Non-equilibrium QCD dynamics on the lattice

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TIFR ICTS School
"THE MYRIAD COLORFUL WAYS OF UNDERSTANDING EXTREME QCD MATTER"

Bangalore, India April 2019

Universität Bielefeld

CRC-TR 211
Strong-interaction matter
under extreme conditions

Classical-statistical approxmiation

Classical-statistical field theory provides powerful way to approximate non-equilibrium quantum dynamics

=> sign problem free*, direct access to many observables

Various derivations based on alternative approaches
-> Wigner-Well formalism, …

Different names for semi-classical approximation of quantum field dynamics

- classical-statistical approximation
- truncated Wigner approxation

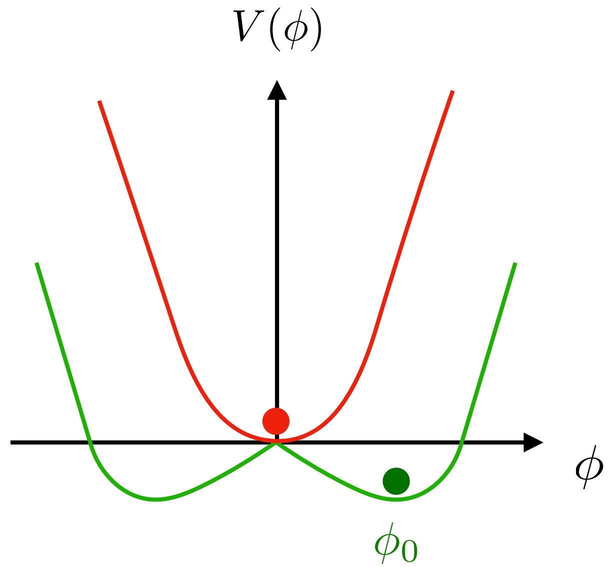
Question: What are possible applications? What is the nature of quantum corrections/range of applicability?

*iff Wigner function is positive semi-definite

Example: Critical dynamics of scalar fields

We consider scalar field theory with classical action

$$S_{\mathrm{cl}}[\phi] = \int_{t,\mathbf{x}} \frac{1}{2}(\partial_\mu\phi)(\partial^\mu\phi) - J\phi - \frac{m^2}{2}\phi^2 - \frac{\lambda}{4!}\phi^4$$



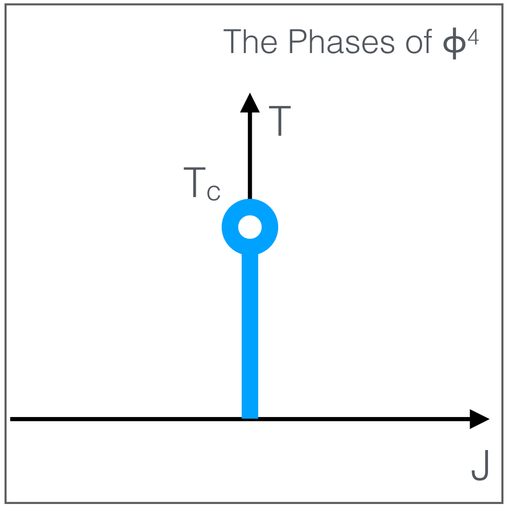
when $m^2<0$ the model will have a second order phase-transition at finite temperature T_c

$$\phi(t) = \lim_{J\to 0}\lim_{V\to\infty}\langle\phi(t)\rangle_T = \phi_0 \qquad \text{for} \qquad T < T_c$$

$$\phi(t) = \lim_{J\to 0}\lim_{V\to\infty}\langle\phi(t)\rangle_T = 0 \qquad \text{for} \qquad T > T_c$$

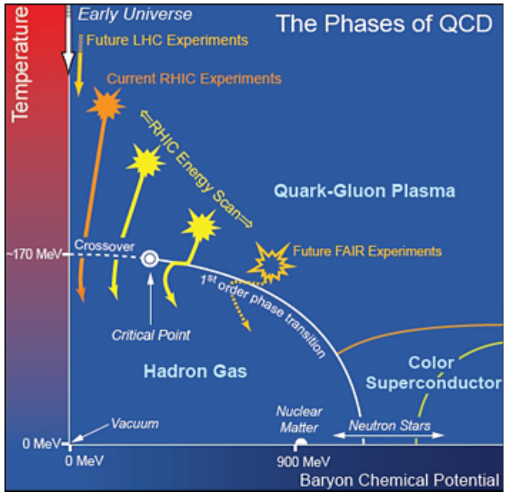
Example: Critical dynamics of scalar fields

Spatial correlation length ξ_s diverges at the critical point of a second order phase transition



Near the critical point the macroscopic properties are governed by universal scaling laws

$$\xi_s \sim |T-T_c|^{-\nu} \qquad \phi \sim |T-T_c|^{\beta}$$

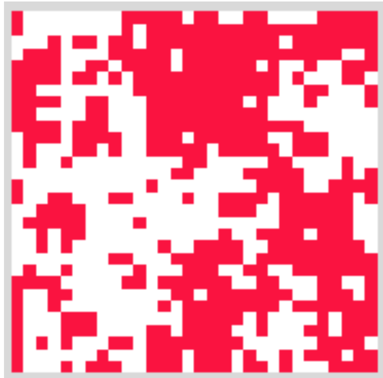


Critical exponents $\alpha, \beta, \gamma, \delta, \nu, \eta$ identical for different microscopic realizations within the same universality class

Static universality classes

dimensionality, symmetry breaking pattern

Example: Critical dynamics of scalar fields



Dynamics near the critical point subject to critical slowing down

-> Divergence of the temporal correlation length ξ_t

Characterized in terms of dynamical critical exponent *z*

$$\xi_t \sim \xi_s^z \sim |T-T_c|^{-\nu z}$$

Dynamical constraints (e.g conservational laws) affect the long time dynamics of the system

static universality class

3D Ising model (Z_2)

no conservation laws (Model A) … conserved order parameter (Model B) … energy-momentum conservation (Model C)

dynamic universality classes

Dynamical universality classes classified by Halperin & Hohenberg '77

Example: Critical dynamics of scalar fields

Since symmetries and conserved quantities are the same for classical and quantum system* can study critical dynamics within CSA

Since thermal equilibrium is a time translation invariant state, all equal time time correlation functions $\langle\hat{\phi}(t,\mathbf{x})\rangle \equiv \phi(t,\mathbf{x})$, … are effectively static quantities only

Interesting dynamical information is contained in unequal time correlation functions $\langle\hat{\phi}(t,\mathbf{x})\hat{\phi}(t,\mathbf{y})\rangle$

Generally there are two independent two-point correlation functions corresponding to the two different operator orderings e.g.

$$F(t,\mathbf{x},t'\mathbf{y}) = \frac{1}{2}\langle\{\hat{\phi}(t,\mathbf{x}),\hat{\phi}(t',\mathbf{y})\}\rangle - \phi(t,\mathbf{x})\phi(t',\mathbf{y})$$

Statistical two-point function

$$\rho(t,\mathbf{x},t',\mathbf{y}) = i\langle[\hat{\phi}(t,\mathbf{x}),\hat{\phi}(t',\mathbf{y})]\rangle$$

Spectral function

*No quantum anomalies in this case

Example: Critical dynamics of scalar fields

Different two-point correlation functions contain different information

Quantum theory

$$F(t,\mathbf{x},t'\mathbf{y}) = \frac{1}{2}\langle\{\hat{\phi}(t,\mathbf{x}),\hat{\phi}(t',\mathbf{y})\}\rangle - \phi(t,\mathbf{x})\phi(t',\mathbf{y})$$

$$\rho(t,\mathbf{x},t',\mathbf{y}) = i\langle[\hat{\phi}(t,\mathbf{x}),\hat{\phi}(t',\mathbf{y})]\rangle$$

Classical-statistical theory

$$F(t,\mathbf{x},t',\mathbf{y}) = \langle\phi(t,\mathbf{x})\phi(t',\mathbf{y})\rangle - \phi(t,\mathbf{x})\phi(t',\mathbf{y})$$

$$\rho(t,\mathbf{x},t',\mathbf{y}) = -\langle\{\phi(t,\mathbf{x}),\phi(t',\mathbf{y})\}_{\mathrm{PB}}\rangle \overset{*}{=} \left\langle\frac{\delta\phi(t,x)}{\delta\pi(t',y)}\right\rangle$$

Statistical function F~<ϕϕ> -> actual excitations present in the system

Spectral function ρ~<δϕ/δπ> -> possible excitations of the systems

In thermal equilibrium fluctuation dissipation relation implies

$F(\omega,p) = -i\,(n_{BE}(\omega)+1/2)\,\rho(\omega,p)$

$F(\omega,p) = -i\,T/\omega\,\rho(\omega,p)$

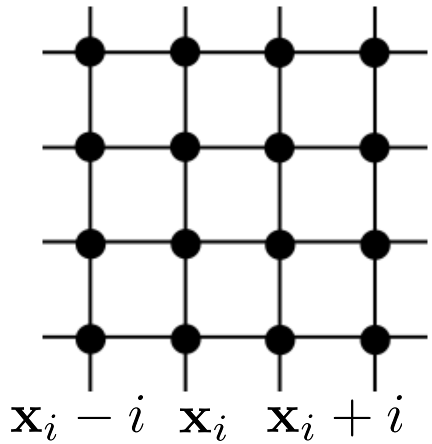
only one independent two-point function

$$^*\{A(x),B(y)\}_{\mathrm{PB}} = \int d^d\mathbf{z}\left[\frac{\delta A(x)}{\delta\phi(\mathbf{z})}\frac{\delta B(y)}{\delta\pi(\mathbf{z})} - \frac{\delta A(x)}{\delta\pi(\mathbf{z})}\frac{\delta B(y)}{\delta\phi(\mathbf{z})}\right]$$

Example: Critical dynamics of scalar fields

Classical-statistical field theory study of critical dynamics

0 Discretize classical scalar field theory on a lattice to make problem finite dimensional



Hamiltonian formalism

Discretization on a spatial lattice

$$\phi(t,\mathbf{x}) \to \phi(t,\mathbf{x}_i) \qquad \pi(t,\mathbf{x}) \to \pi(t,\mathbf{x}_i)$$

$$H[\phi,\pi] = a_s^d \sum_{x_i} \frac{\pi(\mathbf{x}_i)^2}{2} + \frac{1}{2}\left(\frac{\phi(\mathbf{x}_i) - \phi(\mathbf{x}_i - i)}{a_s}\right)^2 + \frac{m^2}{2}\phi^2(\mathbf{x}_i) + \frac{\lambda}{4!}\phi^4(\mathbf{x}_i)$$

1 IC: Since we are interested in equilibrium dynamics near a critical point, relevant initial conditions correspond to classical thermal ensemble

$$P[\phi_0,\pi_0] \propto e^{-\beta H[\phi_0,\pi_0]}$$

-> Generate initial field configurations according to classical thermal weight (e.g. Metropolis,Langevin,HMC)

Example: Critical dynamics of scalar fields

2 Dynamics: Classical EOMs obtained from Hamilton's equations

$$\partial_t \phi(t, \mathbf{x}_i) = +a_s^{-d} \frac{\partial H}{\partial \pi(\mathbf{x}_i)} \qquad \boxed{\partial_t \phi(t, \mathbf{x}_i) = \pi(t, \mathbf{x}_i)}$$

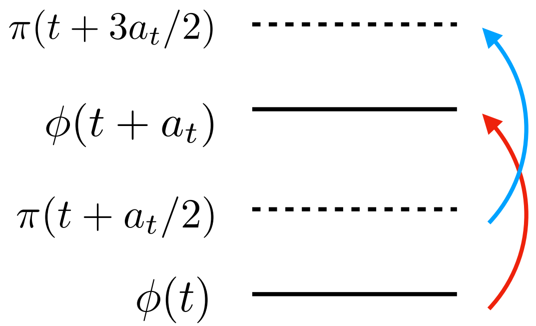
$$\partial_t \pi(t, \mathbf{x}_i) = -a_s^{-d} \frac{\partial H}{\partial \phi(\mathbf{x}_i)} \qquad \boxed{\partial_t \pi(t, \mathbf{x}_i) = \frac{\phi(t, \mathbf{x}_i + i) - 2\phi(t, \mathbf{x}_i) + \phi(t, \mathbf{x}_i - i)}{a_S^2} - m^2 \phi(t, \mathbf{x}_i) - \frac{\lambda}{6} \phi^3(t, \mathbf{x}_i)}$$

Discretize time step a_t to obtain numerical solution

-> need $a_t << a_s$ to guarantee stability of numerical solution

-> simplectic integrators highly efficient

most commonly used scheme is leap-frog



Sequential updates to calculate real-time evolution up to t_{Max}

Example: Critical dynamics of scalar fields

3 Observables: Since fields ϕ(t) are known at any given instant of time simply calculate observable of interest from field

$$\phi = \frac{1}{N_s^3} \sum_{\mathbf{x}_i} \phi(t, \mathbf{x}_i) \qquad \rho(t, t', \mathbf{x}_i, \mathbf{y}_i) = -\{\phi(t, \mathbf{x}), \phi(t', \mathbf{y})\}_{\mathrm{PB}}$$

Can exploit KMS relation to avoid calculation of Poisson-Bracket

$$F(\omega, \mathbf{p}_i) = -i\frac{T}{\omega}\rho(\omega, \mathbf{p}_i) \qquad \rho(t-t', \mathbf{p}_i) = -\frac{1}{T}\partial_{t-t'}F(t-t', \mathbf{p}_i)$$

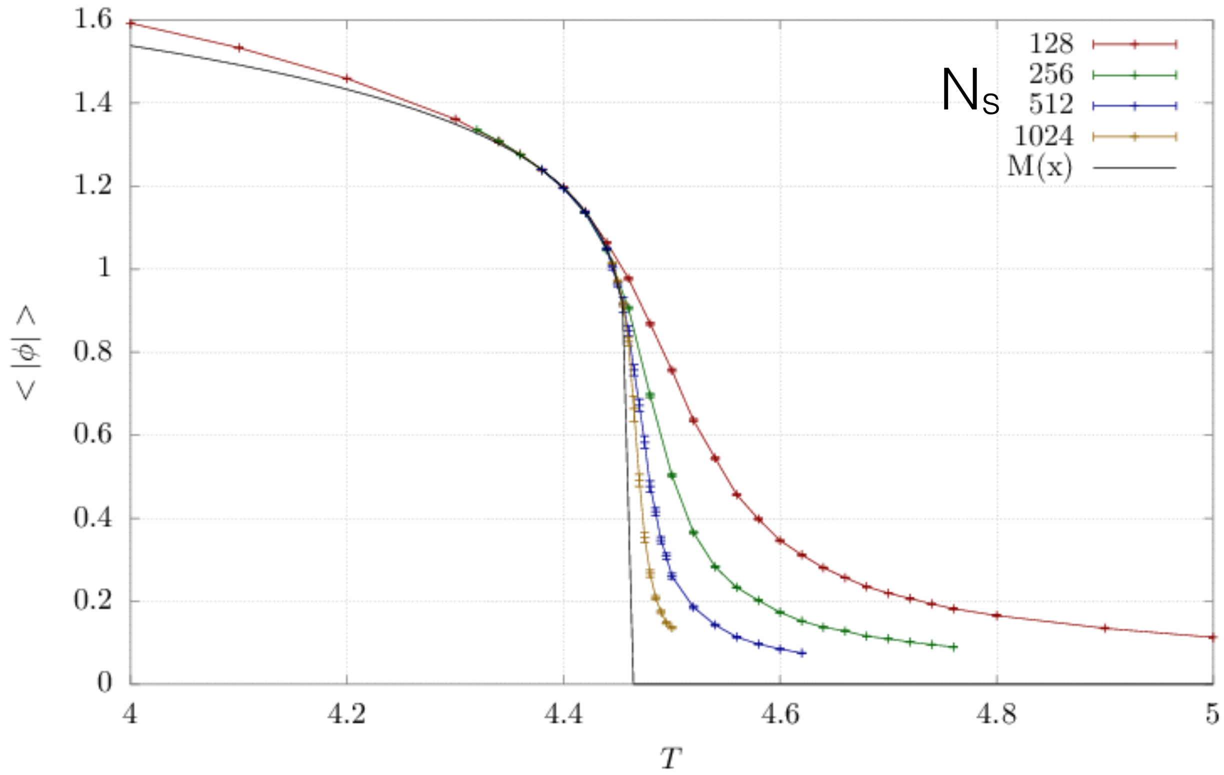
$$\rho(t-t', \mathbf{p}_i) = -\frac{1}{2VT}\sum_{x_i, y_i} e^{-i\mathbf{p}_i(\mathbf{x}_i - \mathbf{y}_i)}\Big(\pi(t, \mathbf{x}_i)\phi(t', \mathbf{y}_i) - \phi(t, \mathbf{x}_i)\pi(t', \mathbf{y}_i)\Big)$$

=> only need to calculate equal/un-equal time correlation functions

4 Statistical averaging by repeating steps 1-3

Example: Critical dynamics of scalar fields

Identifying critical point for fixed microscopic parameters (m^2,λ,a_s)



Challenge: Critical divergence of correlation length near T_c limited by lattice size; phased transition is washed out in finite system

d=2 can beat problem with sufficiently large lattices
d=3 increasingly challenging due to numerical cost

Example: Critical dynamics of scalar fields

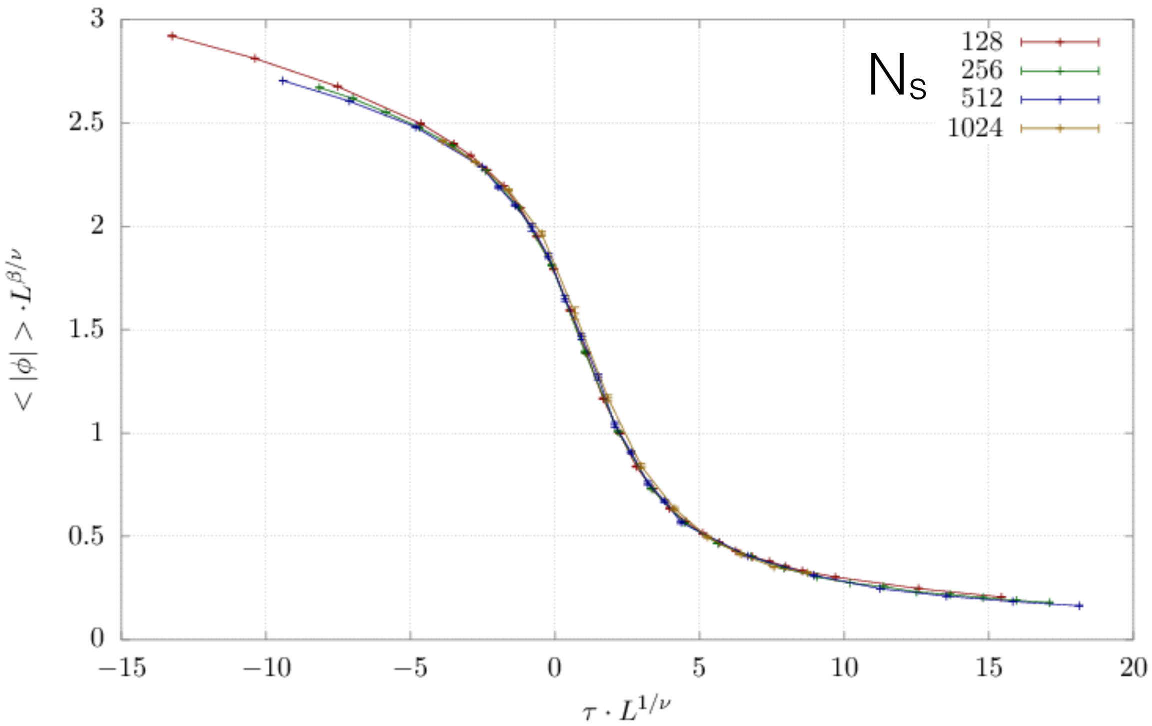
Scaling relations for infinite system

$$\tau = \frac{T - T_c}{T_c} \qquad \xi_s(\tau) \sim \tau^{-\nu} \qquad \phi(\tau) \sim \xi_s(\tau)^{-\beta/\nu}$$

finite system

$$\phi(\tau, L) \sim \xi_s(\tau)^{-\beta/\nu} \Phi(L/\xi_s(\tau))$$

finite size scaling $L^{\beta/\nu}\phi(\tau, L) \sim (L/\xi_s(\tau))^{\beta/\nu}\Phi(L/\xi_s(\tau)) \sim (L\tau^{1/\nu})^{\beta/\nu}\Phi(L\tau^{1/\nu})$



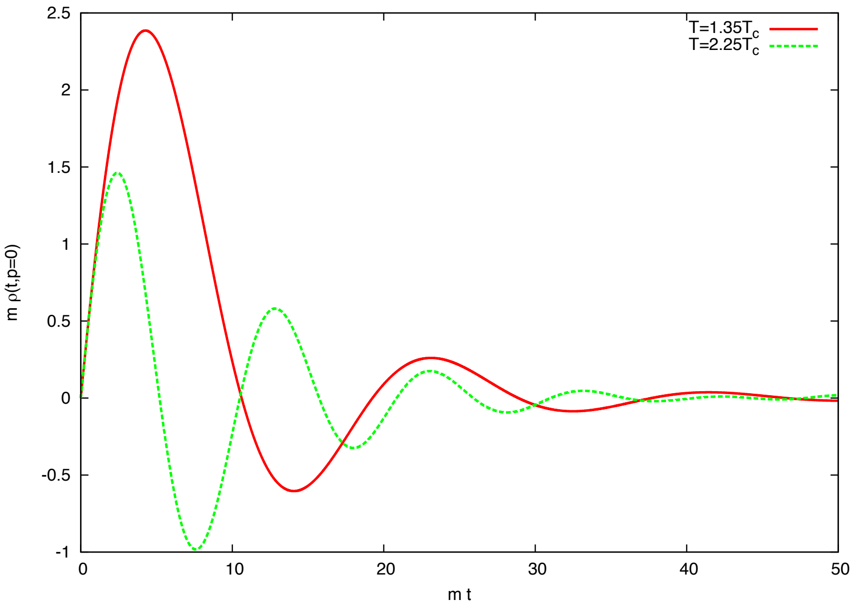
=> Based on combination of observables one can obtain precise estimates of T_c and critical exponents

Example: Critical dynamics of scalar fields

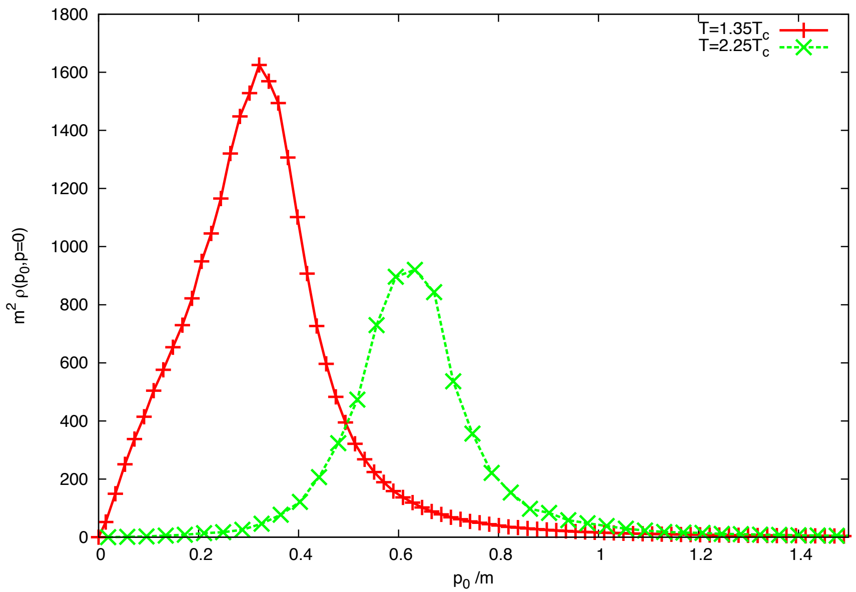
Spectral functions from classical-statistical simulations (d=2)

$$\rho_{\text{free}}(t, \mathbf{p}=0) = \omega_0(T)^{-1} \sin(\omega_0(T)\ t)$$

$$\tilde{\rho}_{\text{free}}(\omega, \mathbf{p}=0) = 2\pi i\ \text{sign}(\omega)\ \delta(\omega^2 - \omega_0(T)^2)$$



time domain



frequency domain

=> Broadening of quasi-particle peaks due to interactions

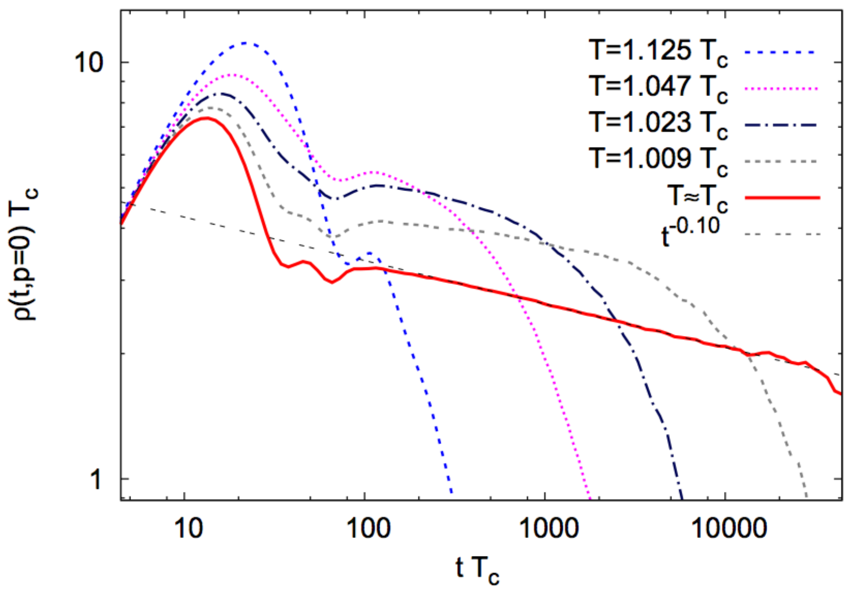
Berges, Sexty, SS NPB832 (2010) 228-240

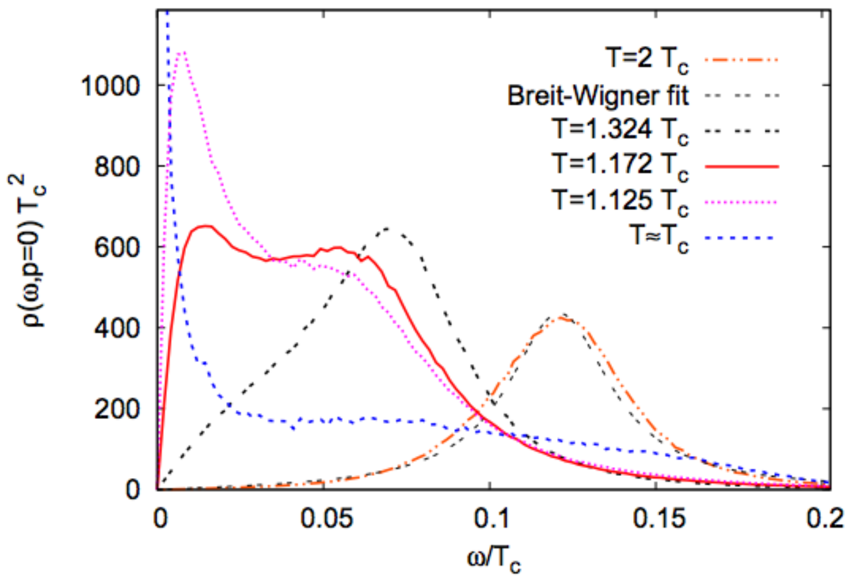
Example: Critical dynamics of scalar fields

Spectral functions from classical-statistical simulations (d=2)

$$\rho_{\text{critical}}(t, \mathbf{p}=0) \sim t^{\frac{2-\eta-z}{z}} \exp(-t/\xi_t(\tau))$$

$$\tilde{\rho}_{\text{critical}}(\omega, \mathbf{p}=0) \sim \omega^{-\frac{2-\eta}{z}}$$





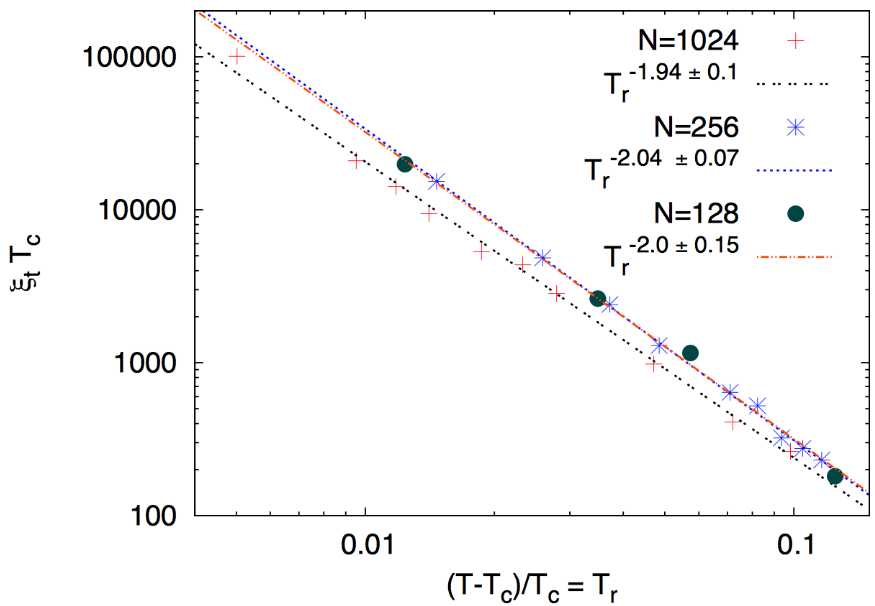
=> Change from relativistic quasi-particle to relaxation dynamics

Berges, Sexty, SS NPB832 (2010) 228-240

Example: Critical dynamics of scalar fields

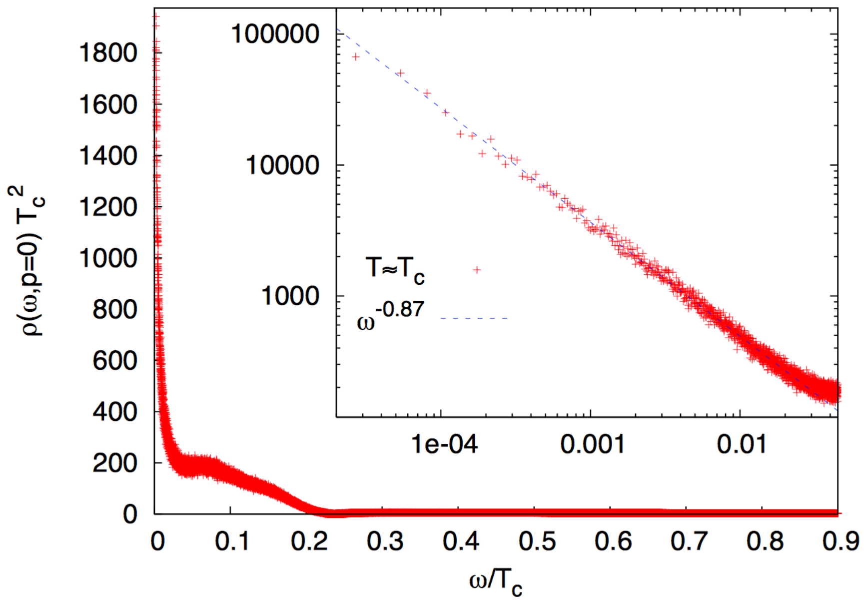
Extraction of dynamic critical exponent *z* (d=2)

$$\xi_t \sim \tau^{-\nu z}$$



Divergence of temporal correlation length

$$\tilde{\rho}_{\mathrm{critical}}(\omega, \mathbf{p}=0) \sim \omega^{-\frac{2-\eta}{z}}$$



Critical spectral function

=> Different extractions yield z=2.05±0.15 consistent with Model C

Berges, Sexty, SS NPB832 (2010) 228-240

Example: Non-equilibrium phase-transitions

Near critical point auto-correlation time diverges

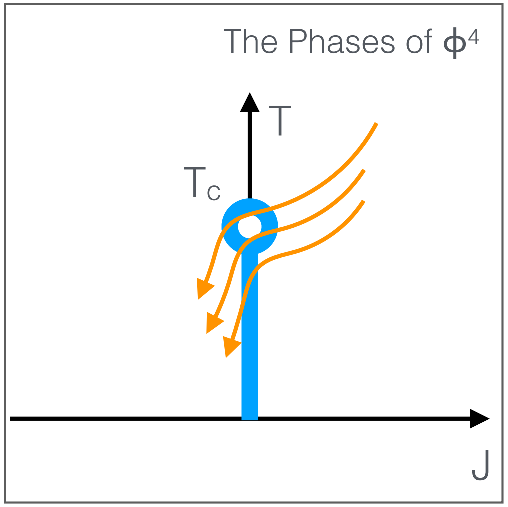
=> system will fall out of equilibrium when approaching critical point at finite rate

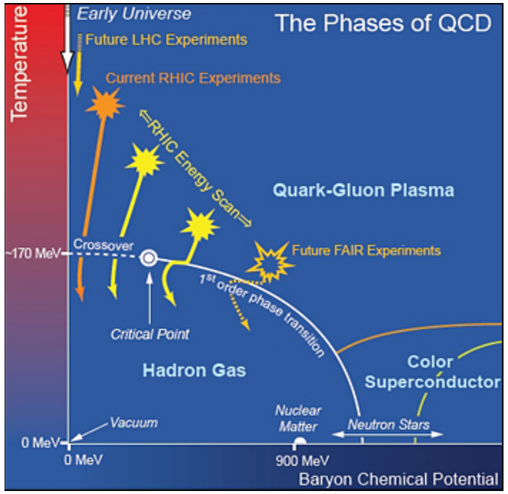
Highly relevant to search of QCD critical point in HIC

Berdnikov, Rajagopal PRD 61 (2000) 105017
Mukherjee,Venugopalan,Yin, PRL 17 (2016) no.22, 222301
…

Possibility to benchmark QCD studies from first principles in scalar fields theories

Caveat: Dynamic universality class of QCD model H; Scalar field theory model A/C

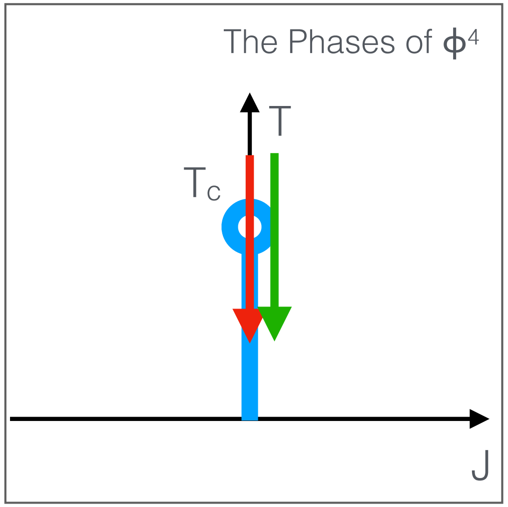




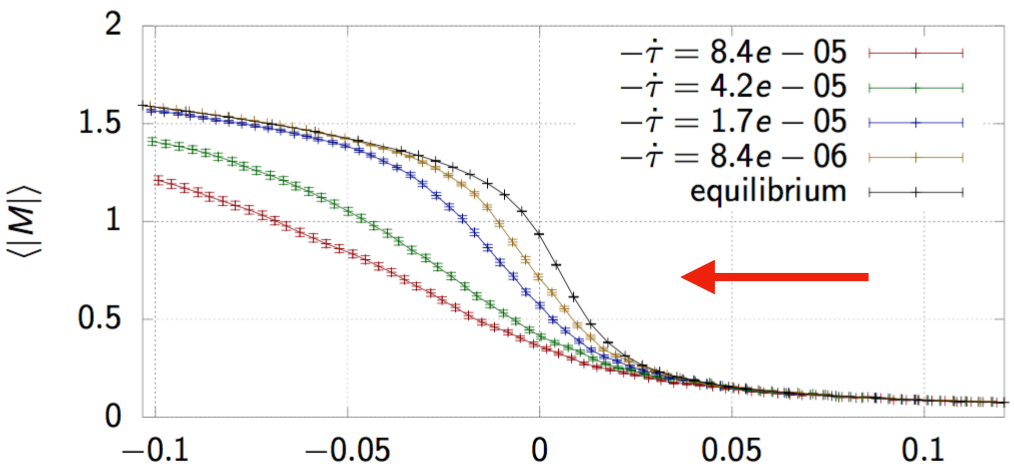
Example: Non-equilibrium phase-transitions

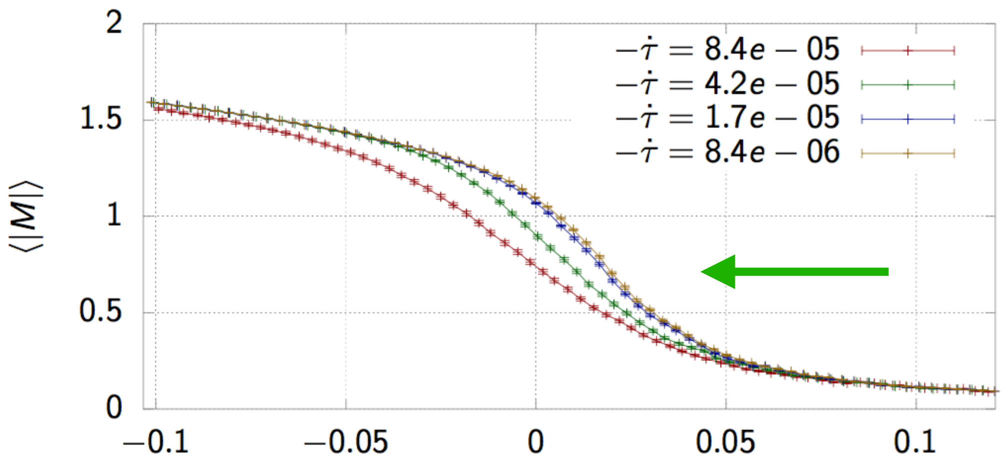
Can realize time dependent T,J by coupling the order parameter field a heat bath

$$\partial_t \phi(t,\mathbf{x}_i) = +a_s^{-d} \frac{\partial H}{\partial \pi(\mathbf{x}_i)}$$
$$\partial_t \pi(t,\mathbf{x}_i) = -a_s^{-d} \frac{\partial H}{\partial \phi(\mathbf{x}_i)} - \gamma \pi(t,\mathbf{x}_i) + \sqrt{2\gamma T(t)}\xi(t)$$



Extremely rich dynamics depending on trajectory in the phase diagram





Challenging to obtain statistics for fluctuation observables

Quantum versus classical-statistical field theory

So far exploited universality near critical point to describe QFT dynamics semi-classically

Before we can meaningfully apply to non-equilibrium QFT, we should understand range of applicability and corrections to CSA

$$\int_{\varphi_0}^{\varphi_f} D\varphi \int D\chi \exp\Big[-i\underbrace{\int_{t,\mathbf{x}} \chi(x)\Big(\partial_\mu\partial^\mu\varphi(x) + m^2\varphi(x) + \frac{\lambda}{6}\varphi^3(x)\Big)}_{\text{included in CSA}} - \underbrace{\frac{i\lambda\hbar^2}{24}\int_{t,\mathbf{x}} \chi^3(x)\varphi(x)}_{\text{neglected in CSA}}\Big]$$

Decompose action into “free” and “interacting” parts ($\hbar$=1 from now on)

$$S_0[\varphi,\chi] = \int_{t,\mathbf{x}} \chi(x)(-\partial_\mu\partial^\mu - m^2)\varphi(x)$$

=> CSA is exact for free theory (λ=0)

Quantum versus classical-statistical field theory

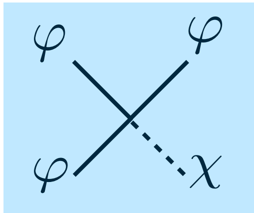
Question: What are corrections? Range of applicability?

$$\int_{\varphi_0}^{\varphi_f} D\varphi \int D\chi \exp\Big[-i \underbrace{\int_{t,\mathbf{x}} \chi(x)\Big(\partial_\mu\partial^\mu\varphi(x) + m^2\varphi(x) + \frac{\lambda}{6}\varphi^3(x)\Big)}_{\text{included in CSA}} - \underbrace{\frac{i\lambda\hbar^2}{24}\int_{t,\mathbf{x}} \chi^3(x)\varphi(x)}_{\text{neglected in CSA}}\Big]$$

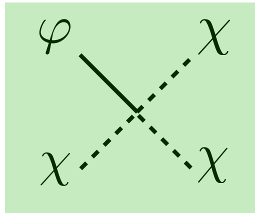
Diagrammatic analysis of interaction terms

$$S_I[\varphi,\chi] = \frac{\lambda}{6}\int_{t,\mathbf{x}} \chi(x)\varphi^3(x) + \frac{\lambda}{24}\int_{t,\mathbf{x}} \chi^3(x)\varphi(x)$$

classical vertex



quantum vertex



CSA is non-perturbative expansion (all orders in classical vertex)

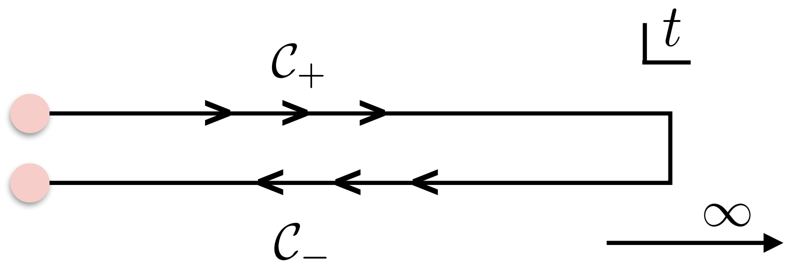
CSA neglects powers of χ compared to φ

-> Expansion in "$|\chi| << |\varphi|$"

Quantum versus classical-statistical field theory

Need to analyze more carefully in terms of correlation functions

=> recall that $\varphi^{+/-}$ correlation functions correspond to expectation values of time ordered operators along the Schwinger-Keldysh contour



$$\langle\varphi^+(t,\mathbf{x})\rangle \equiv \left.\frac{\delta Z[J,R]}{i\delta J^+(t,\mathbf{x})}\right|_{J=R=0} = \langle\hat{\phi}(t,\mathbf{x})\rangle$$

$$\langle\varphi^-(t,\mathbf{x})\rangle \equiv \left.\frac{\delta Z[J,R]}{i\delta J^-(t,\mathbf{x})}\right|_{J=R=0} = \langle\hat{\phi}(t,\mathbf{x})\rangle$$

$$\xrightarrow[\chi = \varphi^+ - \varphi^-]{\varphi = \frac{\varphi^+ + \varphi^-}{2}}$$

change of variables

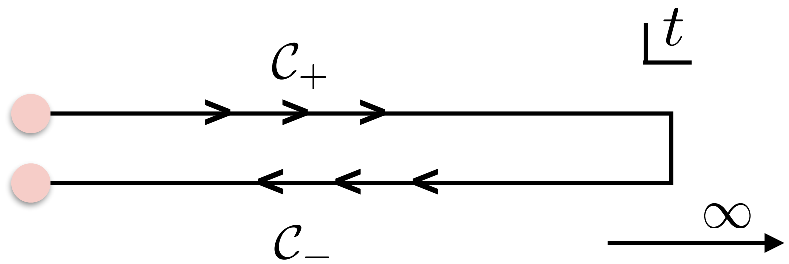
$$\langle\varphi(t,\mathbf{x})\rangle = \langle\hat{\phi}(t,\mathbf{x})\rangle \equiv \phi(t,\mathbf{x})$$

$$\langle\chi(t,\mathbf{x})\rangle = 0$$

Classicality condition "$|\chi| << |\varphi|$" always satisfied at the level of one-point functions

Quantum versus classical-statistical field theory

Need to analyze higher order correlation functions



$$\langle \varphi^+(t,\mathbf{x})\varphi^+(t',\mathbf{y})\rangle = \langle \mathcal{T}\hat{\phi}(t,\mathbf{x})\hat{\phi}(t',\mathbf{y})\rangle = \theta(t'-t)\langle\hat{\phi}(t',\mathbf{y})\hat{\phi}(t,\mathbf{x})\rangle + \theta(t-t')\langle\hat{\phi}(t,\mathbf{x})\hat{\phi}(t',\mathbf{y})\rangle$$

$$\langle \varphi^-(t,\mathbf{x})\varphi^-(t',\mathbf{y})\rangle = \langle \bar{\mathcal{T}}\hat{\phi}(t,\mathbf{x})\hat{\phi}(t',\mathbf{y})\rangle = \theta(t-t')\langle\hat{\phi}(t',\mathbf{y})\hat{\phi}(t,\mathbf{x})\rangle + \theta(t'-t)\langle\hat{\phi}(t,\mathbf{x})\hat{\phi}(t',\mathbf{y})\rangle$$

$$\langle \varphi^+(t,\mathbf{x})\varphi^-(t',\mathbf{y})\rangle = \langle\hat{\phi}(t',\mathbf{y})\hat{\phi}(t,\mathbf{x})\rangle$$

$$\langle \varphi^-(t,\mathbf{x})\varphi^+(t',\mathbf{y})\rangle = \langle\hat{\phi}(t,\mathbf{x})\hat{\phi}(t',\mathbf{y})\rangle$$

Generally there are two independent two-point correlation functions corresponding to the two different operator orderings e.g.

Wightman functions: $G^>(t,\mathbf{x},t',\mathbf{y}) = \langle\hat{\phi}(t,\mathbf{x})\hat{\phi}(t',\mathbf{y})\rangle$ $\quad G^<(t,\mathbf{x},t',\mathbf{y}) = \langle\hat{\phi}(t',\mathbf{y})\hat{\phi}(t,\mathbf{x})\rangle$

Statistical & spectral function:

$$F(t,\mathbf{x},t'\mathbf{y}) = \frac{1}{2}\langle\{\hat{\phi}(t,\mathbf{x}),\hat{\phi}(t',\mathbf{y})\}\rangle - \phi(t,\mathbf{x})\phi(t',\mathbf{y})$$

$$\rho(t,\mathbf{x},t',\mathbf{y}) = i\langle[\hat{\phi}(t,\mathbf{x}),\hat{\phi}(t',\mathbf{y})]\rangle$$

Quantum versus classical-statistical field theory

By performing change of variables we find

$$\langle\varphi^+(t,\mathbf{x})\varphi^+(t',\mathbf{y})\rangle$$
$$\langle\varphi^-(t,\mathbf{x})\varphi^-(t',\mathbf{y})\rangle$$
$$\langle\varphi^+(t,\mathbf{x})\varphi^-(t',\mathbf{y})\rangle$$
$$\langle\varphi^-(t,\mathbf{x})\varphi^+(t',\mathbf{y})\rangle$$

$$\xrightarrow[\chi = \varphi^+ - \varphi^-]{\varphi = \frac{\varphi^+ + \varphi^-}{2}}$$

change of variables

$$\begin{aligned}
\langle\varphi(t,\mathbf{x})\varphi(t',\mathbf{y})\rangle &= F(t,\mathbf{x},t',\mathbf{y}) + \phi(t,\mathbf{x})\phi(t',\mathbf{y}) \\
\langle\varphi(t,\mathbf{x})\chi(t',\mathbf{y})\rangle &= -iG_R(t,\mathbf{x},t'\mathbf{y}) \\
\langle\chi(t,\mathbf{x})\varphi(t',\mathbf{y})\rangle &= -iG_A(t,\mathbf{x},t'\mathbf{y}) \\
\langle\chi(t,\mathbf{x})\chi(t',\mathbf{y})\rangle &= \quad 0
\end{aligned}$$

where retarded & advanced propagators are again given in terms of the spectral function

$$\begin{aligned}
G_R(t,\mathbf{x},t'\mathbf{y}) &= +i\theta(t-t')\langle[\hat\phi(t,\mathbf{x}),\hat\phi(t,\mathbf{y})]\rangle = +\theta(t-t')\rho(t,\mathbf{x},t'\mathbf{y}) \\
G_A(t,\mathbf{x},t'\mathbf{y}) &= -i\theta(t'-t)\langle[\hat\phi(t,\mathbf{x}),\hat\phi(t,\mathbf{y})]\rangle = -\theta(t-t')\rho(t,\mathbf{x},t'\mathbf{y})
\end{aligned}$$

Classicality condition "$|\chi| << |\varphi|$" means

$$|F(t,\mathbf{x},t',\mathbf{y}) + \phi(t,\mathbf{x})\phi(t',\mathbf{y})| \gg |\rho(t,\mathbf{x},t',\mathbf{y})|$$

Quantum versus classical-statistical field theory

What does classicality condition mean in practice?

$$|F(t,\mathbf{x},t',\mathbf{y}) + \phi(t,\mathbf{x})\phi(t',\mathbf{y})| \gg |\rho(t,\mathbf{x},t',\mathbf{y})|$$

Statistical function F -> actual excitations present in the system

Spectral function ρ -> possible excitations of the systems

e.g. in thermal equilibrium $\quad |F(\omega,\mathbf{p})| = \Big(n(\omega) + \frac{1}{2}\Big)|\rho(\omega,\mathbf{p})|$

Classical-statistical description accurate in the presence of strong fields/ for highly occupied bosonic quantum fields

=> Correspondence principle

Several interesting problems of this nature in QCD,Cosmology, Cold Atoms

Note that classicality criterion is time dependent; classical-statistical description typically breaks down after some time