KK ('23)]

$$\left[-\frac{\partial}{\partial \log \rho}\bigg|_{T,N} + \frac{1}{d}\sum_{i=1}^{n} x_i^{\mu}\partial_{\mu}^{(i)}\right] c^{(n)}(\{x_i\}) - \delta_{n0}V\rho - \delta_{n1} = -\frac{\beta}{d}\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n} d^d y_i\right)\sum_{i=1}^{n}\sum_{\mu=1}^{d} y_i^{\mu}\frac{\partial v_n(\{y_i\})}{\partial y_i^{\mu}} \times \frac{\delta^n G_{\lambda}^{(n)}(\{y_i\})}{\delta\phi(x_1)\cdots\delta\phi(x_n)}$$

- In general, we have to represent $G^{(n)}$ as a functions of $F^{(2)}$ and $c^{(l)}$ as usual
- When only $G^{(1)}$ and $G^{(2)}$ appear in the R.H.S, their functional derivatives are easy to calculate
- Again, they are hierarchical and need some approximations for practical calculations

Q: How do we get a closure equation ?

Closure for inverse propagator in simple Liquid

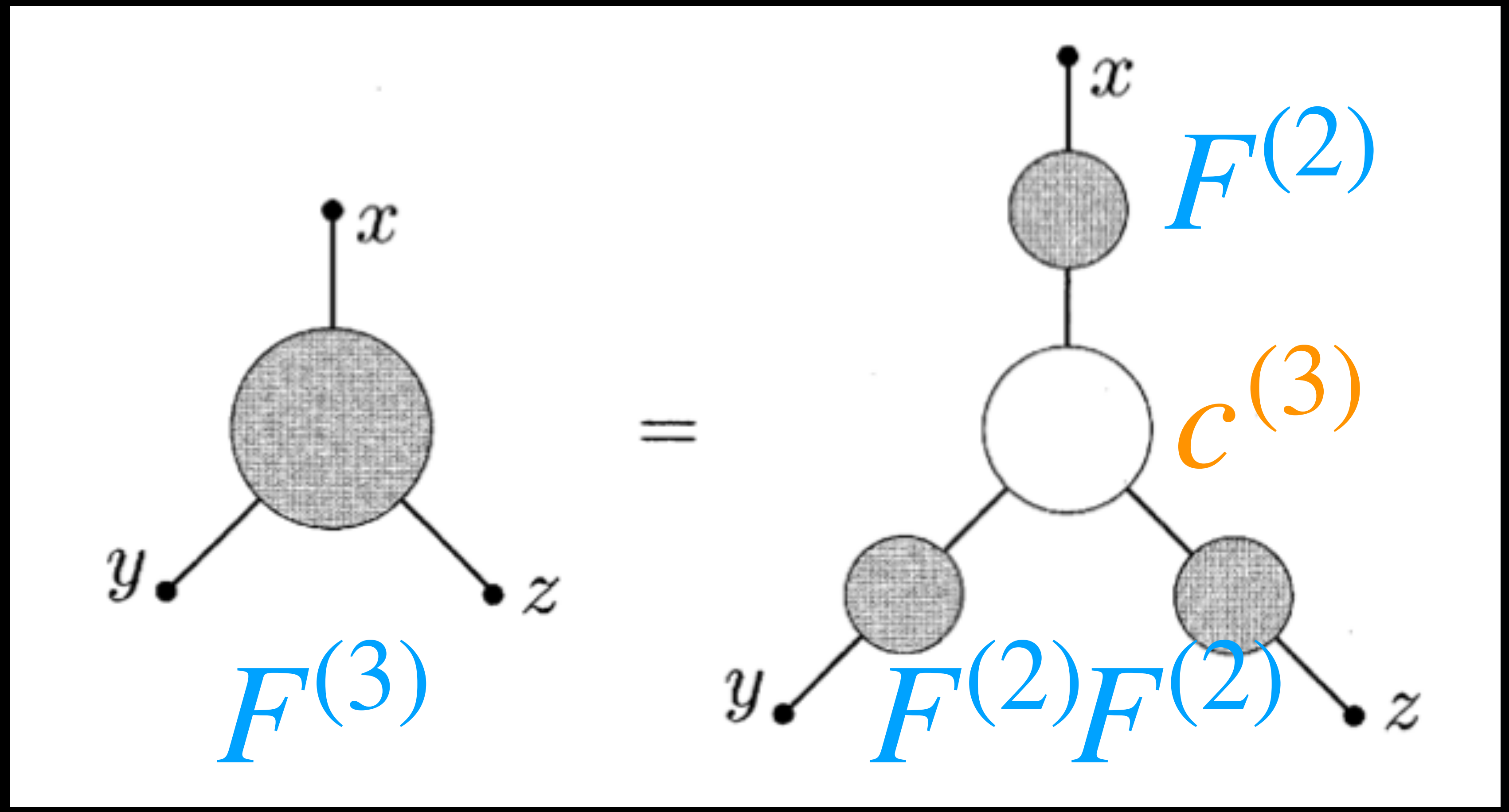
[KK, S.Iso ('18) And ongoing work with Yokota-san]

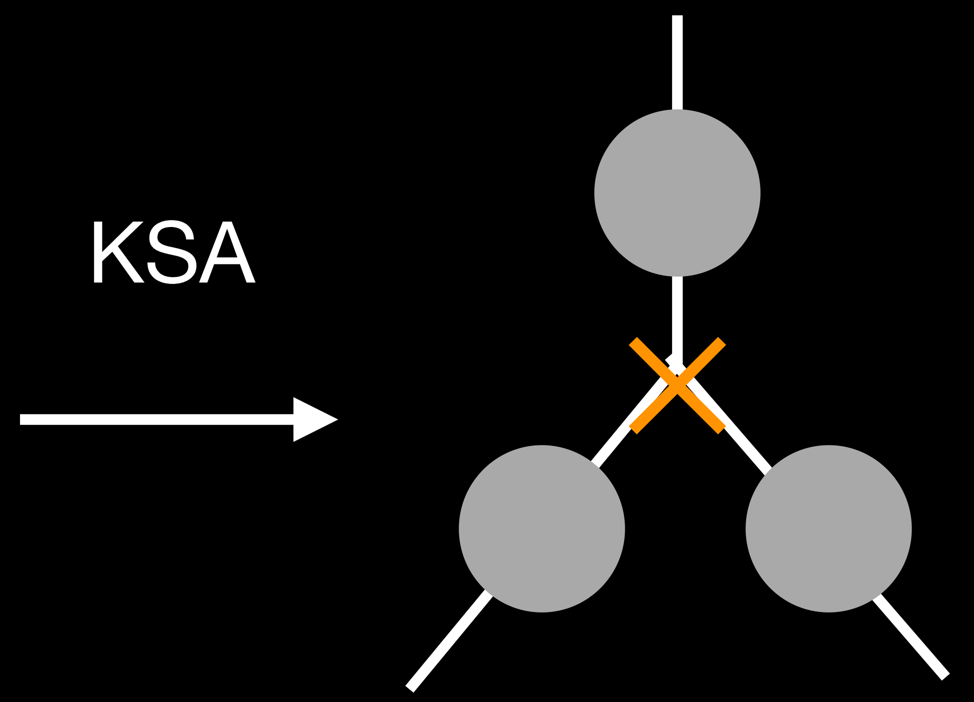
$$\left[-\frac{\partial}{\partial \log \rho}\Big|_{T,N} + \frac{1}{d}(x_1 - x_2)^\mu \partial_\mu \right] c^{(2)}(x_1 - x_2) = -\frac{\beta}{2d}\int d^d y \int d^d y' (y - y')^\mu \frac{\partial v(y - y')}{\partial y^\mu}$$

$$\times \left[F^{(2)} \cdot c^{(4)}(x_1, x_2) \cdot F^{(2)} + 2F^{(2)} \cdot c^{(3)}(x_1) \cdot F^{(2)} \cdot c^{(3)}(x_2) \cdot F^{(2)} + 2\delta^{(d)}(x_1 - y)\delta^{(d)}(x_2 - y') \right]$$

- In 1PI formalism, approximations (truncations) can be studied systematically

e.g. Kirkwood superposition approximation (KSA)





Replace $c^{(n)}$ by ideal gas case $c^{(n)}_{\rm ideal}$!

$$= \quad c^{(3)}_{\rm ideal} = \frac{1}{\rho^2}\delta^{(d)}(x_1 - x_3)\delta^{(d)}(x_2 - x_3)$$

Cont'd

∴ Closure equation for the inverse propagator in simple Liquid

$$\left[-\frac{\partial}{\partial \log \rho}\bigg|_{T,N} + \frac{1}{d}(x_1 - x_2)^\mu \partial_\mu\right] c^{(2)}(x_1 - x_2) = -\frac{\beta}{2d}\int d^d y \int d^d y' (y - y')^\mu \frac{\partial v(y - y')}{\partial y^\mu}$$

Note $F^{(2)} = -c^{(2)^{-1}}$

$$\times \left[-\frac{2\delta^{(d)}(x_1 - x_2)}{\rho^3} F^{(2)}(y) F^{(2)}(y') + \frac{2}{\rho^4} F^{(2)}(x_1 - x_2) F^{(2)}(x_1 - y) F^{(2)}(x_2 - y') + 2\delta^{(d)}(x_1 - y)\delta^{(d)}(x_2 - y')\right]$$

contact term — nontrivial term — constant term

- It is difficult to solve this analytically → needs numerical approach
- The R.H.S is just a convolution → One loop expression in momentum space
- In principle, we can further improve the truncation based on the Virial expansion

$$c^{(n)} = c^{(n)}_{\text{ideal}} \;\rightarrow\; c^{(n)}_{\text{ideal}} + \sum_{m=1}^{\infty} \rho^{i-(n-1)} c^{(n)}_i$$

e.g. $c^{(3)}_1 = 0\ , \quad c^{(3)}_2 \sim f \cdot f \cdot f$

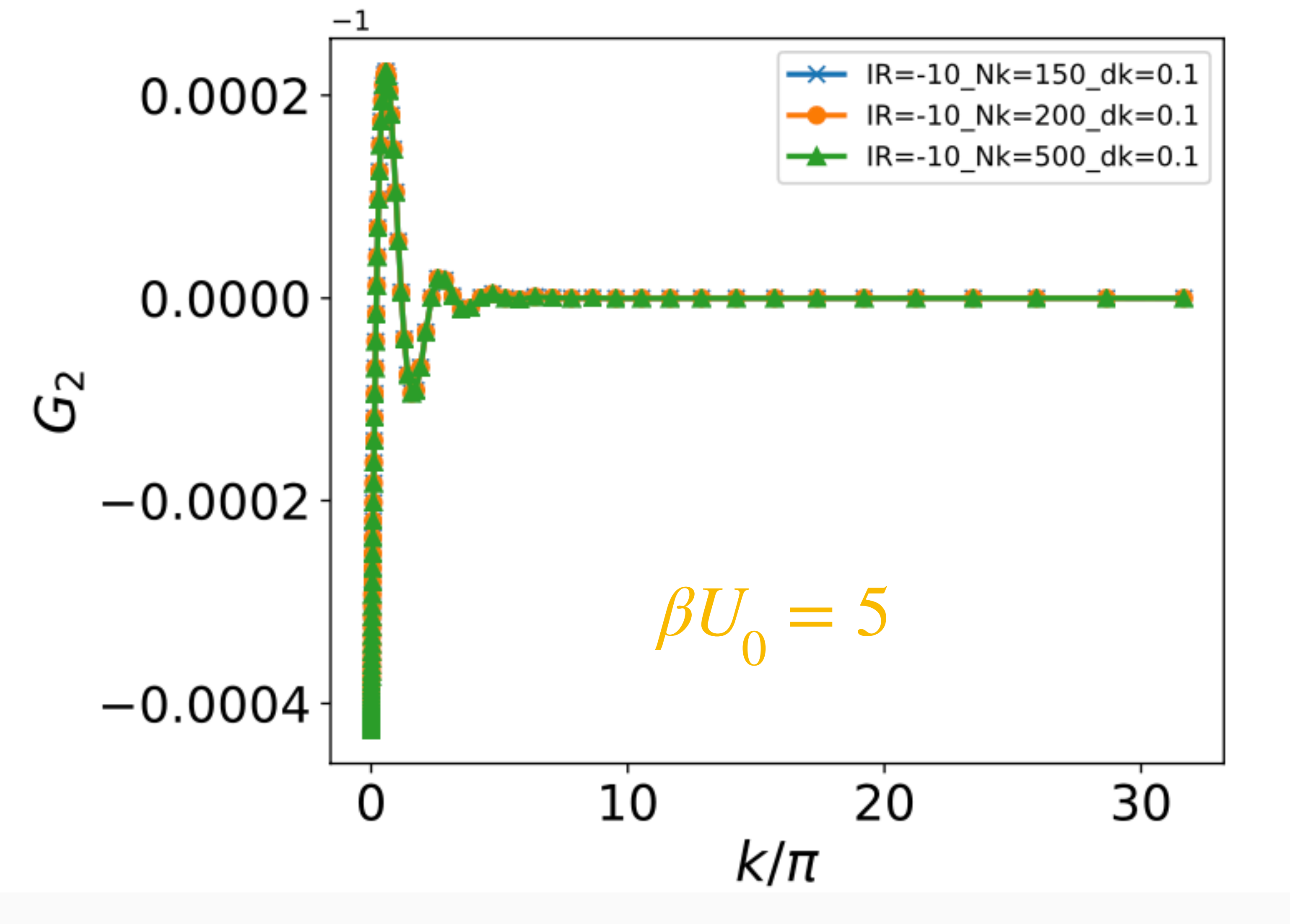
$f = e^{\beta v} - 1$ =Mayer's f function

First attempt in hard-sphere system

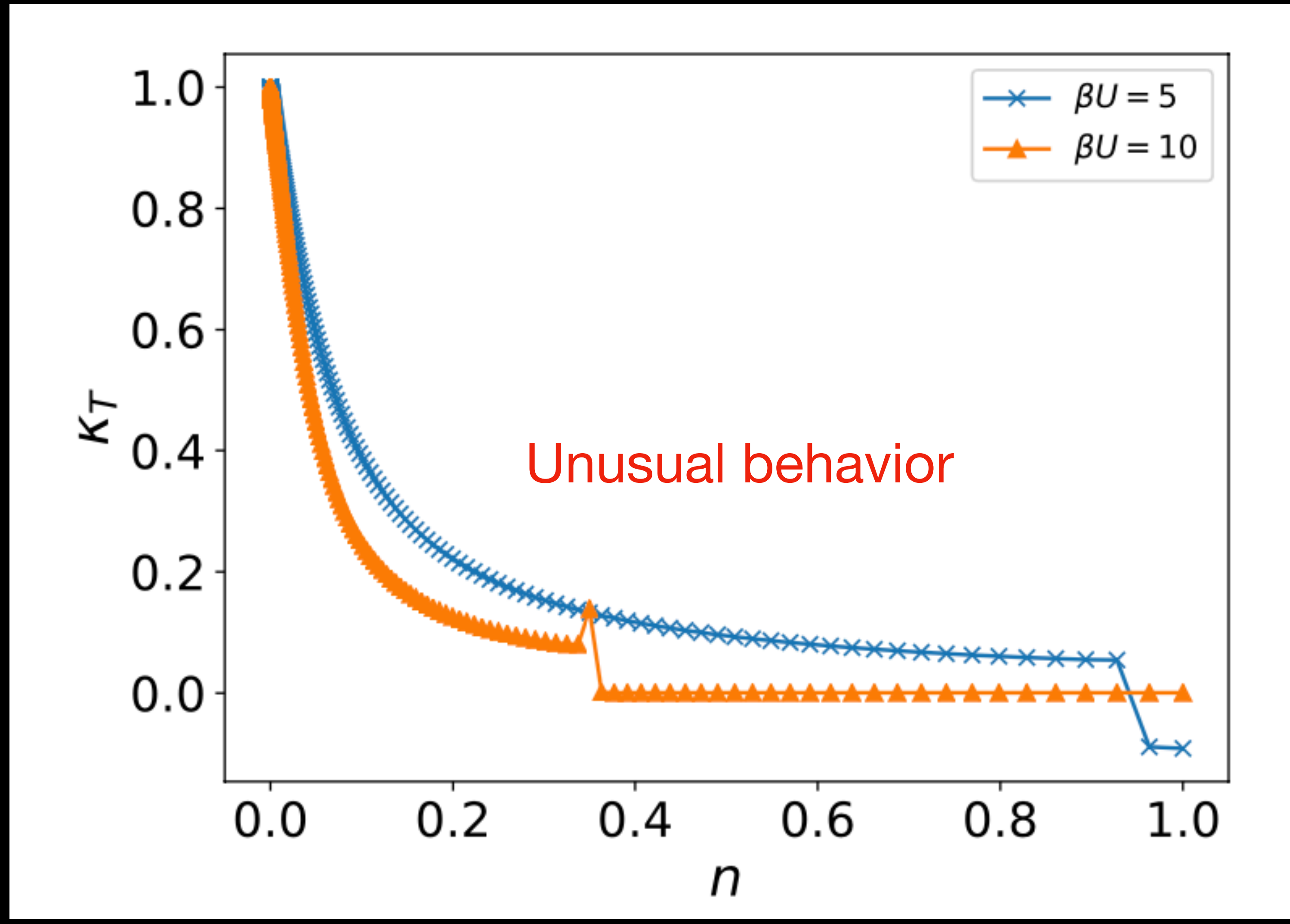
$v(x) = U_0 \times \theta(a - |x|)$

Fourier mode of $c^{(2)}$

Different colors
= Different UV cut off scales
in momentum integration



Compressibility $\kappa_T = \frac{1}{T}\frac{\partial n}{\partial p}$



In the left plot, we realized that we focused on very high density region (i.e. packing fraction $\eta \gg 1$)

→ Need to refine the calculations. In progress with Yokota-san (RIKEN)

Plan of Talk

1. General flow approach in statistical mechanics
2. Classical liquids systems (HRT and DRG)
3. Optimized cut off and critical phenomena in HRT (in progress)
4. Summary

How to choose cut-off function ?

Regulator function

$$R_k(x-y) = \beta\left[v_k(x-y) - v(x-y)\right]$$

- We consider HRT in the following.

$$\frac{d(\beta^{-1}\Gamma_k[\rho])}{dk} = \frac{1}{2}\mathrm{Tr}\left[(\partial_k R_k)\left(\Gamma_k^{(2)} + R_k\right)^{-1}\right]$$

- Conventionally, sharp cut-off schemes were often used in HRT

[Parola, Reatto ('84), JM Caillol ('06)]

e.g.

$$\tilde{v}_k(p) = \tilde{v}(p) \times \theta_\epsilon(p-k) \rightarrow \tilde{v}(p) \times \theta(p-k)$$

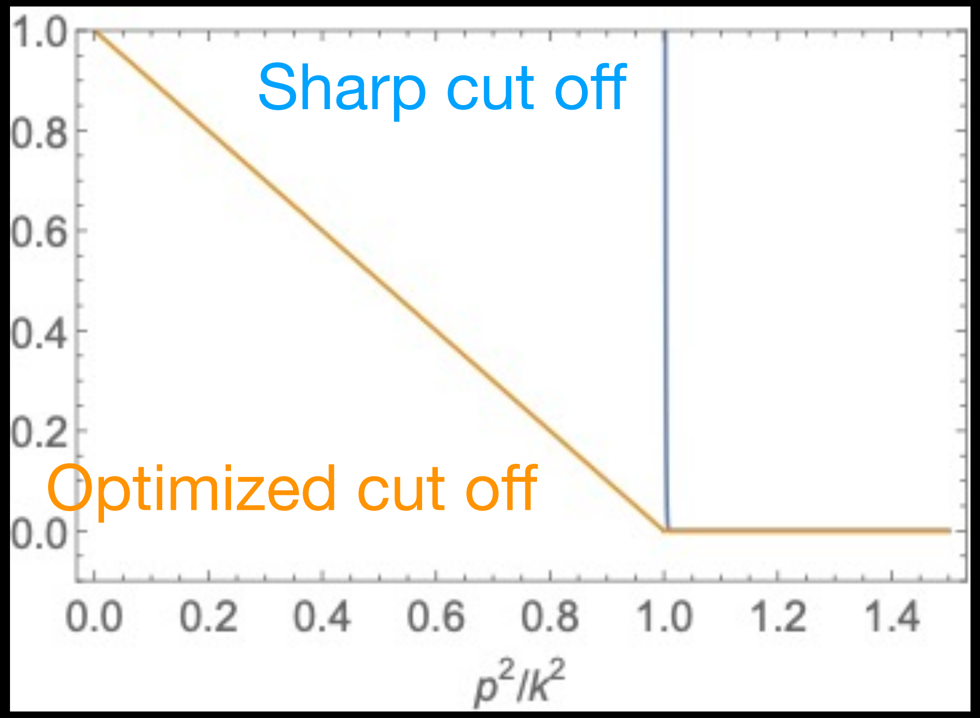
Mild sharp cut off   Ultra sharp cut off

Question: Is this the only way ?
How about functional RG in QFT ?

Cont'd

How to choose cut-off function ?

- In functional RG in QFT, however, people usually take action-independent regulator



$$\tilde{R}_k(p) = \begin{cases} p^2\left[\theta\left(\left(\frac{p}{k}\right)^2 - 1\right)^{-1} - 1\right] & \text{(Sharp cut off)} \\ (k^2 - p^2)\,\theta\left(1 - \left(\frac{p}{k}\right)^2\right) & \text{(Optimized sharp cut off)} \end{cases}$$

[Litim (2001)]

In these cases, the flow equation does not depend on the microscopic (bare) action.

∴ The microscopic information only appears as the initial condition $\Gamma_{k=\Lambda}[\phi] = S_\Lambda[\phi]$

Why not using the similar cut-off scheme in liquid systems ?

Optical cut off in classical liquids

[Work in progress]

- We propose to use the optimized cut-off regulator

$$\tilde{R}_k(p) = \frac{Z_k}{K^{d+2}}(k^2 - p^2)\theta\left(1 - \frac{p^2}{k^2}\right)$$

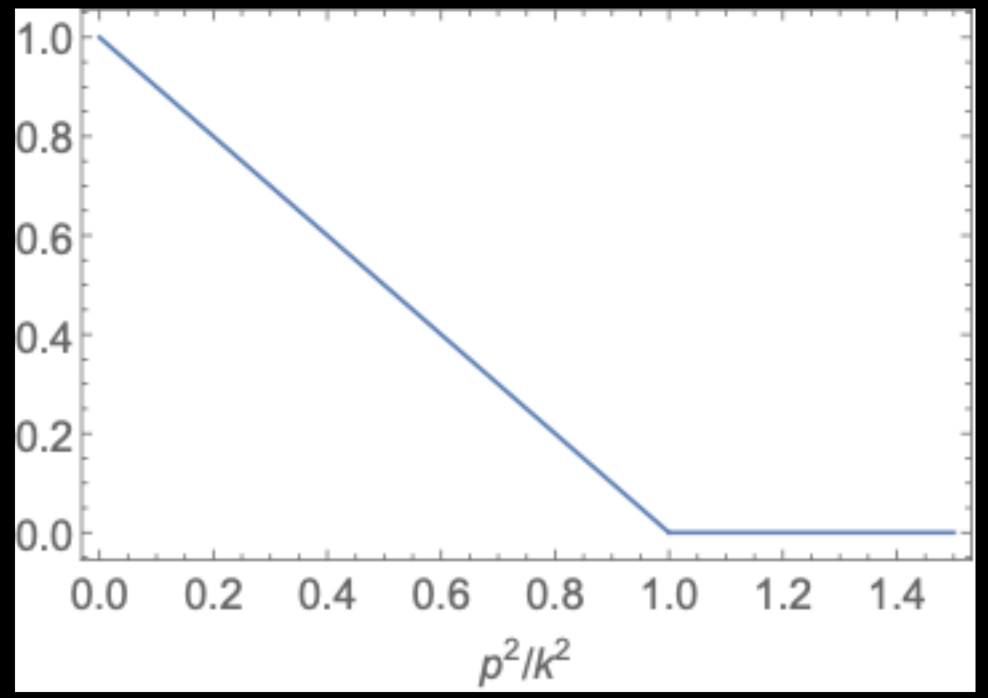
Z_k = wave function renormalization
K = some dimension 1 parameter
(e.g. $K = a^{-1}$ = microscopic scale)

- The flow equation becomes

$$N_d = \frac{\mathrm{Area}(S^{d-1})}{(2\pi)^d}$$

$$\frac{1}{V_d}\frac{d(\beta\Gamma_k[\rho])}{dk} = \frac{N_d Z_k k^{d-1}}{2}\int_0^1 dy \frac{y^{\frac{d-2}{2}}}{K^{d+2}\tilde{c}^{(2)}(p) + Z_k(1-y)}$$

$\tilde{R}_k(p)$



This is still exact (no approximation yet)

Integration in the R.H.S can be done analytically under the Local potential Approximation (LPA)
→ One of the advantages of the optical cut-off scheme !

LPA in optical cut-off scheme

[Work in progress]

- LPA

$$\beta\Gamma_k[\rho] = \frac{1}{K^{d+2}}\int d^dx \left(\frac{Z_k}{2}(\partial_\mu\rho)^2 + U_k(\rho)\right) \longrightarrow \tilde{c}^{(2)}(p) = Z_k p^2 + U_k''(\rho)$$

$$\therefore \quad \frac{1}{K^{d+2}k^d}\frac{dU_k[\rho]}{d\log k} = \frac{N_d}{1 + Z_k^{-1}k^{-2}U_k''(\rho)}$$

(Flow equation for the local potential $U_k(\rho)$)

- Another good point of this scheme = LPA is consistent with the ideal-gas initial condition

$$\beta\Gamma_{\mathrm{ideal}}[\rho] = -\int d^dx\rho\left[1 - \log\rho\right] \longleftrightarrow Z_{k=\infty} = 0\ , \quad U_{k=\infty}(\rho) = -K^{d+2}\rho(1 - \log\rho)\ .$$

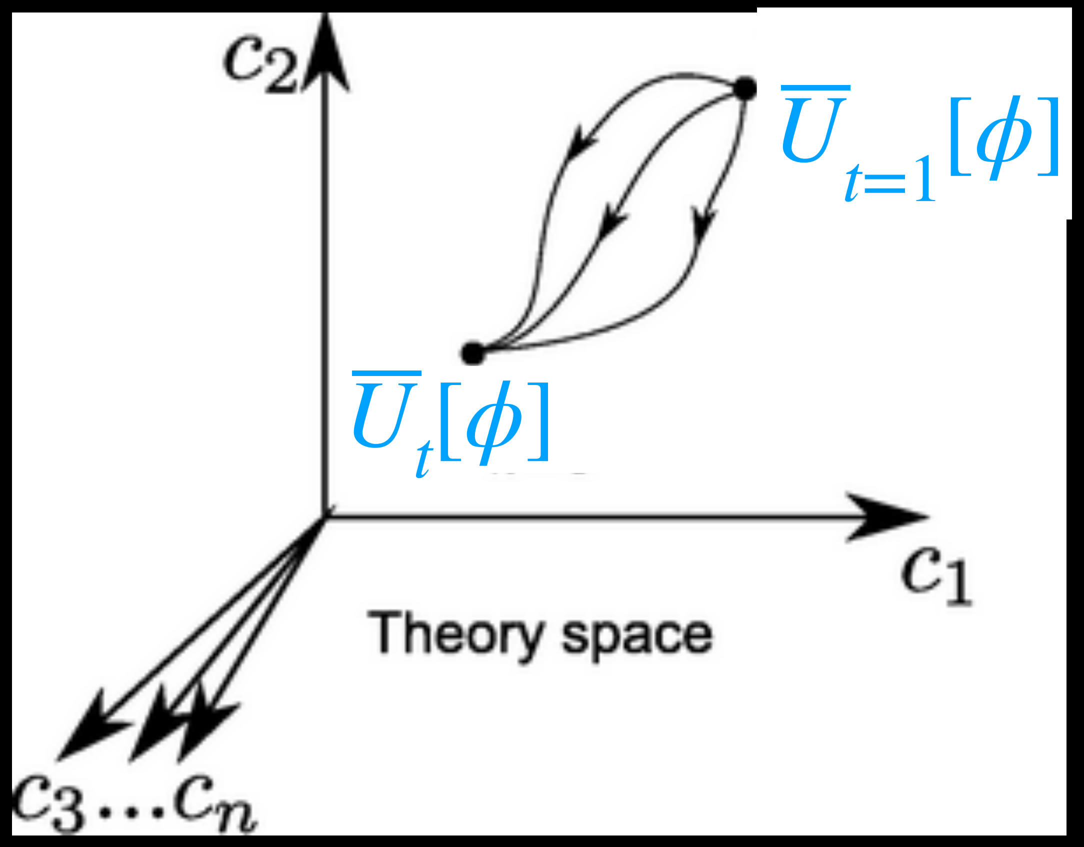
But, once interaction is added, classical liquid system is non-local
Can we come up with a good initial condition within LPA ?
→ Leave this issue and let us focus on critical phenomena for now

Flow equation for dimensionless potential

[Work in progress]

Flow equation $$\frac{1}{K^{d+2}k^d}\frac{dU_k[\rho]}{dt} = \frac{N_d}{1+Z_k k^{-2}U_k''(\rho)}$$ $t = \log k$

- It is convenient to introduce dimensionless variables



$$z = \frac{\rho}{K^{\frac{d+2}{2}}k^{\frac{d-2}{2}}}, \qquad \overline{U}_t(\overline{z}) = \frac{U_k(\rho)}{K^{d+2}k^d},$$

$$\longrightarrow \quad \left(d + \frac{\partial}{\partial t} - \frac{d-2+\eta_k}{2}\frac{\partial}{\partial \log z}\right)\overline{U}_t(z) = \frac{N_d}{1+\overline{U}_t''(z)} - N_d$$

Non-pertubative effects

∴ Fixed point is determined by

$$\left(d - \frac{d-2+\eta_*}{2}\frac{\partial}{\partial \log z}\right)\overline{U}_*(z) = \frac{N_d}{1+\overline{U}_*''(z)} - N_d$$

Second-order differential equation

Polynomial expansion and fixed point

[Work in progress]

$$\left(d + \frac{\partial}{\partial t} - \frac{d-2+\eta_k}{2}\frac{\partial}{\partial \log z}\right)\overline{U}_t(z) = \frac{N_d}{1+\overline{U}_t''(z)} - N_d$$

- We can study fixed point by assuming a $\mathbb{Z}_2$ - invariant polynomial $\overline{U}_t(\overline{\rho}) = \sum_{n=2}^{\infty} \frac{\lambda_{2n}(t)}{(2n)!} z^{2n}$

$\epsilon = 4 - d$

RGEs

$$\frac{d\lambda_2}{dt} + 2\lambda_2 = -\frac{N_d}{(1+\lambda_2)^2}\lambda_4$$

$$\frac{d\lambda_4}{dt} + \epsilon\lambda_4 = \frac{N_d}{(1+\lambda_2)^2}\left(-\lambda_4 + \frac{6\lambda_4^2}{1+\lambda_2}\right)$$

$$\frac{d\lambda_6}{dt} + 2(3-d)\lambda_6 = \frac{N_d}{(1+\lambda_2)^2}\left(-\lambda_8 + \frac{20\lambda_2\lambda_4}{1+\lambda_2} - \frac{90\lambda_2\lambda_4^3}{(1+\lambda_2)^2}\right)$$

$$\cdots$$

Wilson-Fischer fixed point

$$\begin{cases} \lambda_{2*} = -\dfrac{\epsilon}{12+\epsilon} \\ \lambda_{4*} = \dfrac{288\epsilon}{N_d(12+\epsilon)^3} \end{cases}$$

for $\lambda_n = 0 \ (n \geq 6)$

Critical exponent in Polynomial expansion

[Work in progress]

- Linearlized flow around the fixed point (Note: we haven't used epsilon expansion yet)

$$\frac{d\delta\lambda_2}{dt} = -\left(2 - \frac{\varepsilon}{3}\right)\delta\lambda_2 - \frac{N_d(12+\varepsilon)^2}{144}\delta\lambda_4$$

$$\frac{d\delta\lambda_4}{dt} = -\frac{72\varepsilon^2}{N_d(12+\varepsilon)^2}\delta\lambda_2 + \varepsilon\delta\lambda_4$$

Diagonalization →

$$-\frac{d}{dt}\begin{pmatrix}\delta\lambda_2 \\ \delta\lambda_4\end{pmatrix} = \begin{pmatrix} a_1 & 0 \\ 0 & a_2 \end{pmatrix}\begin{pmatrix}\delta\lambda_2 \\ \delta\lambda_4\end{pmatrix}$$

$$a_1 = \frac{6 - 4\varepsilon + \sqrt{36 + 24\varepsilon + 22\varepsilon^2}}{6} \underset{\varepsilon \ll 1}{\to} 2 - \frac{\varepsilon}{3}$$

Matches the leading result of epsilon expansion

However…

$$\nu = \frac{1}{a_1} \simeq 0.54 \quad (\varepsilon = 1)$$

which is much smaller than the observed value $\nu \simeq 0.63$

→ Higher-order vertices should be included in the present formalism
or
Polynomial expansion itself may not be appropriate

What to do next

- Want to improve the calculations of critical exponents without relying on polynomial expansion

Actually, critical exponents in LPA have been already studied in many literatures

Table form arXiv: 2006. 04853

N	Correlation-length exponent ν	Include higher derivative terms								Conformal Bootstrap
	LPA	DE_2	DE_4	DE_6	LPA″	BMW	MC	PT	ϵ-exp	CB
0	0.5925	0.5879(13)	0.5876(2)	–	–	0.589	0.58759700(40)	0.5882(11)	0.5874(3)	0.5876(12)
1	0.650	0.6308(27)	0.62989(25)	0.63012(16)	0.631	0.632	0.63002(10)	0.6304(13)	0.6292(5)	0.629971(4)
2	0.7090	0.6725(52)	0.6716(6)	–	0.679	0.674	0.67169(7)	0.6703(15)	0.6690(10)	0.6718(1)

- How does Localness appear in classical liquid system at around critical point ?

- Classical liquid system is non-local in nature. Thus, it would be better to consider non-local potential approximation like

$$\Gamma_{\mathrm{NLPA}}[\rho] = \int d^d x \int d^d y \left(\frac{Z_k(x,y)}{2} (\partial\rho(x))(\partial\rho(y)) + U(\rho(x),\rho(y)) \right) \ ?$$

Summary

- We discussed general functional flow approach in equilibrium systems

$$\frac{d(-\beta\Gamma[\{\lambda_a\};\phi])}{d\lambda_a} = -\beta\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n}d^d x_i\right)\frac{\partial v_n}{\partial\lambda_a}\times G^{(n)}(\{x_i\};J_\phi)$$

- Once we get a flow equation, what we should do is (1) to find/introduce a good parameter and (2) to find a good approximation/truncation to solve the flow equation for a given system

- Classical liquid system is a good application field of flow approach: HRT, DRG, and more

- Even after some approximation/truncation, numerical calculations are still necessary

- In my opinion, there is still plenty of rooms for analytical studies
  e.g. critical phenomena, phase transitions, new closure equations, etc…

Thank you for your attention !

Backup

Nambu's discussion

[Y. Nambu (87)]

- Grand potential of Ideal gas $$-\beta W_{\mathrm{ideal}} = \exp\left(\beta\mu + \log(VT^{\alpha}m^{-\alpha+3})\right) \quad , \quad \alpha = \frac{3}{2} \text{ for } d = 3$$
- On the other hand, consider two-loop RGE of gauge coupling

$$\frac{dg^2}{d\log M} = \beta(g^2) = b_1 g^4 + b_2 b^6 \longrightarrow \frac{1}{g^2} = \frac{1}{g_0^2} - b_1 \log\left(\frac{M}{M_0}\right) - \frac{b_2}{b_1}\log\left(\frac{g^2}{g_0}\right) + \cdots \quad \bigstar$$

- By putting $$g^2 \to T\,, \quad M \to V^{-1/d} \quad \frac{d}{b_1} \to \mu\,, \quad d\frac{b_2}{b_1} \to \alpha$$

$$\bigstar \longrightarrow \frac{\mu}{T_0} = \frac{\mu}{T} + \log\left(\frac{VT^{\alpha}}{V_0 T_0^{\alpha}}\right) \propto \log(-\beta W_{\mathrm{ideal}})$$

∴ RGE = adiabatic process such that W=constant in Ideal gas

But, the above identifications look very weird

Callan Symanzik equations

[KK, arXiv:2309.10496]

- Consider a situation such that the variation of a parameter $t := \lambda_0$ can be compensated by the changes of other variables

$$\Gamma[\{t-\delta t, \lambda_k, V\}; \phi] = \Gamma[\{t, \lambda_k+\delta\lambda_k, V+\delta V\}; \phi+\delta\phi]$$

- In this case, the t-derivative is related to the derivatives of other variables.

$$-\frac{d(-\beta\Gamma[\{t,\lambda_k,V\},\phi])}{dt} = \left(\sum_k \frac{\delta\lambda_k}{\delta t}\frac{\partial}{\partial\lambda_k} + \frac{\delta V}{\delta t}\frac{\partial}{\partial V} + \int d^dx \frac{\delta\phi(x)}{\delta t}\frac{\delta}{\delta\phi(x)}\right)\Gamma[\{t,\lambda_k,V\},\phi]$$

∴ Using the flow equation in the L.H.S, we obtain

$$\left(\sum_k \frac{\delta\lambda_k}{\delta t}\frac{\partial}{\partial\lambda_k} + \frac{\delta V}{\delta t}\frac{\partial}{\partial V} + \int d^dx \frac{\delta\phi(x)}{\delta t}\frac{\delta}{\delta\phi(x)}\right)\Gamma[\{t,\lambda_k,V\},\phi] = -\beta\sum_{n=1}^{\infty}\frac{1}{n!}\int\left(\prod_{i=1}^{n} d^dx_i\right)\frac{\partial v_n(\{x_i\})}{\partial t}\times G^{(n)}(\{x_i\};J_\phi)$$

Generalized Callan-Symanzik equation

Optimized regulator

$$\frac{d(\beta^{-1}\Gamma_k[\rho])}{dk} = \frac{1}{2}\mathrm{Tr}\left[(\partial_k R_k)\left(\Gamma_k^{(2)} + R_k\right)^{-1}\right]$$

- Optimization criterion = maximize the minimum of inverse propagator

Maximize $\min_p(\Gamma_k^{(2)}(p) + R_k(p))$ ← If this is zero, it means the existence of Gapless mode
And the flow might be ill-defined

- But, still so many possible regulators … → Choose a simple one !

e.g. Flat inverse propagator choice

$$m_k^2 + Z_k p^2 + R_k(p) = \text{constant} \quad \text{for } p^2 < k^2$$

with the conditions

$$R_k(p) = 0 \text{ for } p > k$$

$$\lim_{k\to 0} R_k(p) = 0$$

→

Simplest one

$$R_k(p) = Z_k(k^2 - p^2)\theta\left(1 - \frac{p^2}{k^2}\right)$$

[Litim ('01)]