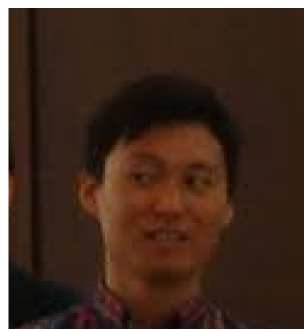
Replica evolution of classical field in 4+1 dimensional spacetime toward real time dynamics of quantum field

Akira Ohnishi[1], H. Matsuda[2], T. Kunihiro[1], T. T. Takahashi[3]

1. YITP, Kyoto U., 2. Dept. Phys., Kyoto U., 3. NCT, Gunma

arXiv:submit/3309636 [hep-lat] 5 August 2020

Asia-Pacific Symposium for Lattice Field Theory (APLAT 2020), Aug. 4-7, 2020 (on Zoom).

arXiv paper is still “on hold”. Please be patient.

PTEP

Prog. Theor. Exp. Phys. **2015**, 00000 (26 pages)
DOI: 10.1093/ptep/0000000000

Replica evolution of classical field in 4+1 dimensional spacetime toward real time dynamics of quantum field †

Akira Ohnishi[1], Hidefumi Matsuda[2], Teiji Kunihiro[1], and Toru T. Takahashi[3]

[1] *Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan*
[*] *E-mail: ohnishi@yukawa.kyoto-u.ac.jp*
[2] *Department of Physics, Faculty of Science, Kyoto University, Kyoto 606-8502, Japan*
[3] *National Institute of Technology, Gunma college, Gunma 371-8530, Japan*

Real-time evolution of replicas of classical field is proposed as an approximate simulator of real-time quantum field dynamics at finite temperatures. We consider N classical field configurations, $(\phi_{\tau\boldsymbol{x}}, \pi_{\tau\boldsymbol{x}})(\tau = 0, 1, \cdots N-1)$, dubbed as replicas, which interact with each other via the τ-derivative terms and evolve with the classical equation of motion. The partition function of replicas is found to be proportional to that of quantum field in the imaginary time formalism. Since the replica index can be regarded as the imaginary time index, the replica evolution is technically the same as the molecular dynamics part of the hybrid Monte-Carlo sampling. Then the replica configurations should reproduce the correct quantum equilibrium distribution after the long-time evolution. At the same time, evolution of the replica-index average of field variables is described by the classical equation of motion when the fluctuations are small. In order to examine the real-time propagation properties of replicas, we first discuss replica evolution in quantum mechanics. Statistical averages of observables are precisely obtained by the initial condition average of replica evolution, and the time evolution of the unequal-time correlation function, $\langle x(t)x(t')\rangle$, in a harmonic oscillator is also described well by the replica evolution in the range $T/\omega > 0.5$. Next, we examine the statistical and dynamical properties of the ϕ^4 theory in the 4+1 dimensional spacetime, which contains three spatial, one replica index or the imaginary time, and one real time. We note that the Rayleigh-Jeans divergence can be removed in replica evolution with $N \geq 2$ when the mass counterterm is taken into account. We also find that the thermal mass obtained from the unequal-time correlation function at zero momentum grows as a function of the coupling as in the perturbative estimate in the small coupling region.

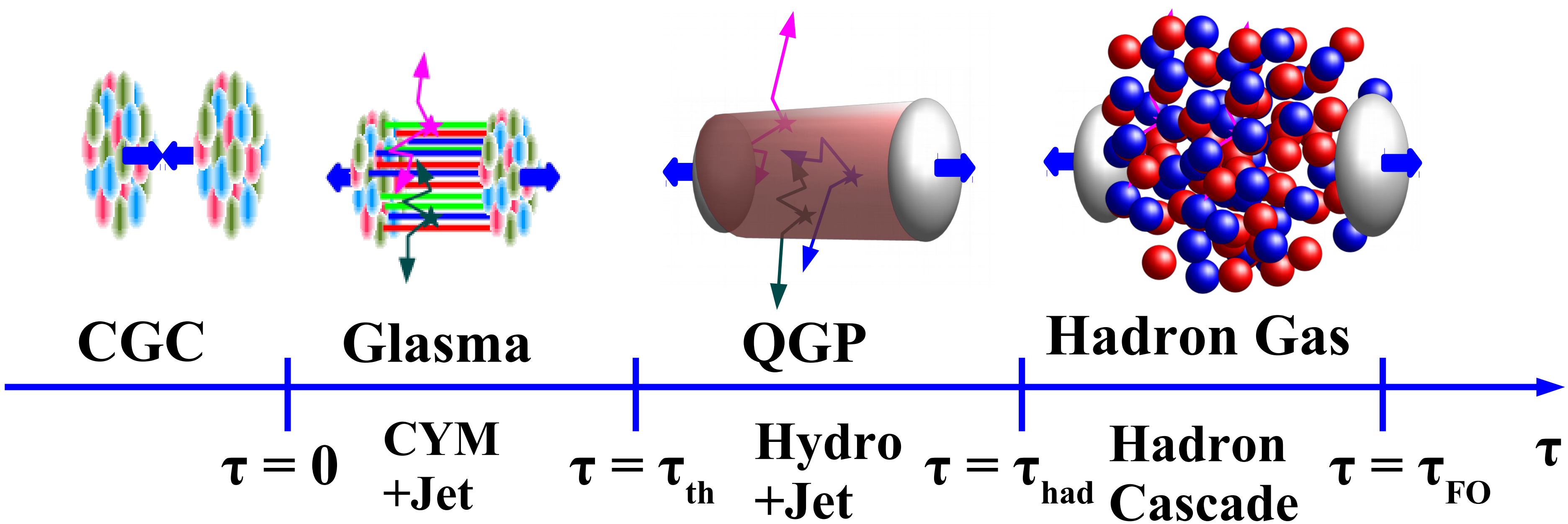
http://www2.yukawa.kyoto-u.ac.jp/~akira.ohnishi/Src/Org/Replica-arXiv.pdf

Contents

- Introduction
- Replica Evolution
- Replica Evolution of a Single Harmonic Oscillator
- Replica Evolution in Scalar Field Theory
  - Momentum distribution and Rayleigh-Jeans divergence
  - Time-correlation function and thermal mass
- Summary

Heavy-Ion Collisions on the Lattice ?

- **Initial Condition: Color Glass Condensate (CGC)**
- **Early Stage: Glasma**
- **Main Stage: Quark Gluon Plasma (QGP)**
- **Final Stage: Hadron Gas**



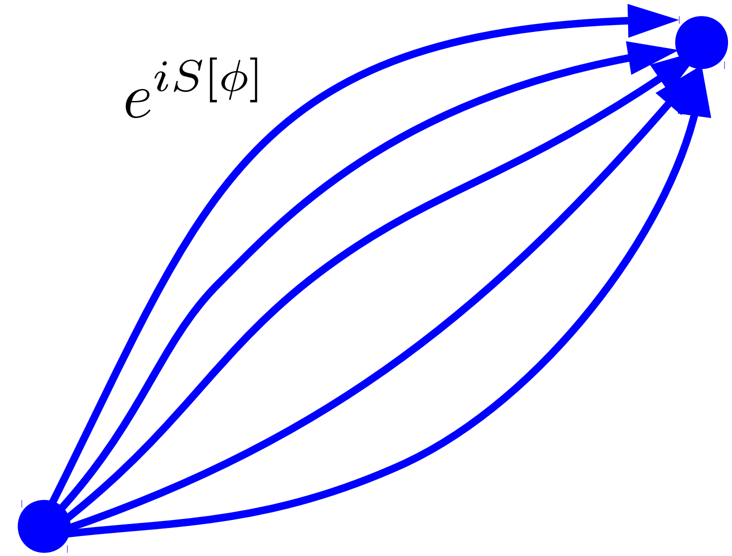
Unreachable Dream ?

Classical Field Evolution

- **Path integral of real time evolution**

$$S_{fi} = \mathcal{N} \int \mathcal{D}\phi \, \langle \Psi(t_f) | \exp\left(iS[\phi]\right) | \Psi(t_i) \rangle$$

  - **Cancellation of amplitudes by exp(iS)** **→ Severe sign problem**



- **Classical Field Evolution**
  - **Euler-Lagrange equation choose path with δS=0 → No sign problem**
  - **Useful in discussing far-from-equilibrium phenomena**
    condensate evolution (Time dep. Gross-Pitaevski), nuclear excitation (TD Hartree-Fock), Inflation, high-energy heavy-ion collisions (classical Yang-Mills), …
  - **But converges to incorrect equilibrium**

$$n_{\boldsymbol{k}} = T/\omega_{\boldsymbol{k}} (\text{Classical}), \quad n_{\boldsymbol{k}} = [\exp(\omega_{\boldsymbol{k}}) \mp 1]^{-1} \, (\text{Quantum})$$

Is ther framework for far-from-equilibrium and around equilibrium ?

Replica evolution

Replica Partition Function (Quantum Mechanics)

- **Part. func. in Classical Mechanics**

$$\mathcal{Z}_C(T) = \int \frac{dxdp}{2\pi} \exp\left[-\frac{H(x,p)}{T}\right] \qquad H = \frac{p^2}{2} + U(x)$$

- **Part. func. in Quantum Mechanics (imag. time formalism)**

$$\mathcal{Z}_Q(T) = \int \mathcal{D}x \exp\left(-S[x]\right) \qquad S = \frac{1}{\xi}\left[\mathcal{V} + \sum_{\tau=1}^{N} U(x_\tau)\right]$$

$$\xi = a/a_\tau, a^3 a_\tau = a^4/\xi, T = \xi/N, \mathcal{V} = \sum_{\tau=1}^{N} \frac{\xi^2}{2}(x_{\tau+1} - x_\tau)^2 \simeq \xi \int_0^{1/T} d\bar{\tau} \frac{1}{2}\left[\frac{\partial x}{\partial \bar{\tau}}\right]^2$$

- **Part. func. in Replicas**
(N classical systems interacting with τ-derivative terms $\mathcal{V}$)

$$\mathcal{Z}_R(\xi) = \int \frac{\mathcal{D}x\mathcal{D}p}{2\pi} \exp\left(-\frac{\mathcal{H}[x,p]}{\xi}\right) \qquad \mathcal{H} = \boxed{\sum_{\tau=1}^{N} \underbrace{\left[\frac{p_\tau^2}{2} + U(x_\tau)\right]}_{H(x_\tau,p_\tau)} + \mathcal{V}} \; \xi S[\phi]$$

$$= (2\pi\xi)^{NL^3/2} Z_Q(T)$$

Part. fn. of N classical systems interacting via V at temp. ξ
∝ Part. fn. of quantum mech. at temp. T=ξ/N (MD in HMC)

Evolution of Replica-Index Average

- **Canonical equation of Motion for replica variables (x_τ, p_τ)**

$$\frac{dx_\tau}{dt} = \frac{\partial \mathcal{H}}{\partial p_\tau} = p_\tau$$

$$\frac{dp_\tau}{dt} = -\frac{\partial \mathcal{H}}{\partial x_\tau} = -\frac{\partial U(x_\tau)}{\partial x_\tau} + \underbrace{\xi^2 (x_{\tau+1} + x_{\tau-1} - 2x_\tau)}_{\tau\text{-derivative terms}}$$

- **Replica index average**

τ-derivative terms

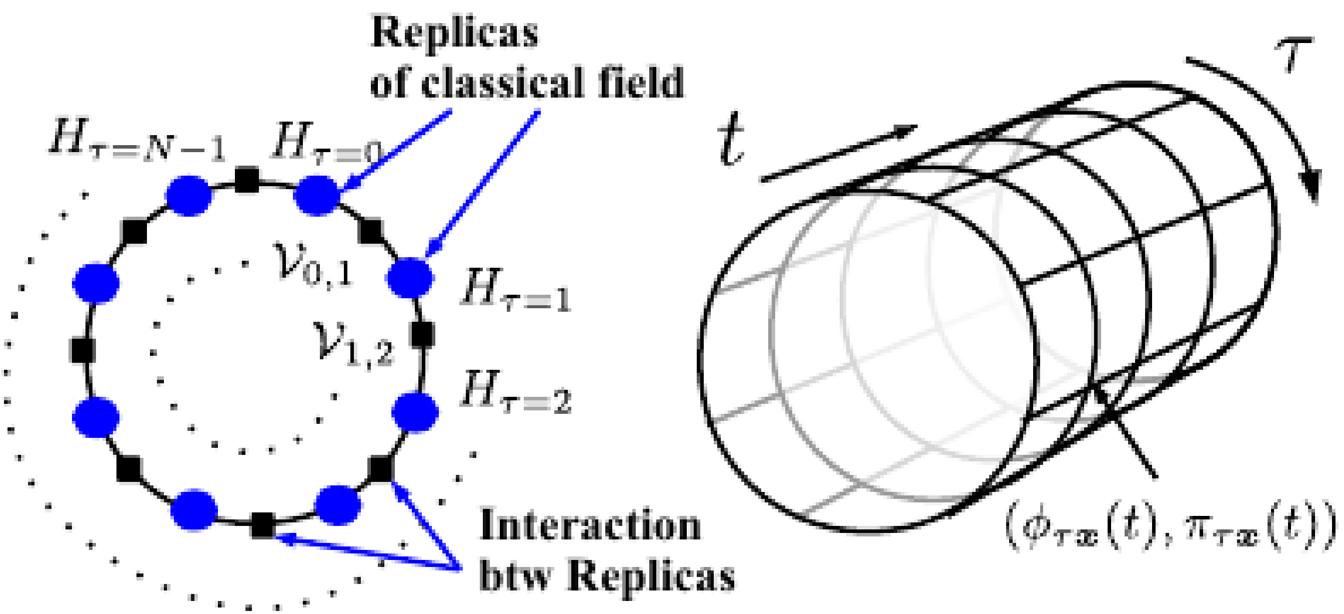
$$\frac{d\widetilde{x}}{dt} = \frac{1}{N}\sum_\tau \frac{dx_\tau}{dt} = \widetilde{p}$$

$$\frac{d\widetilde{p}}{dt} = \frac{1}{N}\sum_\tau \frac{dp_\tau}{dt} = -\frac{1}{N}\sum_\tau \frac{\partial U(x_\tau)}{\partial x_\tau} + 0 \text{ (Ehrenfest's theorem)}$$

$$= -\frac{\partial U(\widetilde{x})}{\partial \widetilde{x}} + \mathcal{O}((\delta x)^2)$$

τ-averaged variables obey classical EOM approximately when fluc. among replicas are small.

Replica Evolution



$$\mathcal{H} = \sum_\tau H_\tau + \sum_\tau \mathcal{V}_{\tau,\tau+1} = \frac{1}{2}\sum_{\tau,\boldsymbol{x}} \pi^2_{\tau,\boldsymbol{x}} + \xi S[\phi]$$

$$\mathcal{Z}_R = \int \mathcal{D}\pi\,\mathcal{D}\phi\,\exp(-\mathcal{H}/\xi) \propto \int \mathcal{D}\phi\,\exp(-S[\phi])$$

Replica Evolution
= Classical Dynamics
with Quantum Statistics in Equilibrium

Replica Evolution

- Replicas = N classical systems interacting with τ-derivative terms (V)

$$\mathcal{V} = \sum_{\tau=1}^{N} \frac{\xi^2}{2}(x_{\tau+1} - x_\tau)^2 \simeq \xi \int_0^{1/T} d\bar{\tau} \frac{1}{2} \left[\frac{\partial x}{\partial \bar{\tau}}\right]^2$$

  - Replica variables (x_τ, p_τ) are assumed to evolve with canonical EOM
  - Long (real) time evolution in 4+1D spacetime (space, τ, t) samples correct quantum statistical configurations of x_τ.
    ~ MD part of HMC
  - Replica index (τ) average of (x_τ, p_τ) obeys the classical EOM.
- Replica evolution of field
  - Replace variables $(x_\tau, p_\tau) \to (\phi_{\tau\boldsymbol{x}}, \pi_{\tau\boldsymbol{x}})$
  - Mass renormalization & Subtracting zero point contribution
- How about dynamical properties of replica evolution ?

I will skip this page...

Replica Evolution of a Single Harmonic Oscillator

Replica Evolution of a Harmonic Oscillator

- **Replica Hamiltonian = N free HO Hamiltonian**

$$\mathcal{H} = \sum_\tau \left[\frac{p_\tau^2}{2} + \frac{\omega^2 x_\tau^2}{2} + \underbrace{\frac{\xi^2}{2}(x_{\tau+1} - x_\tau)^2}_{\mathcal{V}}\right] = \sum_n \left[\frac{\bar{p}_n^2}{2} + \frac{M_n^2 \bar{x}_n^2}{2}\right]$$

$$M_n^2 = \omega^2 + 4\xi^2 \sin^2(\pi n/N)$$

Fourier transf.

- **Expectation value of x^2 in Replica**

Matsubara freq. sum

$$\langle x^2 \rangle = \frac{1}{N}\sum_\tau \langle x_\tau^2 \rangle = \frac{1}{N}\sum_n \langle \bar{x}_n^2 \rangle \overset{\exp(-\mathcal{H}/\xi)}{=} \frac{1}{N}\sum_n \frac{\xi}{M_n^2} = \frac{\coth(\Omega/2T)}{2\omega\sqrt{1+\omega^2/4\xi^2}}$$

$$\Omega = 2\xi \mathrm{arcsinh}(\omega/2\xi)$$

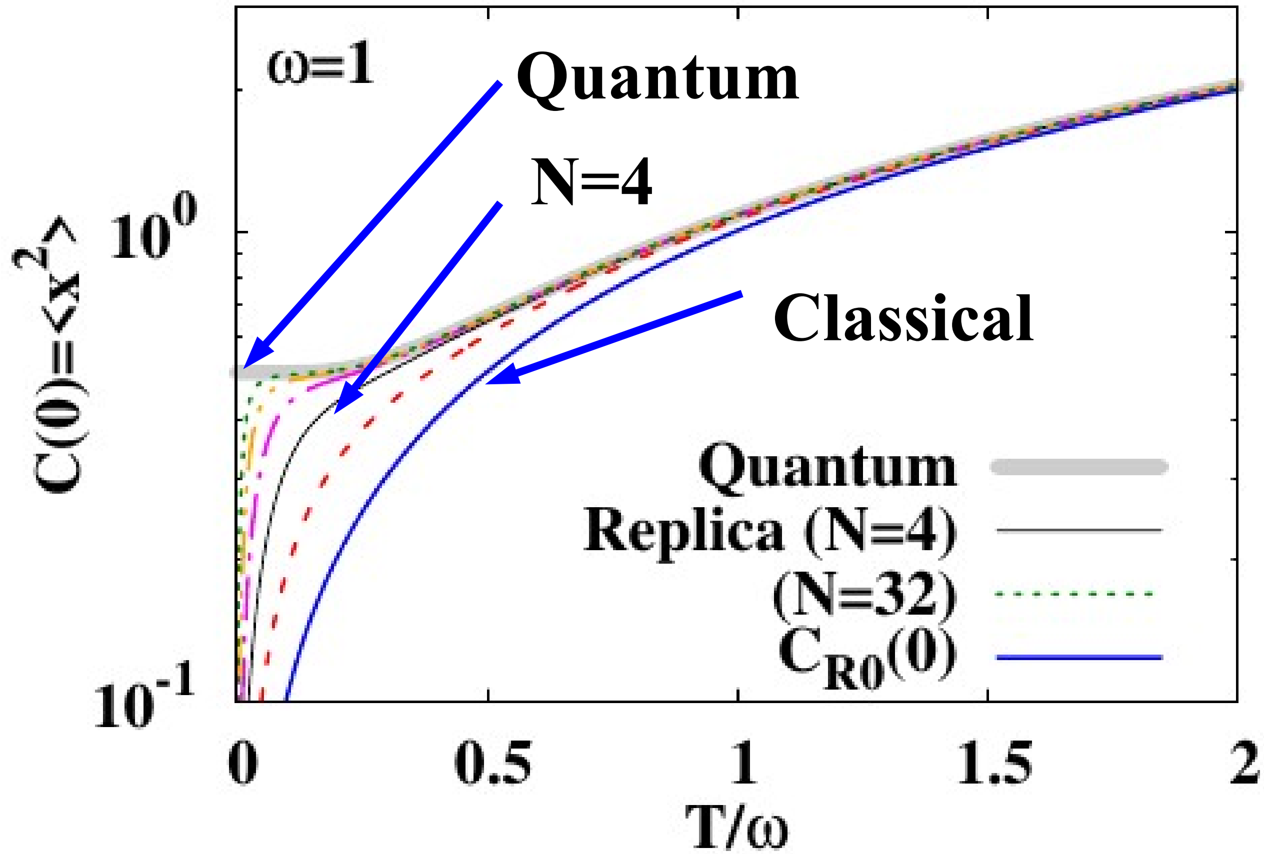
$$\frac{T}{\omega^2}(N=1, \mathrm{Classical})$$

zero point **thermal**

$$\to \frac{\coth(\omega/2T)}{2\omega} = \frac{1}{\omega}\left[\frac{1}{2} + \frac{1}{e^{\omega/T} - 1}\right] (N \to \infty, \mathrm{Quantum})$$

Equal time observables of x are reproduced at $N \to \infty$

Expectation value of x^2



$$\frac{T}{\omega^2}(N=1, \text{Classical}) \to \frac{\coth(\omega/2T)}{2\omega}(N\to\infty, \text{Quantum})$$

Equal time observables of x are reproduced at $N \to \infty$

Time-Correlation Function

- **Time-correlation function (Unequal-time two-point function)**

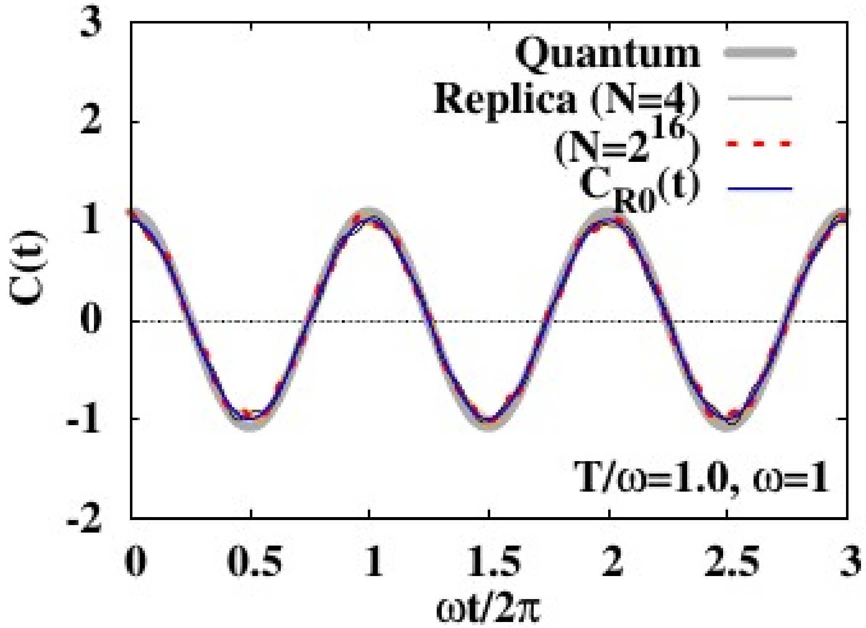
$$C(t) = \left\langle \frac{1}{2}\left[x(t)x(0) + x(0)x(t)\right] \right\rangle$$

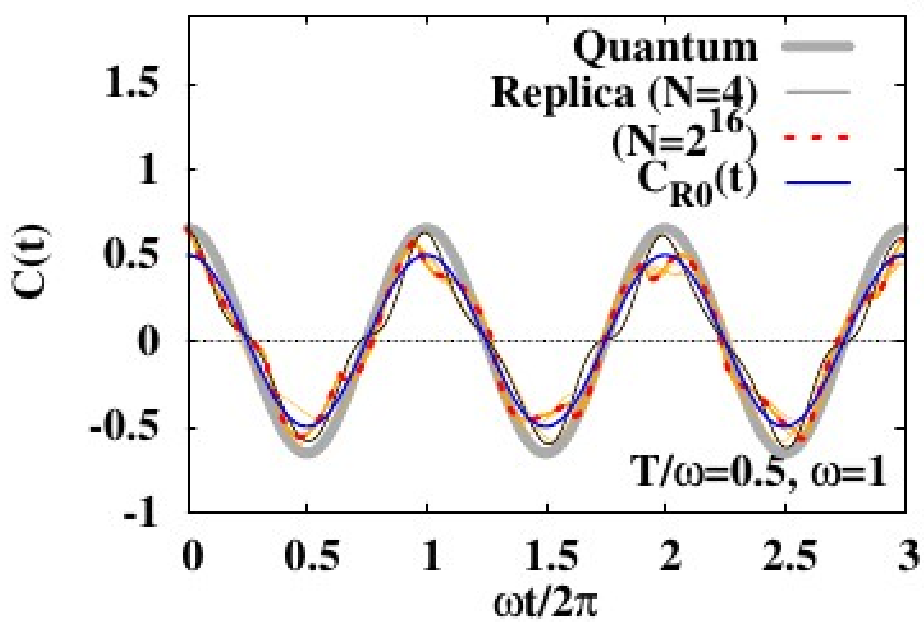
Quantum

$$C_Q(t) = \frac{\coth(\omega/2T)}{2\omega} \cos\omega t$$

Replica

$$C_R(t) = \sum_n \frac{T}{M_n^2} \cos M_n t$$





Not perfect, but $C_R(t)$ roughly explains $C_Q(t)$ at $T/\omega > 0.5$

Replica Evolution in Scalar Field Theory

Replica Evolution in Scalar Field Theory

- **Replica evolution in field theory**
  - **Replace variables** $(x_\tau, p_\tau) \to (\phi_{\tau\boldsymbol{x}}, \pi_{\tau\boldsymbol{x}})$
  - **Mass renormalization & Subtracting zero point contribution**
- **Example: ϕ^4 theory**

$$\mathcal{H} = \sum_{\tau,\boldsymbol{x}} \left[\frac{\pi_{\tau\boldsymbol{x}}^2}{2} + \frac{1}{2}(\nabla\phi_{\tau\boldsymbol{x}})^2 + \frac{m^2}{2}\phi_{\tau\boldsymbol{x}}^2 + \frac{\lambda}{24}\phi_{\tau\boldsymbol{x}}^4 + \overset{\mathcal{V}}{\boxed{\frac{\xi^2}{2}(\phi_{\tau+1,\boldsymbol{x}} - \phi_{\tau\boldsymbol{x}})^2}} \right]$$

$H(\phi_{\tau\boldsymbol{x}}, \pi_{\tau\boldsymbol{x}})$

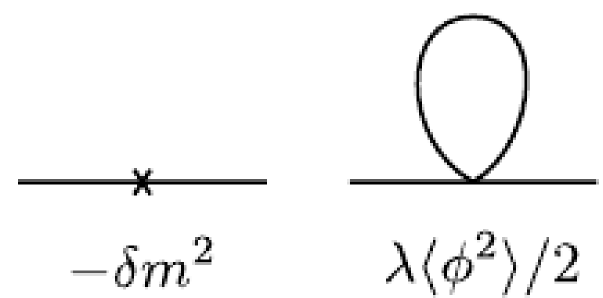
$\xi S[\phi]$

$$-\frac{\delta m^2}{2}\phi_{\tau\boldsymbol{x}}^2$$

  - **Counterterm (one loop)**
    Aarts, Smit ('97), Kapusta, Gale (textbook)

$$\delta m^2 = \frac{\lambda}{2}\langle\phi^2\rangle_{\rm div}$$

$$\langle\phi^2\rangle_{\rm div} = \frac{1}{L^3}\sum_{\boldsymbol{k}} \frac{1}{2\omega_{\boldsymbol{k}}\sqrt{1 + (\omega_{\boldsymbol{k}}/2\xi)^2}}$$



- **Momentum distribution in replica**

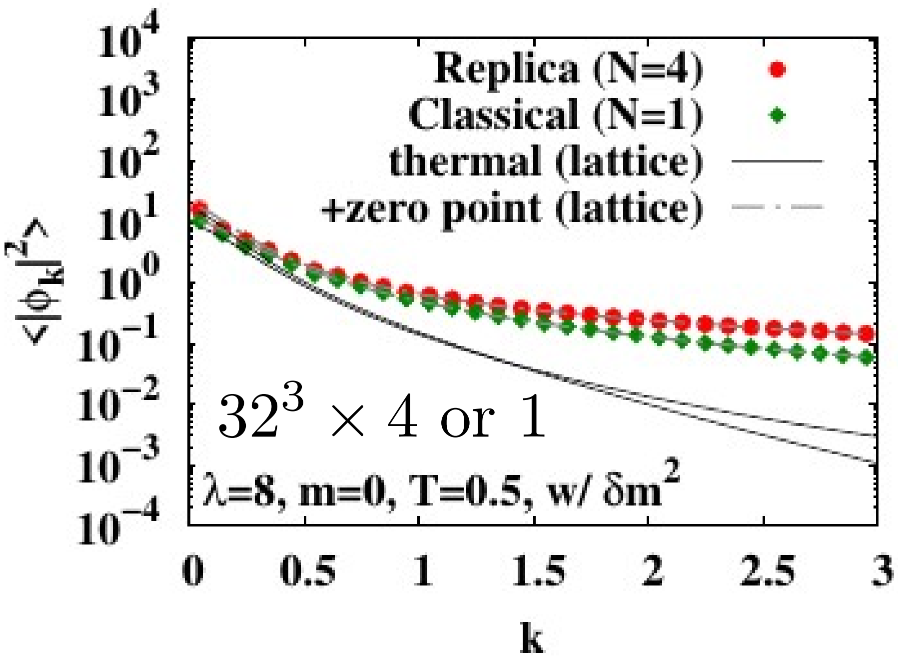
$$\langle|\phi_{\boldsymbol{k}}|^2\rangle = \frac{1}{N}\sum_n \langle\phi_{n\boldsymbol{k}}\phi^*_{n\boldsymbol{k}}\rangle \overset{\uparrow}{=} \frac{1}{\omega_{\boldsymbol{k}}\sqrt{1+(\omega_{\boldsymbol{k}}/2\xi)^2}}\left[\underline{\frac{1}{2}} + \underline{\frac{1}{e^{\Omega_{\boldsymbol{k}}/T}-1}}\right]$$

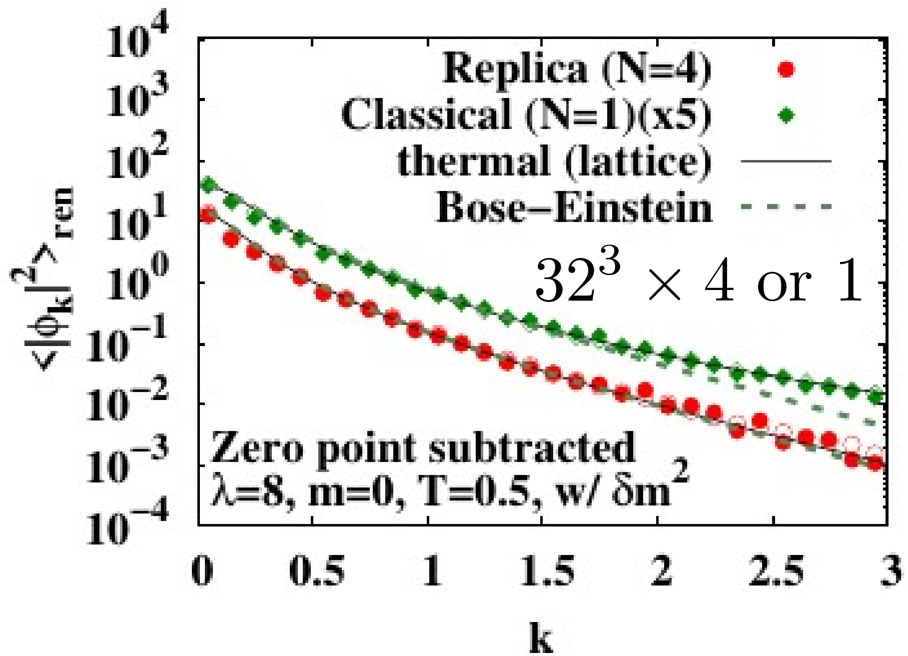
Free field, Matsubara sum

Zero point

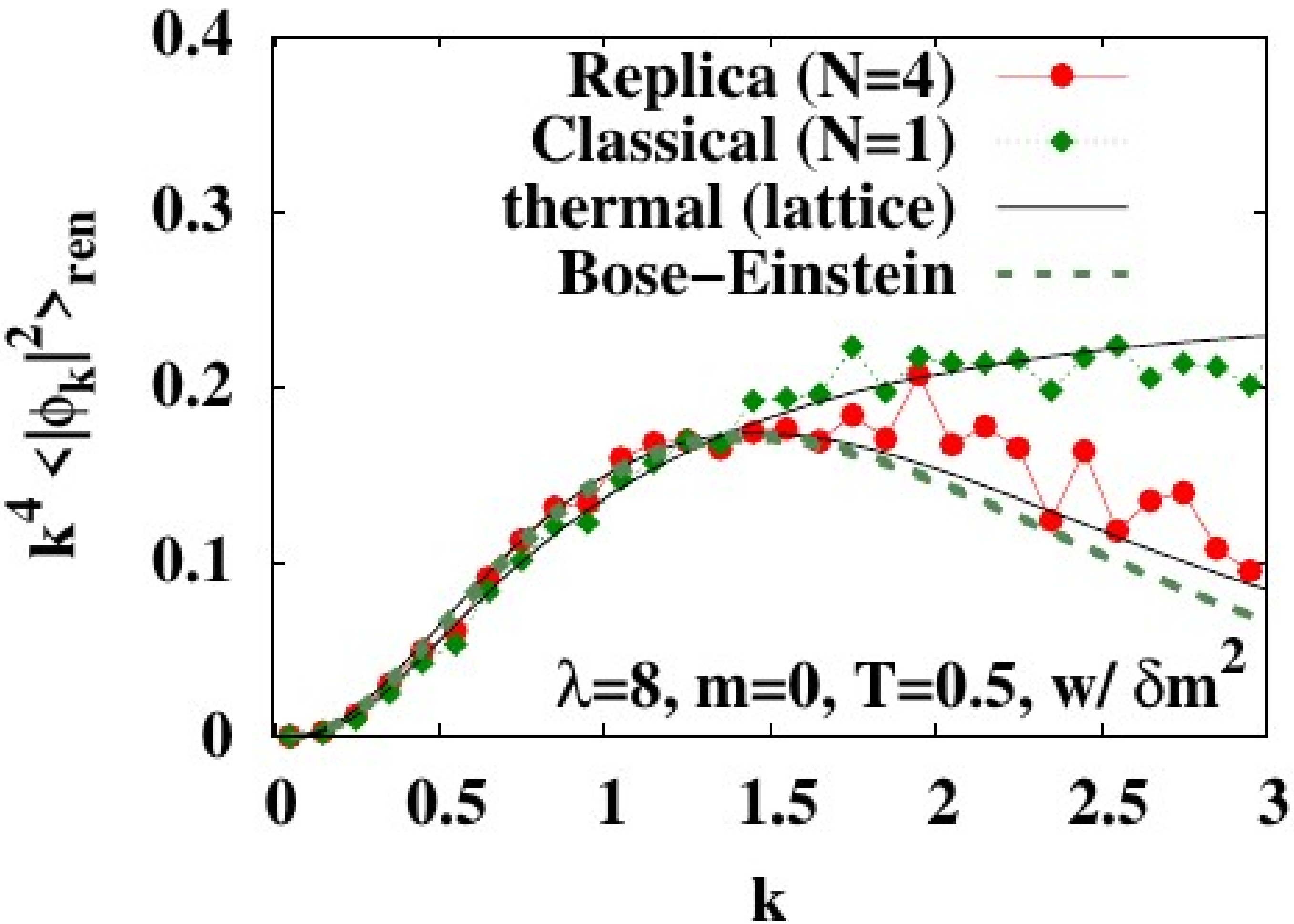
Thermal → Bose-Einstein

  - **By subtracting the zero point part, we can avoid equipartition & Rayleigh-Jeans divergence.**





Momentum Distribution



$$\frac{1}{N}\sum_{\tau \boldsymbol{x}} \frac{1}{2}(\boldsymbol{\nabla}\phi_{\tau\boldsymbol{x}})^2 = \frac{1}{N}\sum_{n\boldsymbol{k}} \frac{1}{2}\boldsymbol{k}^2|\phi_{n\boldsymbol{k}}|^2 \to L^3 \int \frac{d\boldsymbol{k}}{(2\pi)^3}\boldsymbol{k}^2|\phi_{n\boldsymbol{k}}|^2$$

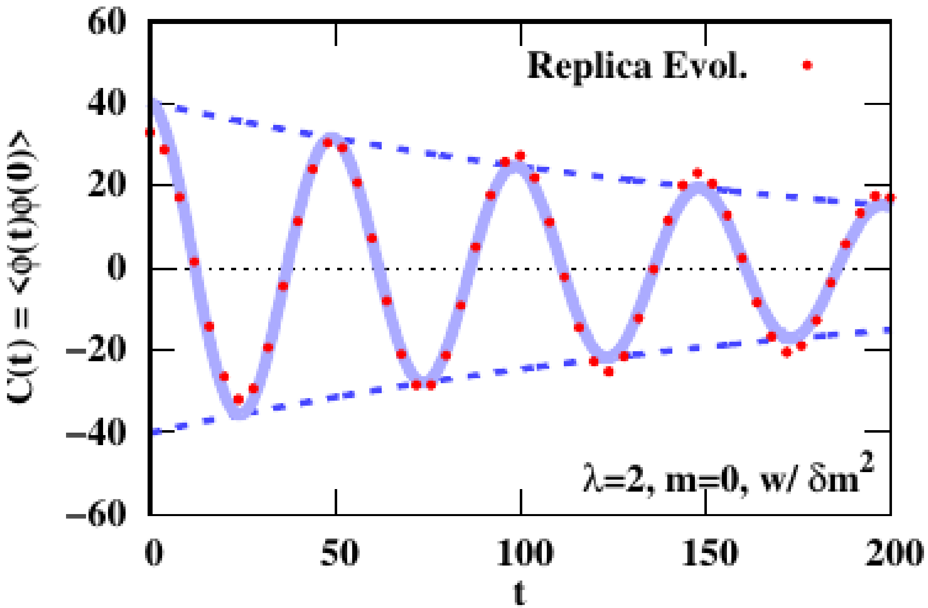
By subtracting the zero point part,
we can avoid the Rayleigh-Jeans divergence of energy.

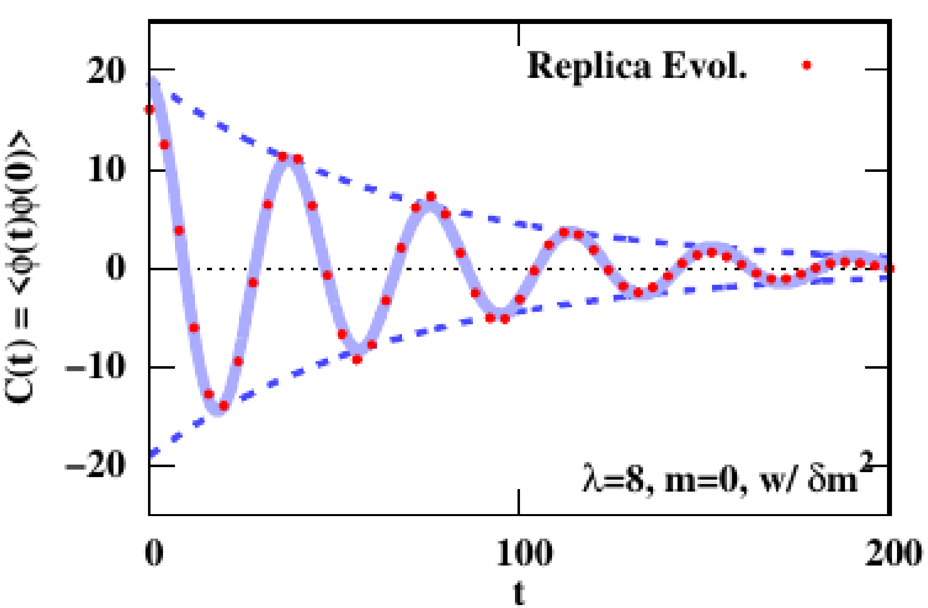
Time-Correlation Function

- **Time-correlation function**
  (unequal-time two-point function at zero momentum)

$$C(t) = \frac{1}{L^3}\sum_{\boldsymbol{x},\boldsymbol{y}}\langle\phi_{\boldsymbol{x}}(t)\phi_{\boldsymbol{y}}(0)\rangle \xrightarrow[\text{free}]{} \sum_n \frac{T}{M_n^2}\cos M_n t$$

- **With interaction (non-zero λ),**
  C(t) shows damped oscillatory behavior.
  → Thermal mass & damping rate



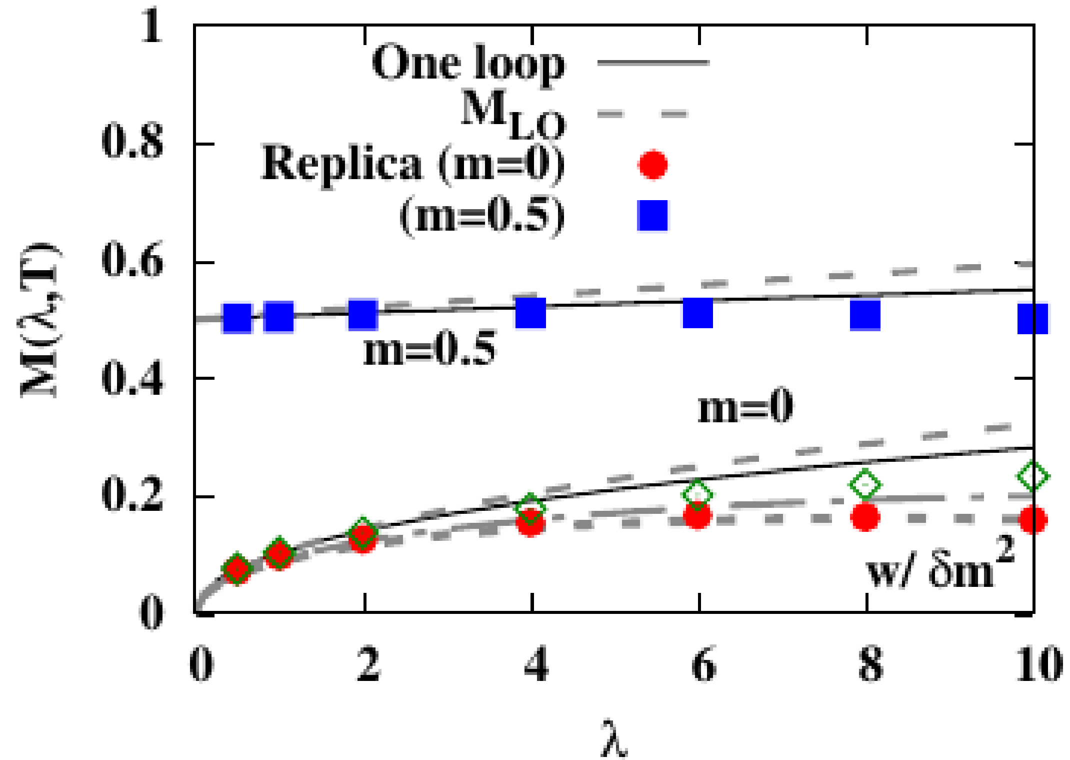


Thermal Mass

- **Thermal Mass**
  - **Leading Order (one-loop)** $M_{\rm LO}^2 = m^2 + \lambda T^2/24.$
  - **Resummed One-Loop** $M_{\rm resum}^2 = \frac{\lambda T^2}{24}\left[1 - \frac{3}{\pi}\sqrt{\frac{\lambda}{24}}\right]$
  - **Two-Loop**

$$M_{2-\rm loop}^2 = \frac{\lambda T^2}{24}\left\{1 - \frac{3}{\pi}\sqrt{\frac{\lambda}{24}} + \frac{\lambda}{(4\pi)^2}\left[\frac{3}{2}\log\left(\frac{T^2}{4\pi\mu^2}\right) + 2\log\left(\frac{\lambda}{24}\right) + \alpha\right]\right\},$$

Kapusta, Gale (textbook)
Parwani ('92, '93)



Thermal mass in Replica Evolution ~ Two-loop results

Summary

- **Replica evolution is proposed as a quantum-statistics-improved classical field framework.**
  - **N classical field configurations evolves with the τ-derivative terms.**
  - **4+1D classical evolution → quantum stat. ensemble (HMC).**
  - **Replica-index (=imag. time) average provides classical field.**
  - **Subtracting zero point part from $< \phi^2 >$**
    → mass renormalization and removing Rayleigh-Jeans divergence
  - **Thermal mass ~ 2-loop perturbation ressults.**
- **To be investigated**
  - **Comparison with previously proposed frameworks.**
    Hard mode effects [Bodeker, McLerran, Smilga ('95), Greiner, B.Muller ('97)], Field-particle sim. [Dumitru, Nara ('05), Dumitru, Nara, Strickland ('07)], 2PI [Aarts, Berges ('02), Hatta, Nishiyama ('12)], …
  - **Formal discussions, e.g. relation to Boltzmann Eq., *A.Muller, Son ('04).***
  - **Shear viscosity *[Matsuda, 6-1C]*, Thermalization, ...**

Thank you for your attention !

AO

Hidefumi Matsuda

Toru T. Takahashi

Teiji Kunihiro

http://www2.yukawa.kyoto-u.ac.jp/~akira.ohnishi/Src/Org/Replica-arXiv.pdf

Lattice Setup

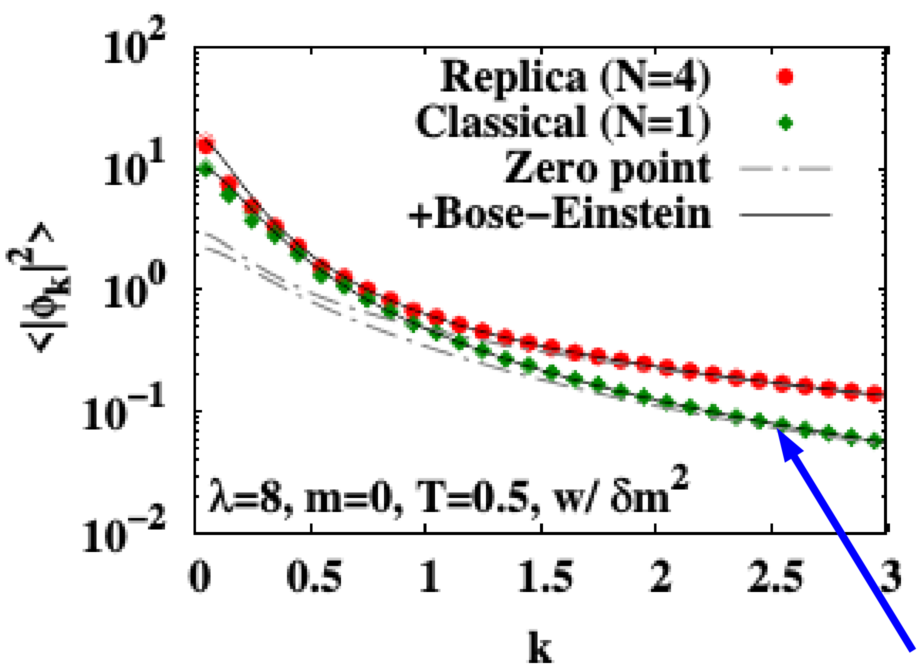
- **Lattice size: 32^3 x 4 (L=32, N=4)**
- **Temperature: T=0.5, Coupling: λ=0.5-10, bare mass:m=0, 0.5**
- **Average over replica index (τ) and replica ensemble (N_{conf}=1000)**
- **Thermal ensemble is prepared by solving the Langevin equation at temperature ξ=NT=2.**
- **EOM is solved in the leap-frog method (reversible !) with the time step of Δt=0.025 until t=500 after equilibration.**
- **A few hours for each (λ, m) on iCore7 PC (w/o MP).**

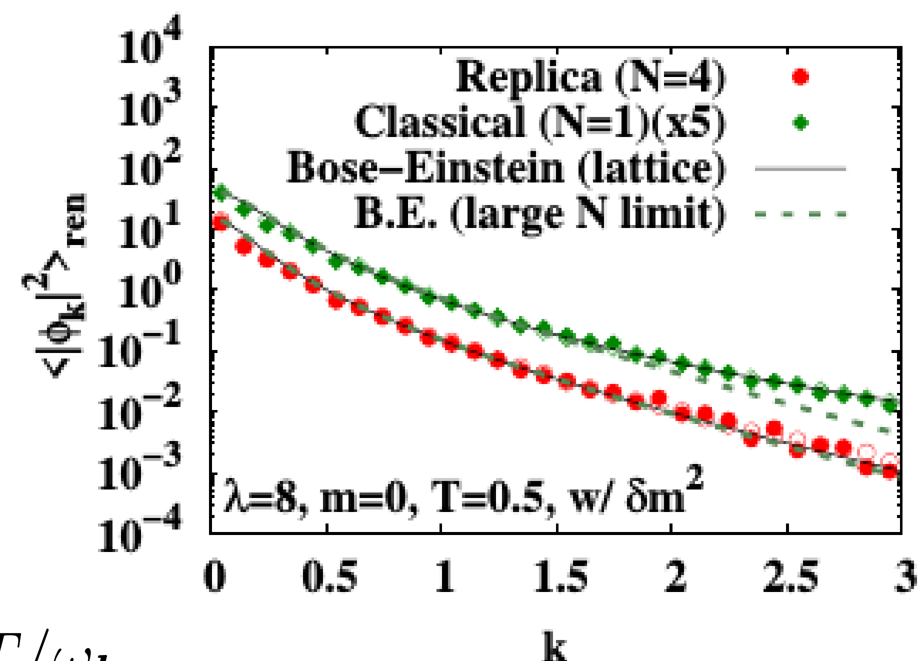
Rayleigh-Jeans Divergence

- **Replica evolution calculation with mass counterterm should give correct quantum field calc. results in the large N lim., but momentum dist. does not necessarily damps exponentially at finite N.**

$$\langle|\phi_{\boldsymbol{k}}|^2\rangle_{\rm ren} \simeq \frac{2NT}{k^2}\underline{\exp(-\Omega_{\boldsymbol{k}}/T)} \underset{k\gg NT}{\longrightarrow} 2(NT)^{2N+1}k^{-2(N+1)}$$

$$\exp(-\Omega_{\boldsymbol{k}}/T) \underset{k\gg NT}{\simeq} (\omega_{\boldsymbol{k}}/NT)^{-2N}$$





$T/\omega_{\boldsymbol{k}}$

Rayleigh-Jeans Divergence

- **With N >= 2, free field energy converges in the replica method.**

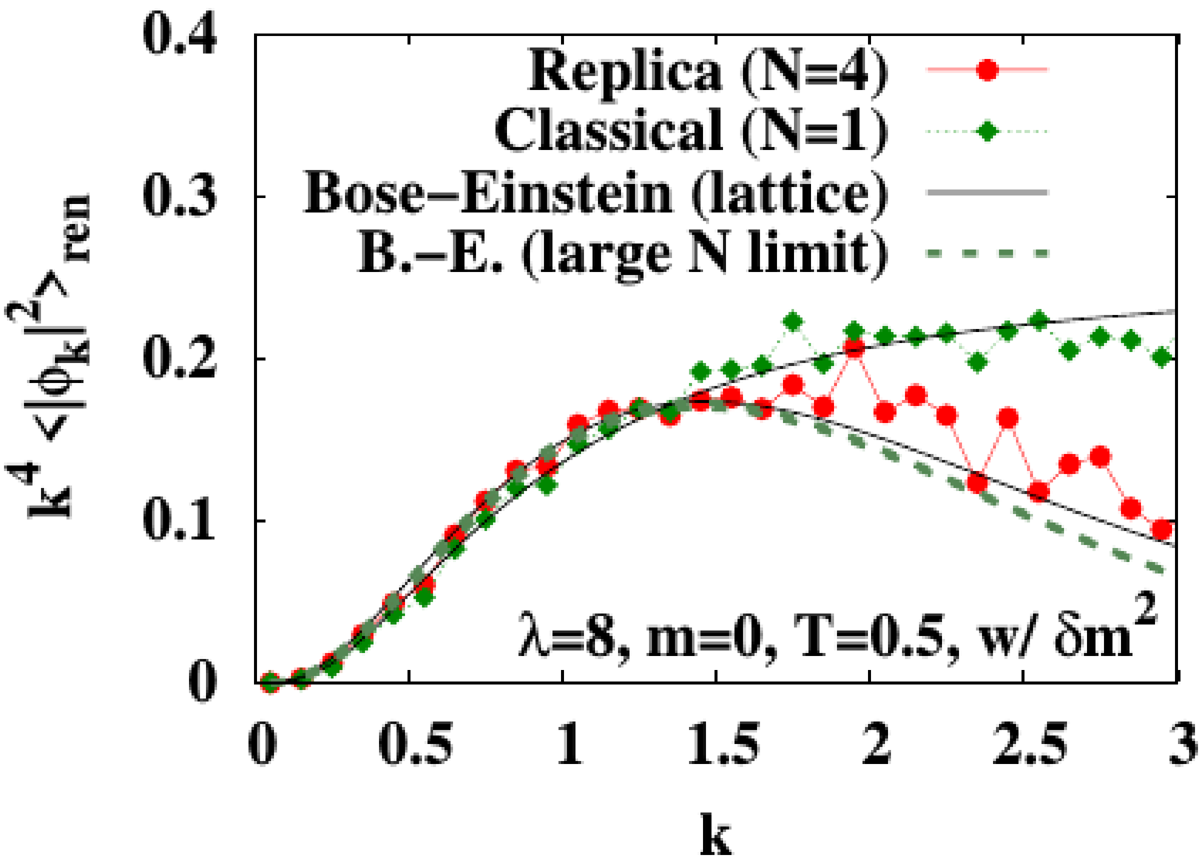
$$\Omega = 2NT\,\mathrm{arcsinh}\,(\omega/2NT) \underset{\omega\gg NT}{\longrightarrow} 2NT\log(\omega/NT)$$

$$\left\langle|\phi_{\boldsymbol{k}}|^2\right\rangle_{\rm ren} \simeq \frac{2NT}{k^2}\exp(-\Omega_{\boldsymbol{k}}/T) \to 2(NT)^{2N+1}k^{-2(N+1)}$$

$$k^4\left\langle|\phi_{\boldsymbol{k}}|^2\right\rangle_{\rm ren} \to 2(NT)^{2N+1}k^{-2(N-1)}$$

- **Convergence cond.**
  2(N-1) > 1 → N > 1.5

We can remove divergence of energy in the replica method (N>=2) with mass counterterm(s).

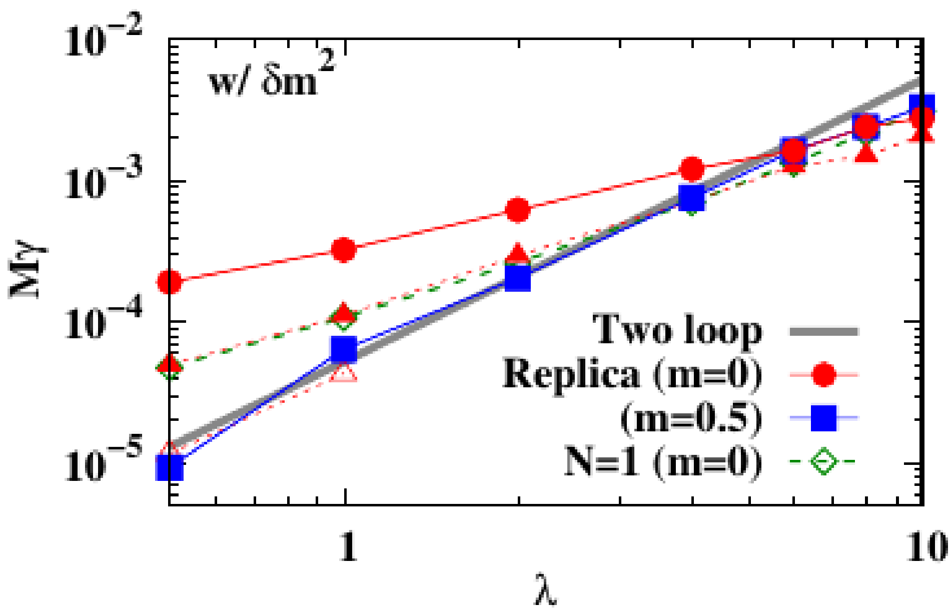


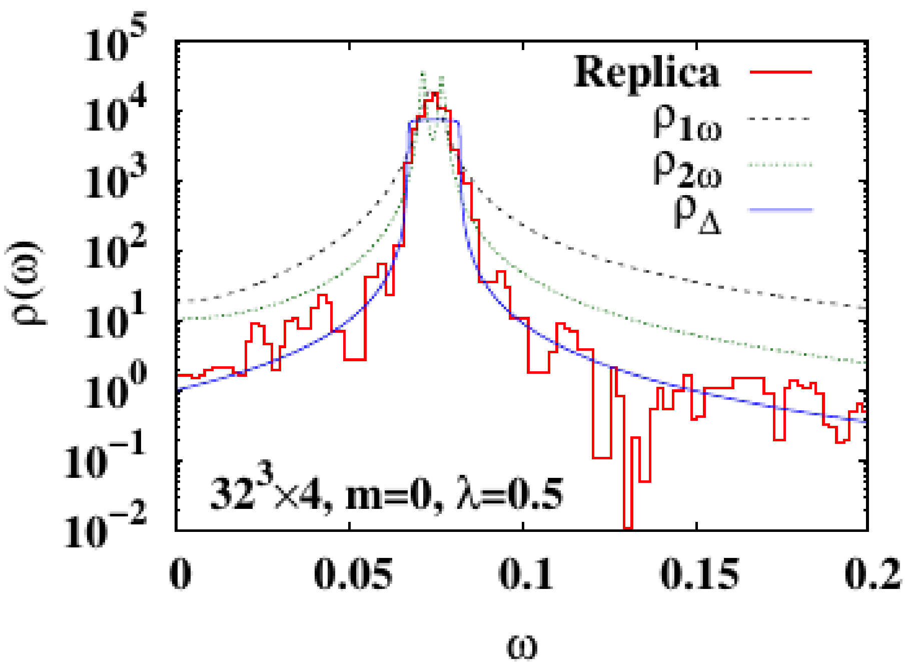
Application to Gauge theories and Fermion Systems

- **Gauge theory**
  - **Temporal component of the gauge field is Wick-rotated in the imaginary time formalism, and replica evolution cannot be applied as it is, except for the case in the temporal gauge (A_0=0).**
- **Fermions**
  - **We do not know (yet) how to handle Grassman number in replica.**
  - **Time-dependent Hartree-Fock theory may help.**

Damping Rate

- **Apparent damping rate in replica evolution is larger than 2-loop results at small coupling. Why ?**
  - **Classical results (N=1) better agrees with 2-loop results.**
    Aarts ('01)
  - **Power spectrum shows wide spread of the mass, but falls off quickly. Fragmentation of zero-momentum single particle mode ?**





Commutator in Classical Dynamics

- **Classical-Quantum Correspondence**

$$[A,B] \to i\hbar\{A,B\}_{\mathrm{PB}} + \mathcal{O}(\hbar^3)$$

- **Unequal-time Poisson bracket** *Aarts ('01)*

$$\langle\frac{1}{2}[\hat{x}_H(t),\hat{x}_H(0)]\rangle \simeq \left\langle\frac{i}{2}\{x(t),x(0)\}_{\mathrm{PB}}\right\rangle$$

$$= \frac{i}{2}\langle\sum_{n,n'}\left[\frac{\partial\bar{x}_n(t)}{\partial\bar{x}_{n'}(t_0)}\frac{\partial\bar{x}_n(0)}{\partial\bar{p}_{n'}(t_0)} - \frac{\partial\bar{x}_n(t)}{\partial\bar{p}_{n'}(t_0)}\frac{\partial\bar{x}_n(0)}{\partial\bar{x}_{n'}(t_0)}\right]\rangle$$

$$\xrightarrow[\mathrm{Free}]{} -\frac{i}{2}\sum_n \frac{1}{M_n}\sin M_n t$$

  - **n=0 term reproduces quantum mechanical result in a HO.**
  - **Unequal-time derivative can be obtained by using the Trotter formula together with Hessian matrix.**
    Kunihiro, Muller, AO, Schafer, Takahashi, Yamamoto ('10)

Previous Attempts

- **Separate soft and hard modes**
  Soft modes still have classical statistics, cutoff needs to be small.
  - **Effective action of soft modes by integrating hard modes**
    → dissipation and fluctuation from integrated hard modes
    D. Bodeker, L. D. McLerran and A. V. Smilga, PRD ('95)52;
    C. Greiner and B. Muller, PRD 55 ('97)1026.
  - **Introducing mass counterterm → Similar results with 2PI**
    e.g. G. Aarts and J. Smit, PLB 393 ('97) 395.
- **Coupled equation of field and particles**
  - **Solve coupled equation of field and particles → faster equilibration**
    A. Dumitru and Y. Nara, PLB 621 ('05) 89.
  - **Two particle irreducible (2PI) effective action approach**
    → Large numerical cost to simulate 3+1D fields
    J. Berges, AIP Conf. Proc. 739('04)1; G. Aarts, J. Berges, PRL 88('02)041603; Y. Hatta, A. Nishiyama, NPA 873('12)47.