

# Nonequilibrium quantum field theory and the lattice

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(hep-ph/0409233)

# Content

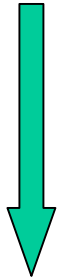
- I. Motivation
- II. Nonequilibrium QFT
- III. Far-from-equilibrium dynamics
- IV. Precision tests on a lattice
- V. Conclusions

# **I. Motivation**

- 1) Early universe**
- 2) Heavy-ion collisions**
- 3) Ultra-cold quantum gases**

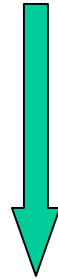
# 1) Early Universe

End of Inflation



*far-from-equilibrium*  
`initial` state

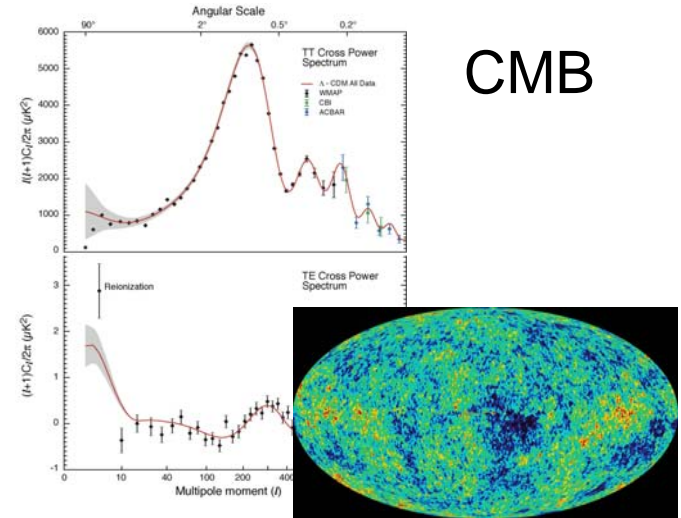
(P)reheating



`entropy`  
production



*time*



CMB

*thermal* spectrum  
with fluctuations

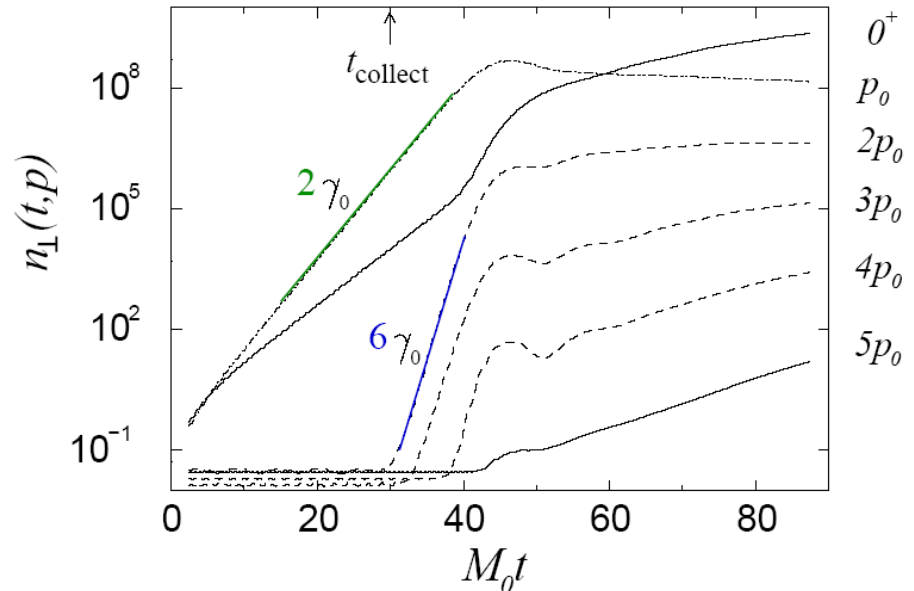
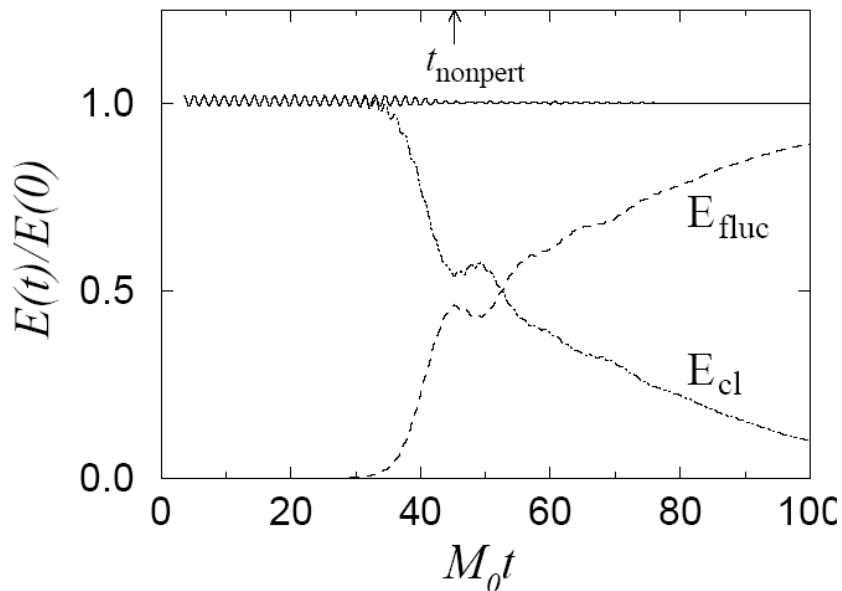
# (P)reheating

## Far-from-equilibrium particle production in quantum field theory

Traschen, Brandenberger, PRD 42 (1990) 2491; Kofman, Linde, Starobinsky, PRL 73 (1994) 3195

CLASSICAL: Khlebnikov, Tkachev, PRL 77 (1996) 219

QUANTUM: Berges, Serreau, PRL 91 (2003) 111601:



## 2) Heavy-ion collisions

Heavy-ion collisions (BNL,CERN,GSI) explore strong interaction matter starting from a transient *nonequilibrium* state

Thermalization ?

Properties of the *equilibrium phase diagram of QCD* ?

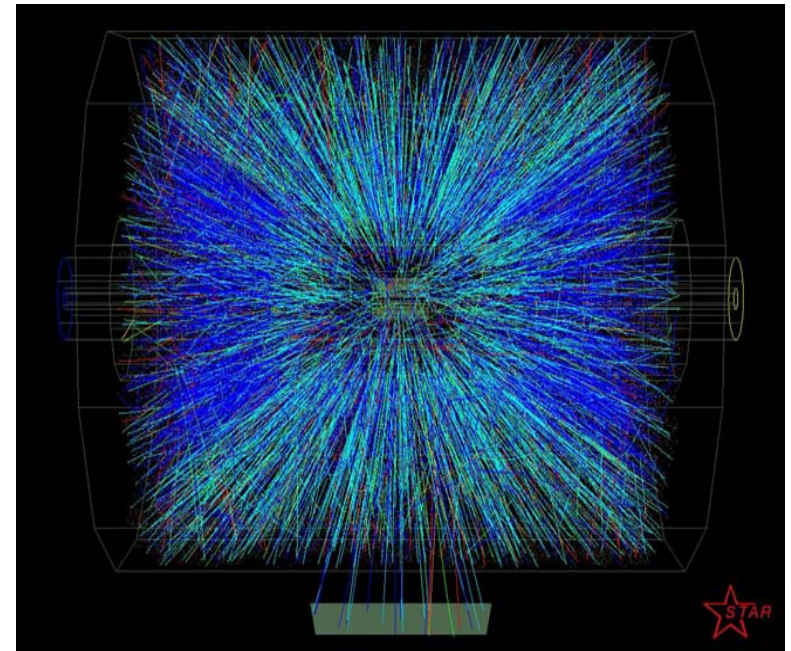
Braun-Munzinger et al., nucl-ex/0411053

*Prethermalization* ?

Berges, Borsanyi, Wetterich, PRL93 (2004)142002

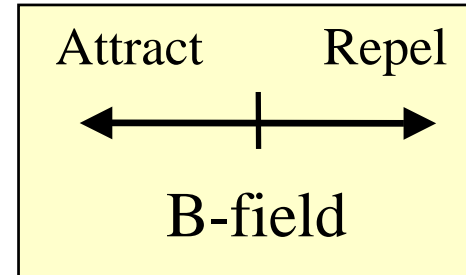
Slowing out of equilibrium near the *QCD critical point*

Rajagopal, Berdnikov, PRD61 (2000) 105017; ...

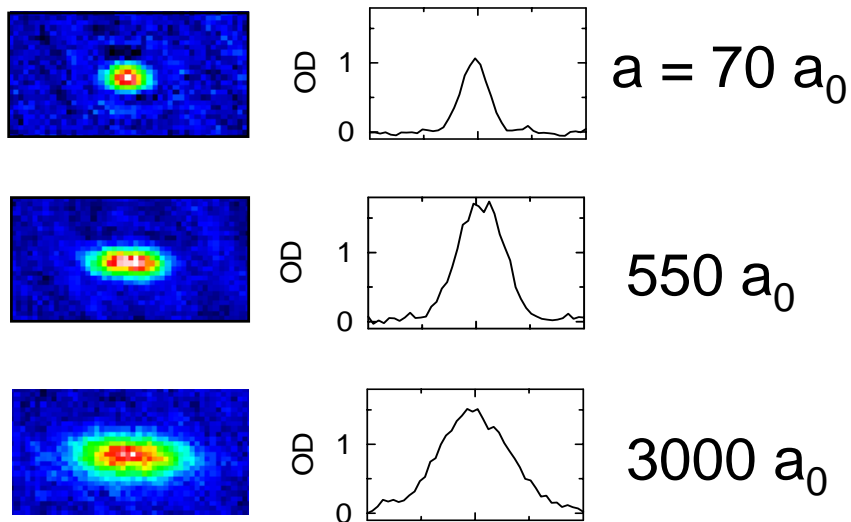


### 3) Ultra-cold quantum gases


 Tunable BEC self-interaction!  
*(Feshbach resonance)*

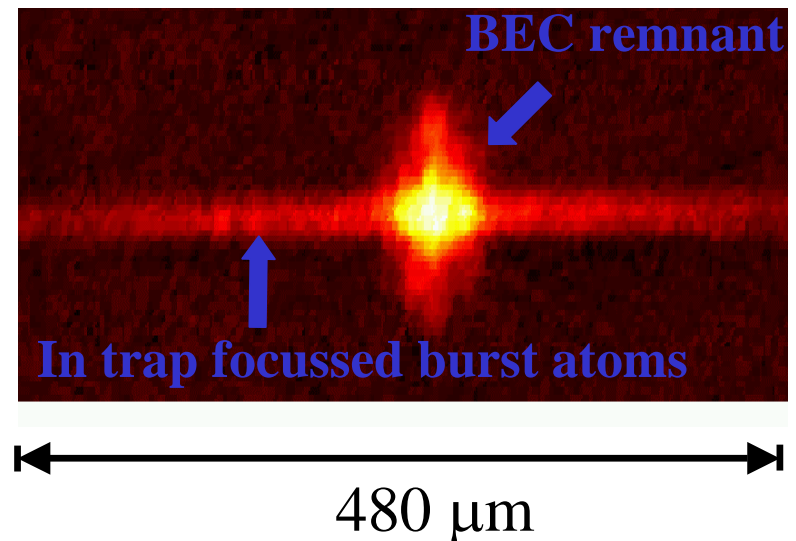


 Measure BEC size, shape:  
*(500 ms)*



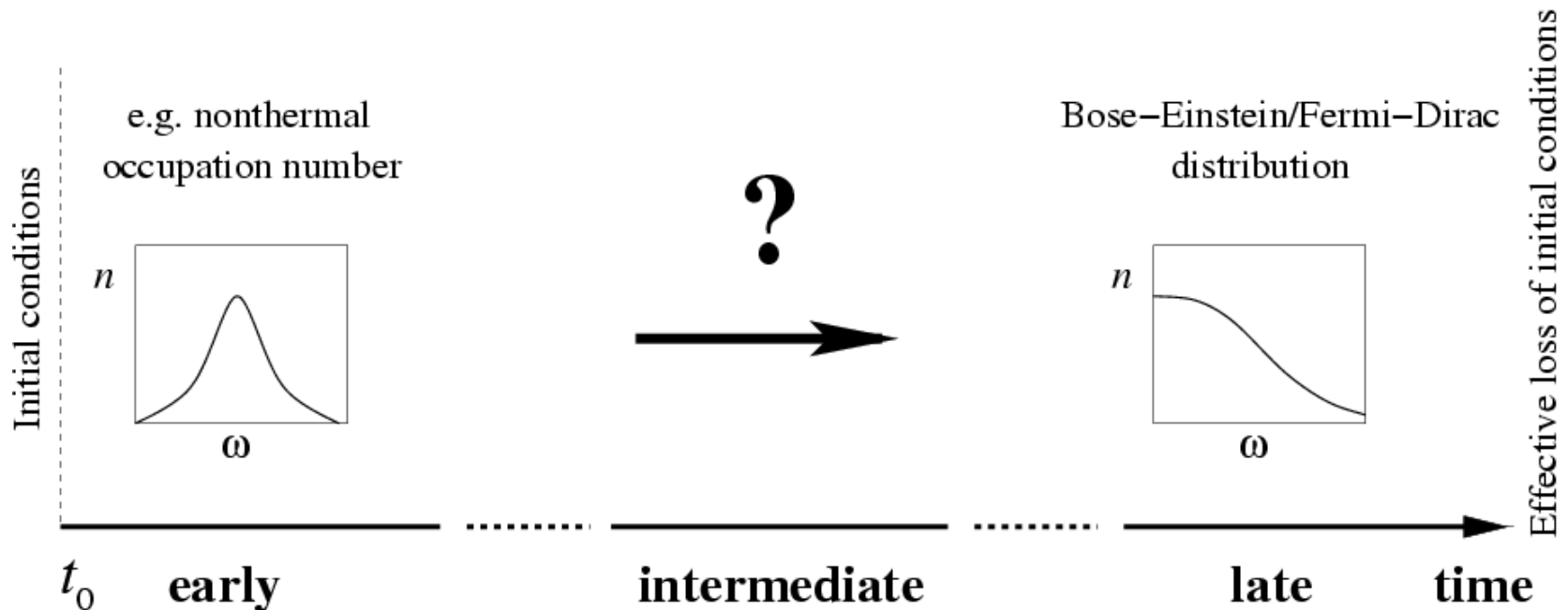
Cornish et al. PRL 85 (2000) 1795

  $B(t)$  faster than atom motion:  
 $(\Delta t \ll 1/\omega_{trap} \sim 10 \text{ ms})$



# Thermalization

- Process of thermalization leads to loss of details about the initial conditions: late-time *'universality'*
- Approach to thermal equilibrium requires *quantum evolution* (*classical* equilibration times are functions of Rayleigh-Jeans cutoff)





# Standard QFT techniques fail out of equilibrium

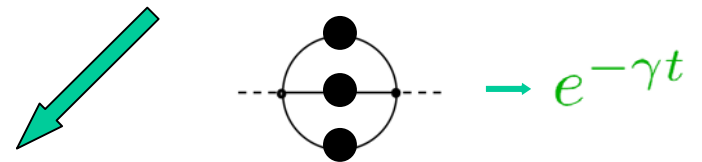
‘Secularity’

➡ uniform approximations in time require infinite pert. orders



‘Universality’

➡ nonlinear dynamics necessary for late-time thermalization



Two-particle irreducible generating functionals

- ➡ systematic 2PI loop-, coupling- or 1/N-expansions available
- ➡ *far-from-equilibrium* dynamics as well as late-time *thermalization* in QFT

Berges, Cox '01; Aarts, Berges '01; Berges '02; Cooper, Dawson, Mihaila '03; Berges, Serreau '03; Berges, Borsanyi, Serreau '03; Cassing, Greiner, Juchem '03; Arrizabalaga, Smit, Tranberg '04 ...

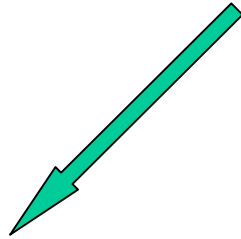
## **II. Nonequilibrium QFT**

- 1) Nonequilibrium generating functional**
- 2) 2PI effective action**
- 3) Time evolution equations**

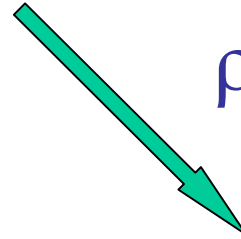
# Nonequilibrium QFT

$$\rho_D \equiv \rho_D^{(\text{eq})}$$

e.g.  $\sim e^{-\beta H}$



$$\rho_D(t=t_0) \neq \rho_D^{(\text{eq})}$$



“Close-to-equilibrium QFT”

“Far-from-equilibrium QFT”

➔ *Thermal equilibrium*  
correlations in real-time

➔ *Nonequilibrium* correlations  
(not necessarily far-from-eq.)

e.g. L.G. Yaffe, NP Proc.Suppl. 106 (2002) 117

- linear response
- transport coefficients
- ...

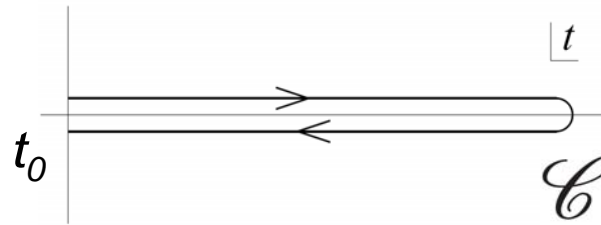
THIS TALK

# Nonequilibrium generating functional

$$Z[J, R; \rho_D] = \underbrace{\int d\varphi^{(1)} d\varphi^{(2)} \langle \varphi^{(1)} | \rho_D(0) | \varphi^{(2)} \rangle}_{\text{initial conditions}} \underbrace{\int_{\varphi^{(1)}}^{\varphi^{(2)}} \mathcal{D}'\varphi e^{i(S[\varphi] + \int_x J(x)\varphi(x) + \frac{1}{2} \int_{xy} R(x,y)\varphi(x)\varphi(y))}}_{\text{quantum dynamics}}$$

*Finite (!)*, closed real-time contour: ( **NO** “ $i\varepsilon$ ” ! No imaginary part)

$$\int_x \equiv \int_{\mathcal{C}} dx^0 \int d^d x$$



$$\langle \varphi^{(1)} | \rho_D(0) | \varphi^{(2)} \rangle = \mathcal{N} e^{if_{\mathcal{C}}[\varphi]}$$

$$f_{\mathcal{C}}[\varphi] = \alpha_0 + \int_x \alpha_1(x)\varphi(x) + \frac{1}{2} \int_{xy} \alpha_2(x,y)\varphi(x)\varphi(y) + \frac{1}{3!} \int_{xyz} \alpha_3(x,y,z)\varphi(x)\varphi(y)\varphi(z) + \dots$$

$$Z[J, R; \rho_D] = \int \mathcal{D}'\varphi e^{i(S[\varphi] + \int_x J(x)\varphi(x) + \frac{1}{2} \int_{xy} R(x,y)\varphi(x)\varphi(y) + \frac{1}{3!} \int_{xyz} \alpha_3(x,y,z)\varphi(x)\varphi(y)\varphi(z) + \dots)}$$

Initial-time sources  $\alpha_i \equiv 0$  for  $t \neq t_0$

# Two-particle irreducible effective action

- Gaussian *initial* density matrix  $\rho_D(0)$ : (i.e.  $\alpha_i = 0$  for  $i > 2$ )

$$Z[J, R; \rho_D(0)] \longrightarrow Z[J, R]$$

(no approximation, just constrains class of initial conditions)

- **2PI effective action** by double Legendre transform:

$$Z[J, R] = \exp(iW[J, R])$$

$$\begin{aligned} \Gamma[\phi, G] &= W[J, R] - \int_x \frac{\delta W[J, R]}{\delta J_a(x)} J_a(x) - \int_{xy} \frac{\delta W[J, R]}{\delta R_{ab}(x, y)} R_{ab}(x, y) \\ &= W[J, R] - \int_x \phi_a(x) J_a(x) - \frac{1}{2} \int_{xy} R_{ab}(x, y) \phi_a(x) \phi_b(y) - \frac{1}{2} \text{Tr} GR \end{aligned}$$

2PI effective action: Luttinger, Ward '60; Baym '62; Cornwall, Jackiw, Tomboulis '74

$$\Gamma[\phi, G] = S[\phi] + \frac{i}{2} \text{Tr} \ln G^{-1} + \frac{i}{2} \text{Tr} G_0^{-1}(\phi) G + \Gamma_2[\phi, G]$$

- Parametrized by macroscopic field:  $\phi(x) = \langle \Phi(x) \rangle$  and
- exact connected propagator:  $G(x, y) = \langle T \Phi(x) \Phi(y) \rangle - \phi(x)\phi(y)$
- $\Gamma_2[\phi, G]$  contains only *two-particle irreducible (2PI) diagrams*

E.g. scalar  $N$ -component field theory to NLO:

$$\Gamma_2[\phi, G] = -\frac{\lambda}{4!N} \int_x G_{aa}(x, x) G_{bb}(x, x) + \frac{i}{2} \text{Tr} \ln \mathbf{B}(G) + \frac{i\lambda^2}{(6N)^2} \int_{xyz} \mathbf{B}^{-1}(x, z; G) G^2(z, y) \phi_a(x) G_{ab}(x, y) \phi_b(y)$$

$$\mathbf{B}(x, y; G) \equiv \delta(x - y) + \frac{i\lambda}{6N} G^2(x, y)$$

Berges '02; Aarts, Ahrensmeier, Baier, Berges, Serreau '02

# Time evolution equations

Equations of motion: (1)  $\frac{\delta\Gamma[\phi, G]}{\delta\phi(x)} = 0$  , (2)  $\frac{\delta\Gamma[\phi, G]}{\delta G(x, y)} = 0$

spectral function  $\sim \langle [\Phi, \Phi] \rangle$

$$G(x, y) = F(x, y) - \frac{i}{2} \rho(x, y) \text{sign}_{\mathcal{C}}(x^0 - y^0)$$

statistical propagator  $\sim \langle \{\Phi, \Phi\} \rangle$

$$[\square_x \delta_{ac} + M_{ac}^2(x)] \rho_{cb}(x, y) = - \int_{y^0}^{x^0} dz \Sigma_{ac}^{\rho}(x, z) \rho_{cb}(z, y)$$

$$[\square_x \delta_{ac} + M_{ac}^2(x)] F_{cb}(x, y) = - \int_0^{x^0} dz \Sigma_{ac}^{\rho}(x, z) F_{cb}(z, y) \\ + \int_0^{y^0} dz \Sigma_{ac}^F(x, z) \rho_{cb}(z, y)$$

$$\left( \left[ \square_x + \frac{\lambda}{6N} \phi^2(x) \right] \delta_{ab} + M_{ab}^2(x; \phi = 0, F) \right) \phi_b(x) \\ = - \int_0^{x^0} dy \Sigma_{ab}^{\rho}(x, y; \phi = 0, F, \rho) \phi_b(y)$$

Nonequilibrium:

$$F \not\sim \rho$$

Equilibrium/Vacuum:  
(fluct.-diss. relation)

$$F \sim \rho$$

📦 In terms of spectral and statistical components the equations for fermionic or gauge fields have very similar structure as well:

↪ In contrast to bosons, for fermions the field anti-commutator corresponds to the spectral function:

$$\begin{aligned}\rho^{(f)}(x, y) &= i\langle\{\psi(x), \bar{\psi}(y)\}\rangle \\ F^{(f)}(x, y) &= \frac{1}{2}\langle[\psi(x), \bar{\psi}(y)]\rangle\end{aligned}$$

Evolution equations are obtained from above by LHS replacement:

$$[\partial^2 + M^2]_x \rho(x, y) \longrightarrow -[i\cancel{\partial}_x - m_f]_x \rho^{(f)}(x, y)$$

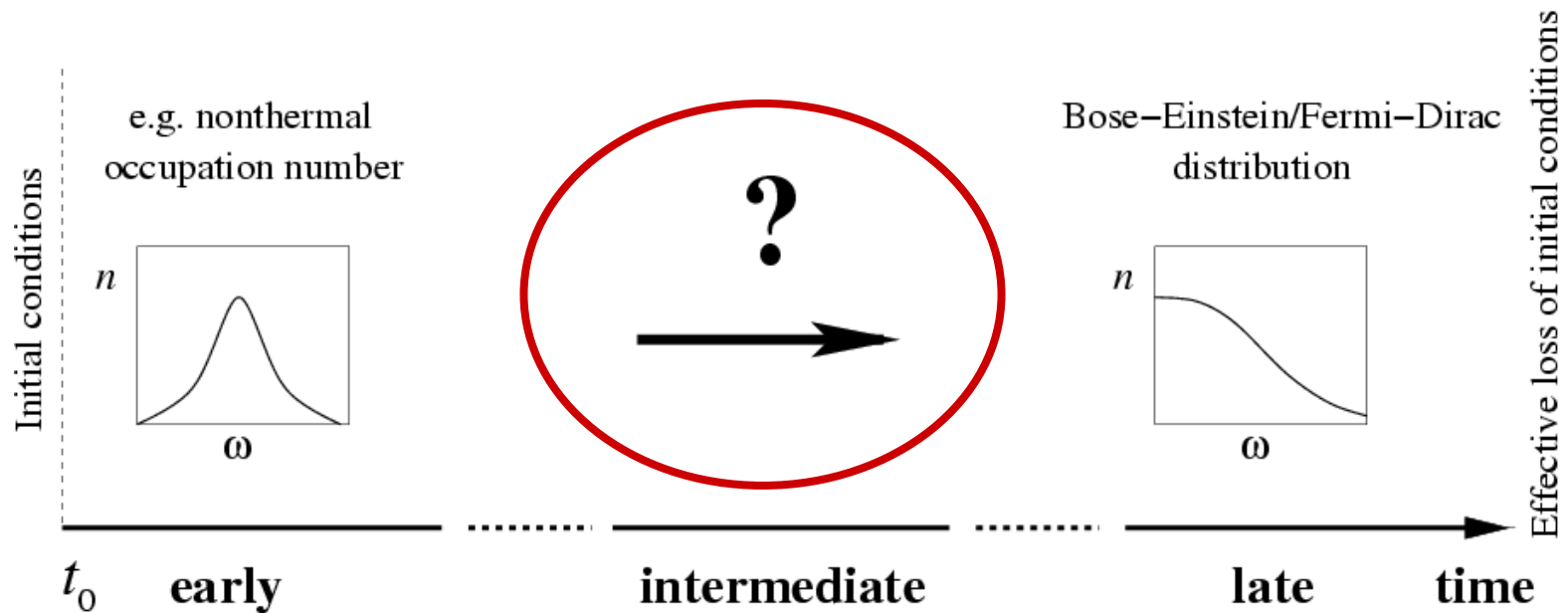
↪ Gauge fields:  $D^{\mu\nu}(x, y) = F_D^{\mu\nu}(x, y) - \frac{i}{2}\rho_D^{\mu\nu}(x, y) \text{sign}_{\mathcal{C}}(x^0 - y^0)$

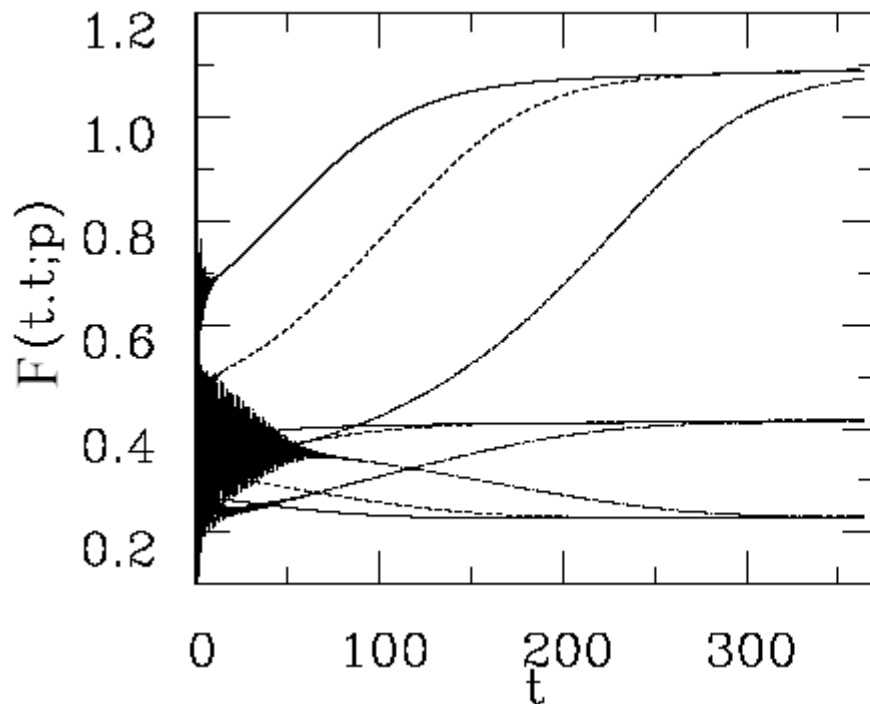
$$[\partial^2 + M^2]_x \rho(x, y) \longrightarrow -[g^\mu{}_\gamma \partial^2 - (1 - \xi^{-1})\partial^\mu \partial_\gamma]_x \rho_D^{\gamma\nu}(x, y)$$

e.g. for covariant gauges and vanishing 'background' fields



# III. Far-from-equilibrium dynamics



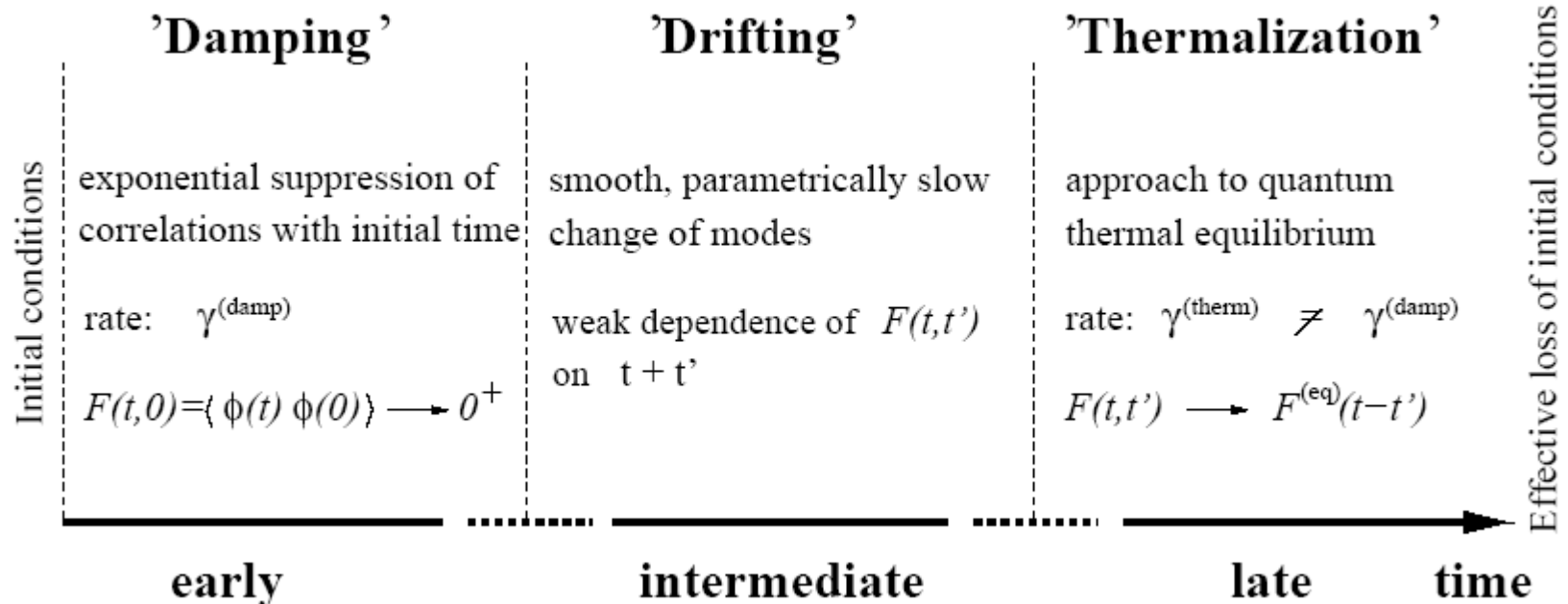


Propagator for (very) different initial conditions with *same*  $\langle E \rangle$

(momenta  $p = 0, 3, 5$ ; all in initial mass units,  $\phi = 0$ )

*scalar  $\phi^4$  in 1+1 d (2PI 3-loop)*

Berges, Cox, PLB 517 (2001) 369



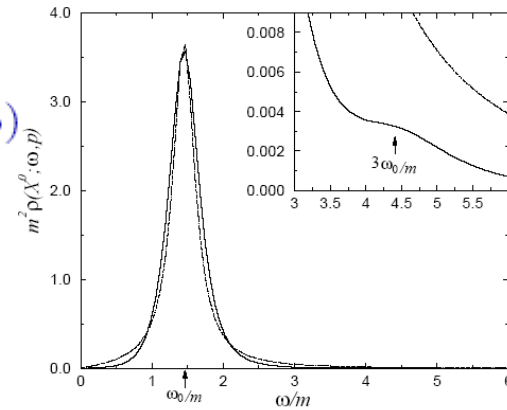
Characteristic time scales for modes are associated to

1. rapid oscillations of correlation functions with period  $\sim 1/\omega_{\mathbf{p}}$

$\rightsquigarrow$  described by 'peak' of spectral function

2. damping of oscillations with inverse rate  $1/\gamma_{\mathbf{p}}^{(\text{damp})}$

$\rightsquigarrow$  described by nonzero 'width'  $\Gamma_{\mathbf{p}} = 2\gamma_{\mathbf{p}}^{(\text{damp})}$   
 (dynamical)



3. 'late-time' thermalization with inverse rate  $1/\gamma_{\mathbf{p}}^{(\text{therm})}$

$\rightsquigarrow$  because of 'off-shell' number changing processes:

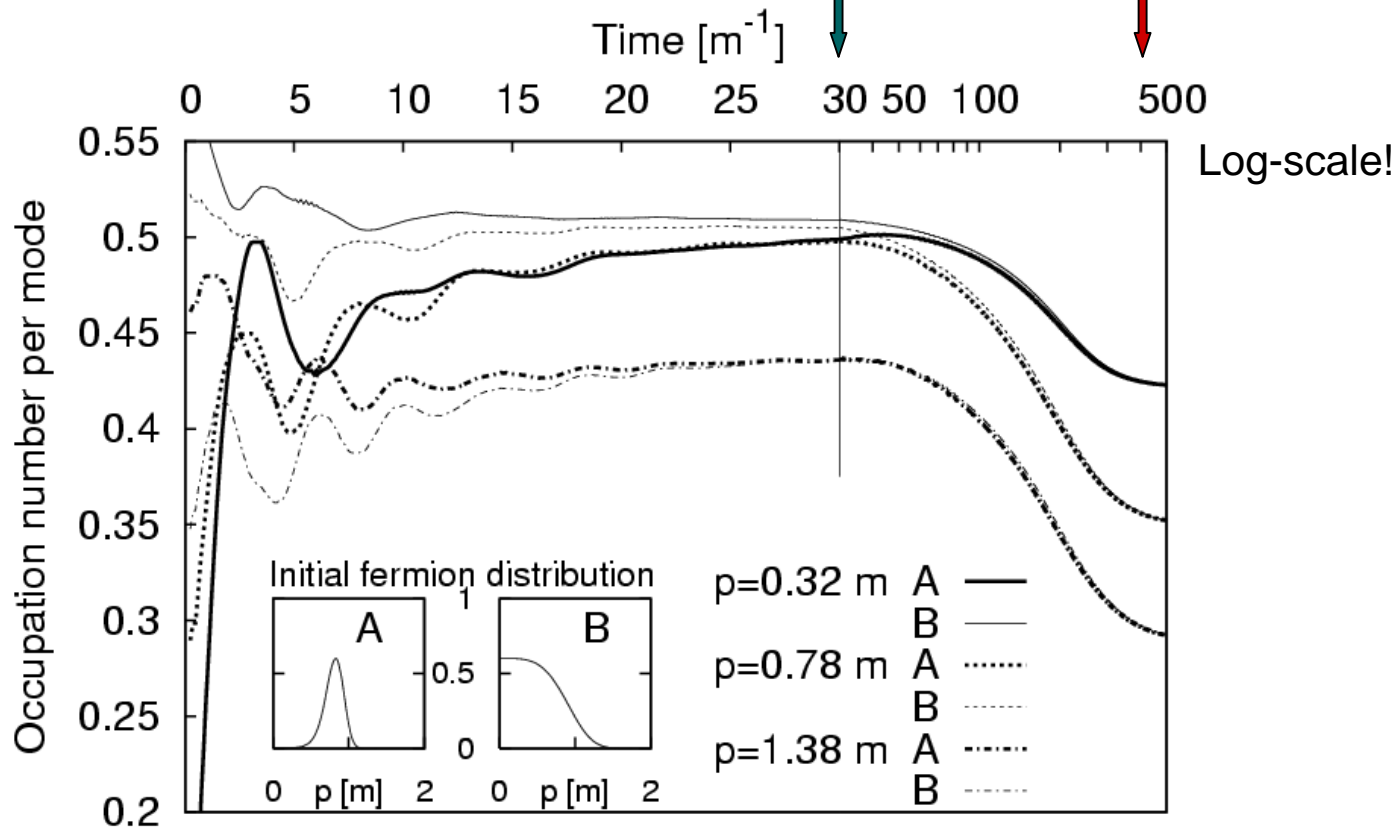
Number changing processes require nonzero 'width'  $\sim \lambda^2/N$  effect in  $\mathcal{O}(\lambda^2/N)$  evolution equation:

$\rightsquigarrow$  parametrically of order  $\lambda^4/N^2$  ("slow!")

Compare to e.g.

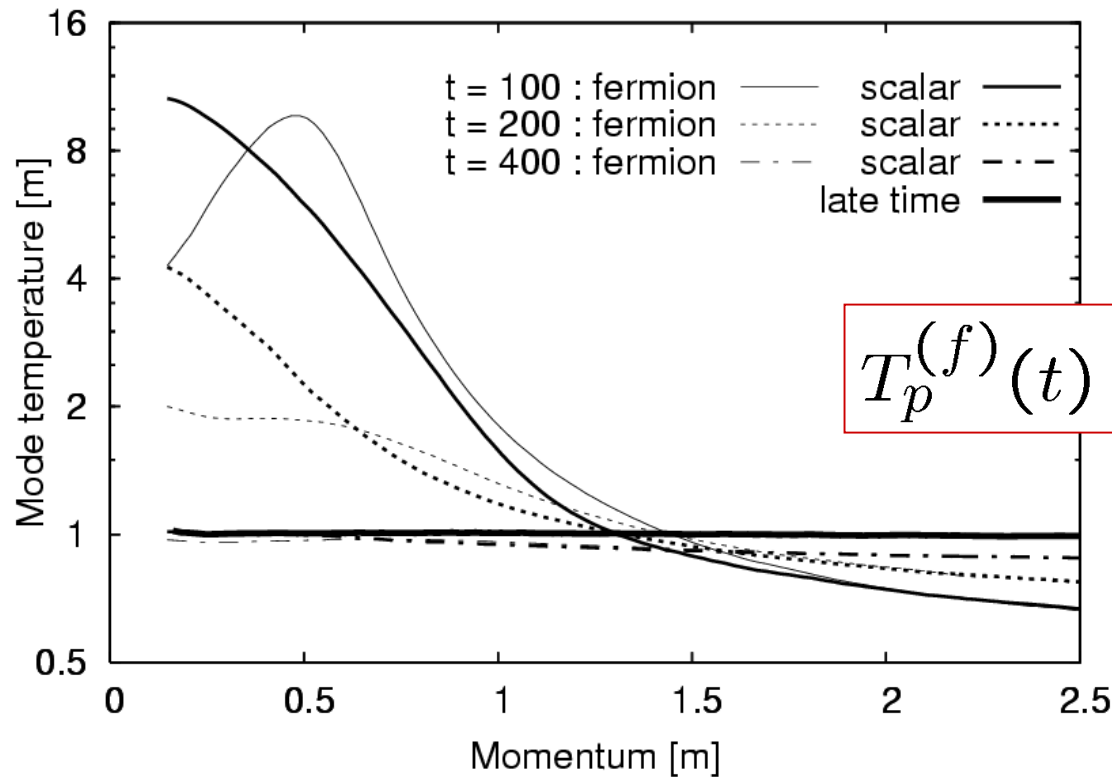
*chiral Yukawa model in 3+1 d (2PI  $1/(N_F=2)$  to NLO)*

Loss of details of initial conditions after  $t_{\text{damp}}$  Thermalization  $t_{\text{therm}}$



# Thermalization

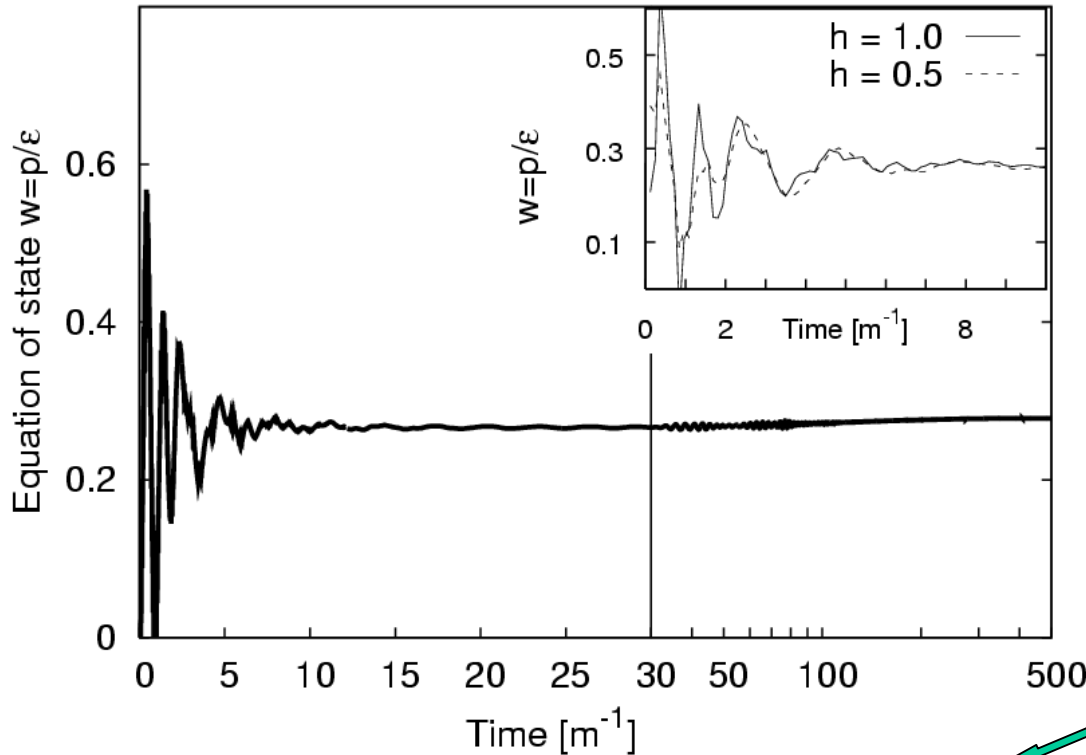
■ 'Mode temperature'  $T_p(t)$ :  $n_p(t) \stackrel{!}{=} \frac{1}{\exp[\omega_p(t)/T_p(t)] \pm 1}$   
 $(n_p \sim \text{tr} \frac{p^i \gamma^i}{p} \langle [\psi, \bar{\psi}] \rangle_p)$



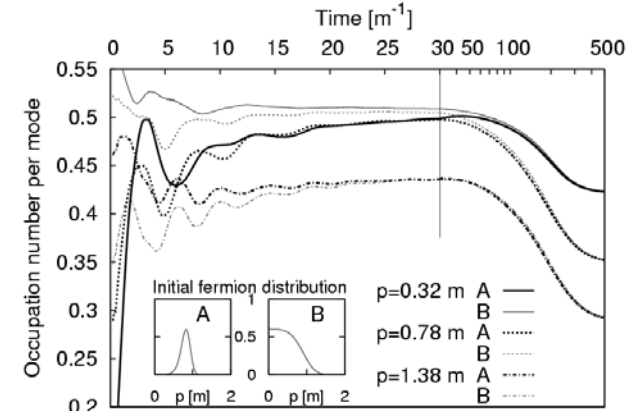
$$T_p^{(f)}(t) = T_p^{(s)}(t) = T_{\text{eq}}$$

Emergence of BE/FD distribution at late times

# Prethermalization



compare:



Prerequisite for hydrodynamics

- Almost time-independent EOS builds up very early, though distributions are far from equilibrium!
- Prethermalization-time independent of interaction details

$$t_{pt} \ll t_{damp} \ll t_{eq}$$

# Application

Estimate of prethermalization time in view of heavy-ion collisions:

- $t_{\text{pt}}$  is rather independent of details of the model like particle content, couplings etc. (‘dephasing’)
- If ‘temperature’, i.e. average kinetic energy per mode, sets the relevant scale we find:

$$T t_{\text{pt}} \simeq 2 - 2.5$$

- For  $T \simeq 400\text{MeV}$  :

$$t_{\text{pt}} \sim 1\text{fm}/c$$

Consistent with observed very early hydrodynamic behavior

## **IV. Precision tests on a lattice**

- 1) Nonequilibrium *classical field simulations***
- 2) Comparison of *simulations* with *classical 2PI***
- 3) Comparison with *quantum 2PI***
- 4) Nonequilibrium *quantum field simulations?***



to 1) Exact classical equation of motion for  $N$ -component field  $\phi_a(x)$ :

$$\left[ \square_x + m^2 + \lambda \phi_b(x) \phi_b(x) / 6N \right] \phi_a(x) = 0$$

Define **classical 'statistical' two-point function**:

$$F_{ab,cl}(x, y) = \langle \phi_a(x) \phi_b(y) \rangle_{cl} \equiv \int D\pi D\phi W[\pi, \phi] \phi_a(x) \phi_b(y)$$

$W[\pi, \phi]$ : normalized probability functional at initial time with canonical momentum  $\pi_a(x) = \partial_t \phi_a(x)$ ,  $\phi_a(0, \mathbf{x}) \equiv \phi_a(\mathbf{x})$ ,  $\pi_a(0, \mathbf{x}) \equiv \pi_a(\mathbf{x})$

Integration over classical phase-space:  $\int D\pi D\phi = \int \prod_{a=1}^N \prod_{\mathbf{x}} d\pi_a(\mathbf{x}) d\phi_a(\mathbf{x})$

Similarly, define **classical spectral function**:

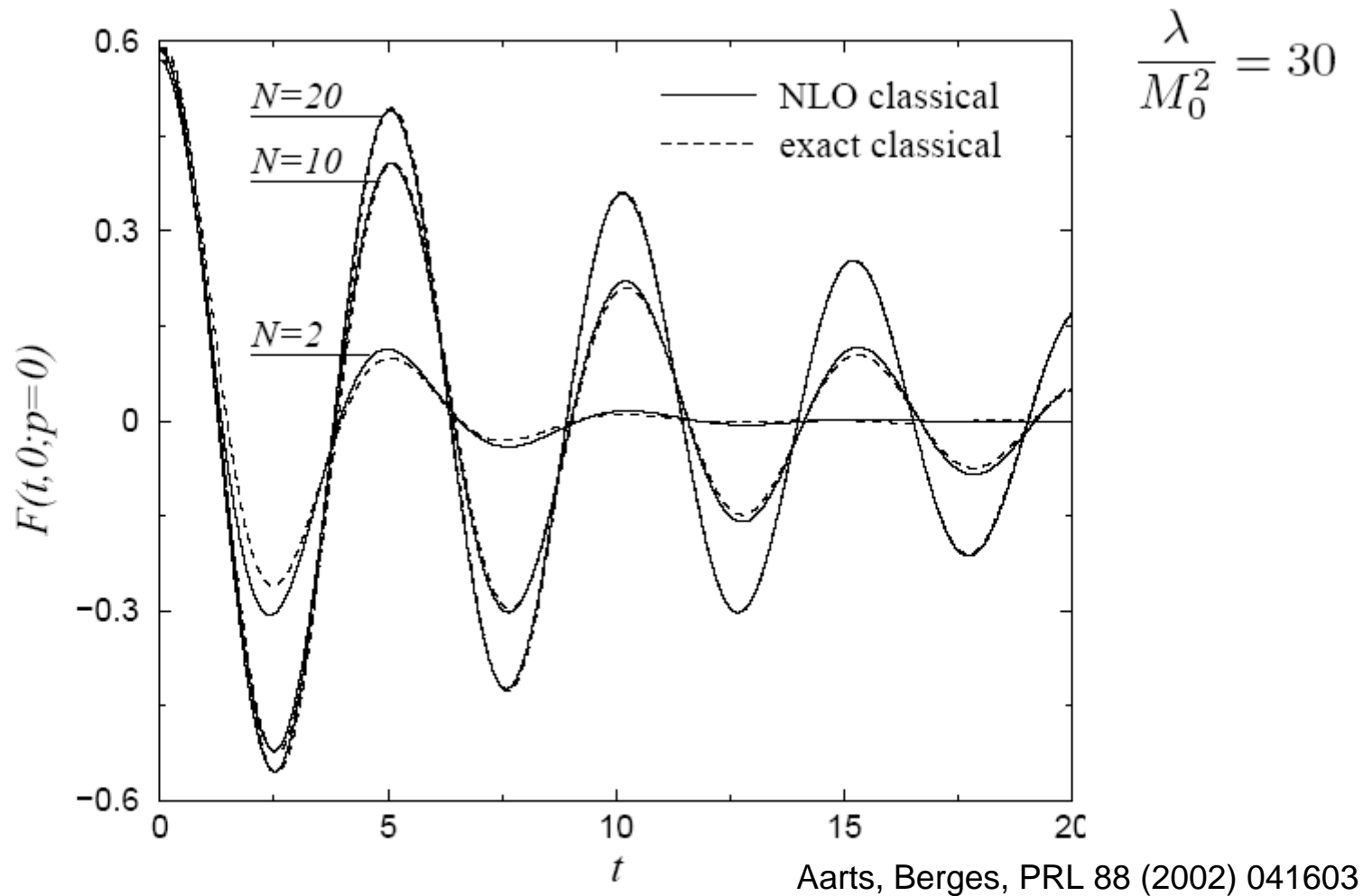
$$\rho_{ab,cl}(x, y) = - \langle \{ \phi_a(x), \phi_b(y) \}_{\text{PoissonBracket}} \rangle_{cl}$$

$$\Rightarrow \rho_{ab,cl}(x, y)|_{x^0=y^0} = 0, \quad \partial_{x^0} \rho_{ab,cl}(x, y)|_{x^0=y^0} = \delta_{ab} \delta(\mathbf{x} - \mathbf{y})$$

$$\{A(x), B(y)\}_{\text{PoissonBracket}} = \sum_{a=1}^N \int d\mathbf{z} \left[ \frac{\delta A(x)}{\delta \phi_a(\mathbf{z})} \frac{\delta B(y)}{\delta \pi_a(\mathbf{z})} - \frac{\delta A(x)}{\delta \pi_a(\mathbf{z})} \frac{\delta B(y)}{\delta \phi_a(\mathbf{z})} \right]$$

# “Early-time” damping (effective loss of details of initial conditions)

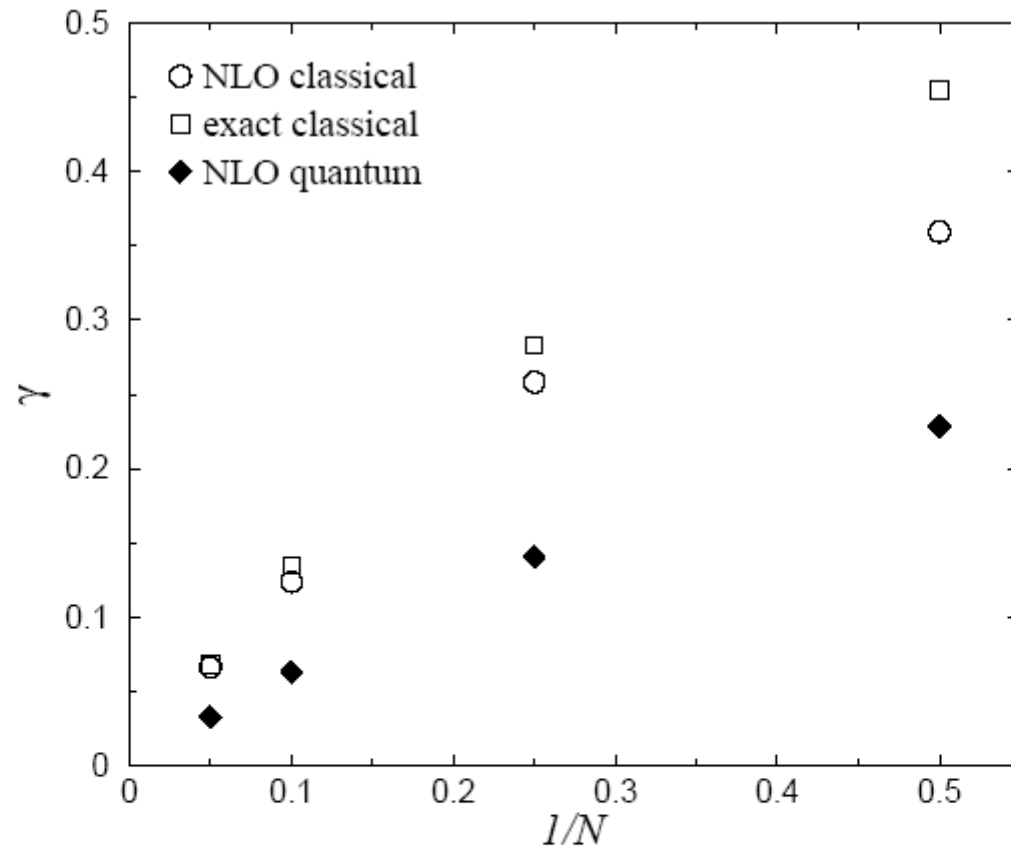
$(1+1)d$



⇒

Convergence of classical *NLO* and *exact* (MC) results already for moderate values of  $N$  (!)

## Parametric behavior/comparison with quantum theory:



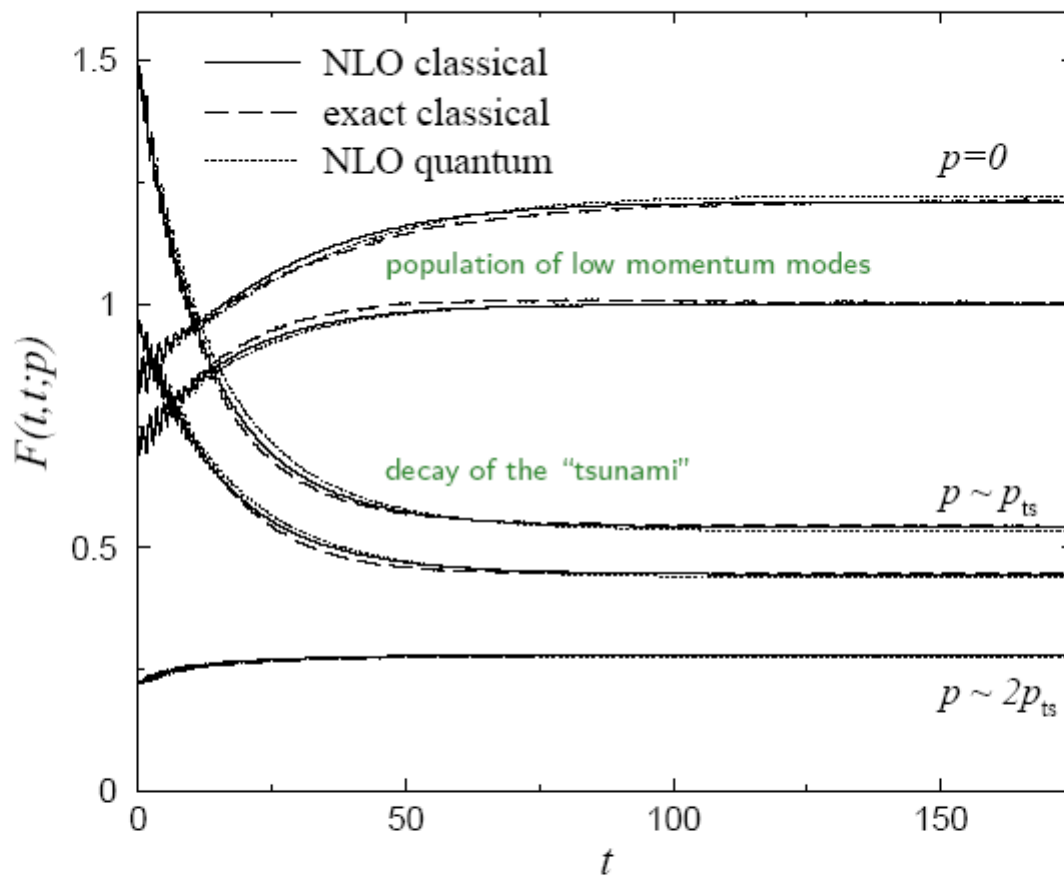
- ▣ Inverse damping rate  $1/\gamma$  scales  $\sim N$  for large  $N$   
 $\rightsquigarrow$  zero damping at LO ( $N \rightarrow \infty$ )
- ▣ Damping *enhanced* if quantum corrections are neglected

Here:  $n_0(p) \ll \frac{1}{2} \rightsquigarrow$  quantum corrections important!

## “Late-time” (i.e. for quantum theory) behavior:

High initial particle number  $n_0$  peaked around  $p = |p_{ts}| \simeq 4M_0$

“Tsunami”:



$$N=4 (!)$$

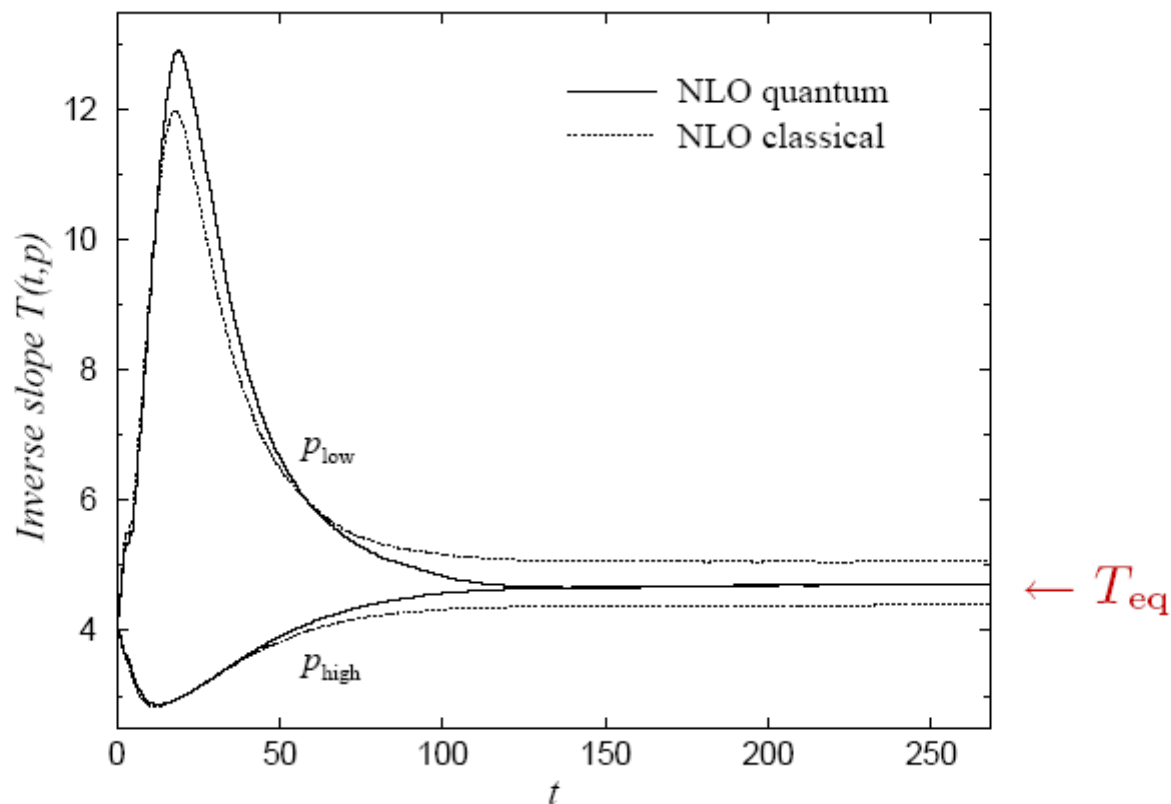
$$\lambda = 12 M_0^{-2}$$

**NLO** quantum evolution well approximated by exact classical result!

Here:  $n_0(p_{ts}) \gg \frac{1}{2}$  and  $n_0(p) \gtrsim 0.35$  for  $p \lesssim 2p_{ts}$

$\leadsto$  small quantum corrections for displayed modes

## Quantum vs. classical thermalization:



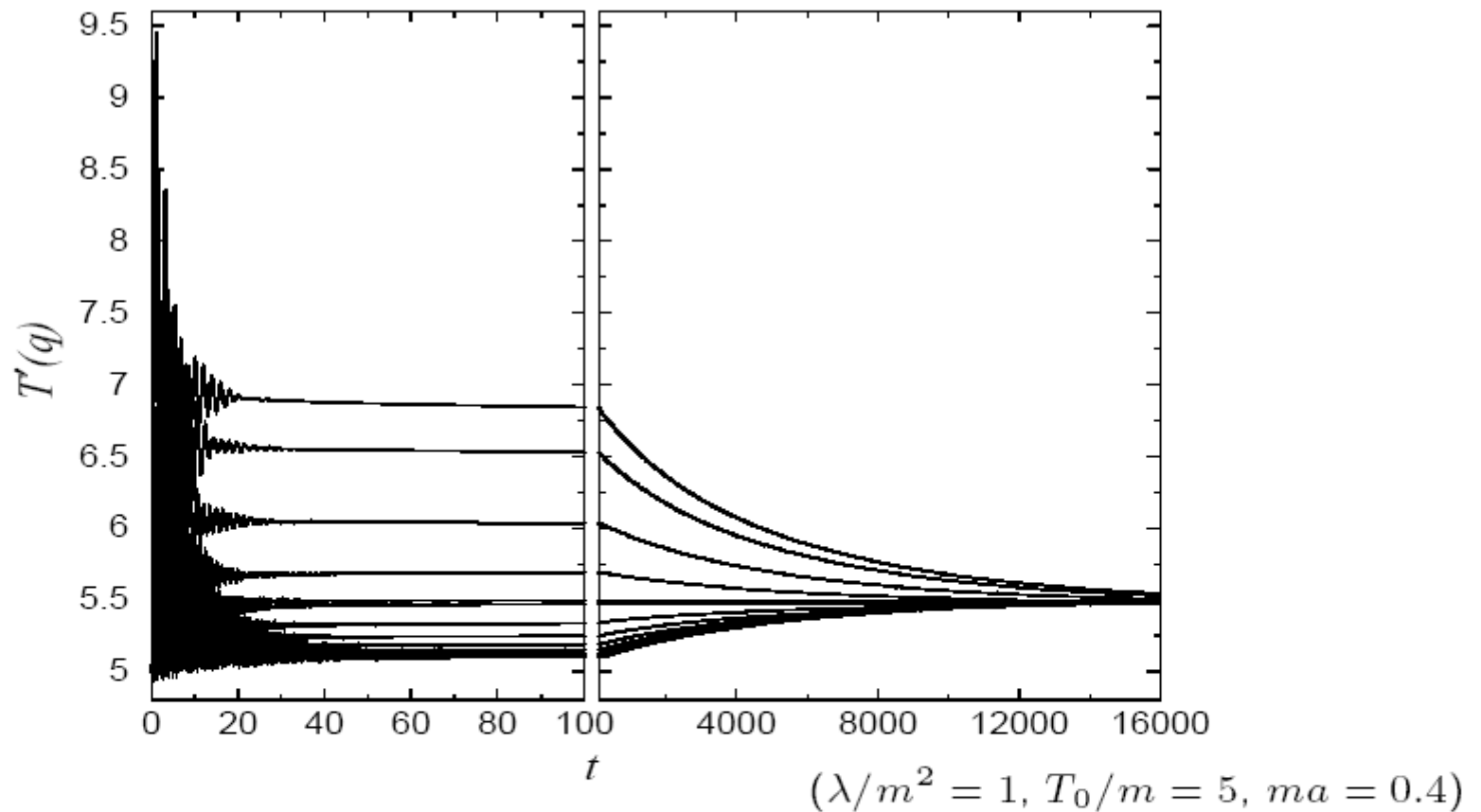
Inverse slope parameter :  $T(t, p) \equiv -n(t, \epsilon_p)[n(t, \epsilon_p) + 1](dn/d\epsilon_p)^{-1}$

$\Rightarrow$  constant for  $n(t, \epsilon_p) = 1/[e^{\epsilon_p/T_{\text{eq}}} - 1]$  (Bose-Einstein)

Classical theory does (of course) not reach Bose-Einstein distribution

Typically classical thermalization time  $\gg$  quantum thermalization time

Classical thermalization example:



Here: classical 2PI 3-loop approximation

J.B., NPA699 (2002) 847

↪ compares well with exact results! Aarts, Bonini, Wetterich, PRD63 (2001) 025012

$$T'(t, p) = \partial_t \partial_{t'} F_{\text{cl}}(t, t'; p)|_{t=t'}$$

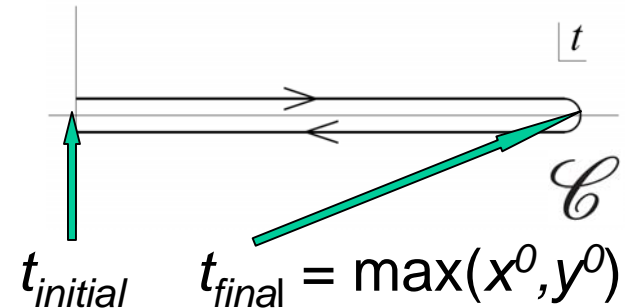
$$\langle \pi_a(t, \mathbf{x}) \pi_b(t, \mathbf{y}) \rangle_{\text{cl}}^{(\text{eq})} = \partial_t \partial_{t'} F_{\text{cl}}^{(\text{eq})}(t, t'; p)|_{t=t'} \delta_{ab} = T_{\text{cl}} \delta(\mathbf{x} - \mathbf{y}) \delta_{ab}$$

# Simulations of nonequilibrium quantum fields?

## Non-positive definite probability measure

→ note again: no “ $i\varepsilon$ ”, finite times

$$\langle T_{\mathcal{C}} \Phi(x) \Phi(y) \rangle = \frac{\delta^2 Z[J, R; \rho_D]}{i\delta J(x) i\delta J(y)} \Big|_{J=R=0}$$



Similar to positivity problems at nonzero chemical potential for baryon number in QCD

→ reweighting? Cf. e.g. Fodor & Katz [hep-lat/0104001](https://arxiv.org/abs/hep-lat/0104001)

very likely not a good idea for nonequilibrium...

(but: interesting short-time/intermediate-time behavior requires relatively small volumes (physical IR-cutoff, cf. UV): enough statistics?)

## ■ Stochastic quantization (complex Langevin equation)

Parisi, Wu '81; ...

- ➡ in principle very well suited, however, not 'safe'  
(not applied so far to nonequilibrium lattice simulations (?))

### Idea

Standard Langevin: 
$$\frac{\partial \phi}{\partial \tau} = -\frac{\partial S(\phi)}{\partial \phi} + \eta(\tau)$$

with white noise  $\langle \eta(\tau) \rangle = 0$  ,  $\langle \eta(\tau) \eta(\tau') \rangle = 2\delta(\tau - \tau')$

Stochastic process described by probability distribution  $P(\phi, \tau)$ ,

Fokker-Planck:

$$\frac{\partial P(\phi, \tau)}{\partial \tau} = \frac{\partial}{\partial \phi} \left( \frac{\partial}{\partial \phi} + \frac{\partial S(\phi)}{\partial \phi} \right) P(\phi, \tau)$$

$P(\phi, \tau) \rightarrow e^{-S(\phi)}$  for  $\tau \rightarrow \infty$  :

$$\langle A \rangle_P = \frac{\int \mathcal{D}\phi A(\phi) P(\phi, \tau)}{\int \mathcal{D}\phi P(\phi, \tau)} \rightarrow \frac{\int \mathcal{D}\phi A(\phi) e^{-S(\phi)}}{\int \mathcal{D}\phi e^{-S(\phi)}}$$



Consider:  $\tau \rightarrow it$  ,  $\phi(\tau) \rightarrow \phi(t)$  ,  $\eta(\tau) \rightarrow -i\eta(t)$

$$\frac{\partial \phi}{\partial t} = -i \frac{\partial S(\phi)}{\partial \phi} + \eta(t), \quad \langle \eta(t) \rangle = 0, \quad \langle \eta(t)\eta(t') \rangle = 2i\delta(t-t')$$

i.e.  $\phi, \eta$  complex!

$$R(\phi, t) \equiv \text{Re} \left( i \frac{\partial S}{\partial \phi} \right), \quad I(\phi, t) \equiv \text{Im} \left( i \frac{\partial S}{\partial \phi} \right)$$

$$\frac{\partial \phi_R}{\partial t} = -iR(\phi, t) + \eta_R(t), \quad \frac{\partial \phi_I}{\partial t} = -iI(\phi, t) + \eta_I(t)$$

$$\langle \eta_R(t) \rangle = \langle \eta_I(t) \rangle = 0 \quad (\star)$$

$$\langle \eta_R(t)\eta_R(t') \rangle = \langle \eta_I(t)\eta_I(t') \rangle = (A + B)\delta(t-t')$$

$$\langle \eta_R(t)\eta_I(t') \rangle = \delta(t-t') \quad , \quad A - B = 1, \quad A > 0, \quad B > 0$$

(Define:  $\eta \equiv (\eta_1 - \eta_2) + i(\eta_1 + \eta_2)$  with  $\eta_1, \eta_2$  real:  $\langle \eta_1 \rangle = \langle \eta_2 \rangle = 0$ ,  $\langle \eta_1 \eta_1 \rangle = A \delta$ ,  $\langle \eta_2 \eta_2 \rangle = B \delta$ ,  $\langle \eta_1 \eta_2 \rangle = 0$ )

Stochastic process (★) described by real positive  $P(\phi_R, \phi_I, t)$ :

$$\begin{aligned} \frac{\partial P(\phi_R, \phi_I, t)}{\partial t} = & \frac{1}{2} \left[ (A+B) \frac{\partial^2}{\partial \phi_R^2} + \frac{\partial^2}{\partial \phi_R \partial \phi_I} + (A+B) \frac{\partial^2}{\partial \phi_I^2} \right] P(\phi_R, \phi_I, t) \\ & + \frac{\partial}{\partial \phi_R} [R(\phi_R, \phi_I, t) P(\phi_R, \phi_I, t)] + \frac{\partial}{\partial \phi_I} [I(\phi_R, \phi_I, t) P(\phi_R, \phi_I, t)] \end{aligned}$$

Note that averages are given by area integral in the complex plane:

$$\langle A \rangle_P = \frac{\int \mathcal{D}\phi_R \mathcal{D}\phi_I A(\phi_R + i\phi_I) P(\phi_R, \phi_I, t)}{\int \mathcal{D}\phi_R \mathcal{D}\phi_I P(\phi_R, \phi_I, t)} = \frac{\int \mathcal{D}\phi_R A(\phi_R) P_{eff}(\phi_R, t)}{\int \mathcal{D}\phi_R P_{eff}(\phi_R, t)}$$

$\uparrow$   
 $\phi_R \rightarrow \phi_R - i\phi_I$

with complex  $P_{eff}(\phi_R, t) = \int \mathcal{D}\phi_I P(\phi_R - i\phi_I, \phi_I, t)$  governed by  
*analytic continuation of Fokker-Planck for real variables:*

$$\frac{\partial P_{eff}(\phi_R, t)}{\partial t} = i \frac{\partial}{\partial \phi_R} \left( \frac{\partial}{\partial \phi_R} + \frac{\partial S(\phi)}{\partial \phi_R} \right) P_{eff}(\phi_R, t)$$

➡ Convergence? Reliability? Not well understood so far...

# Conclusions

- Nonequilibrium real-time evolution in QFT crucial for wide range of phenomena in particle physics and cosmology
- Loop-, coupling- or  $1/N$ -expansions of 2PI effective action so far uniquely suitable to resolve secularity and universality
  - apparently good convergence properties, even for rather strong couplings
  - excellent agreement of *classical simulations* with *2PI quantum* results for large occupation numbers and not too late times
- Non-positive definite probability measure for *quantum simulations*
  - however: no “ $i\varepsilon$ ”, finite times
  - complex Langevin in principle suitable for nonequilibrium, but not well understood so far

Self-energies from 3-loop 2PI effective action (similarly for NLO  $1/N$ ):

to 3) Quantum

$$\phi = 0$$

$$\begin{aligned}\Sigma^F(t, t'; \mathbf{p}) &= -\frac{\lambda^2}{6} \int_{\mathbf{q}, \mathbf{k}} F(t, t'; \mathbf{p} - \mathbf{q} - \mathbf{k}) \\ &\quad \left[ F(t, t'; \mathbf{q}) F(t, t'; \mathbf{k}) - \frac{3}{4} \rho(t, t'; \mathbf{q}) \rho(t, t'; \mathbf{k}) \right] \\ \Sigma^\rho(t, t'; \mathbf{p}) &= -\frac{\lambda^2}{2} \int_{\mathbf{q}, \mathbf{k}} \rho(t, t'; \mathbf{p} - \mathbf{q} - \mathbf{k}) \\ &\quad \left[ F(t, t'; \mathbf{q}) F(t, t'; \mathbf{k}) - \frac{1}{12} \rho(t, t'; \mathbf{q}) \rho(t, t'; \mathbf{k}) \right]\end{aligned}$$

to 2) Classical

$$\begin{aligned}\Sigma_{\text{cl}}^F(t, t'; \mathbf{p}) &= -\frac{\lambda^2}{6} \int_{\mathbf{q}, \mathbf{k}} F(t, t'; \mathbf{p} - \mathbf{q} - \mathbf{k}) F(t, t'; \mathbf{q}) F(t, t'; \mathbf{k}) \\ \Sigma_{\text{cl}}^\rho(t, t'; \mathbf{p}) &= -\frac{\lambda^2}{2} \int_{\mathbf{q}, \mathbf{k}} \rho(t, t'; \mathbf{p} - \mathbf{q} - \mathbf{k}) F(t, t'; \mathbf{q}) F(t, t'; \mathbf{k})\end{aligned}$$

$$\begin{aligned}\Sigma^F &\rightarrow \Sigma_{\text{cl}}^F = \Sigma^F (F^2 \gg \rho^2) \\ \Sigma^\rho &\rightarrow \Sigma_{\text{cl}}^\rho = \Sigma^\rho (F^2 \gg \rho^2)\end{aligned}$$

(LO large- $N$ /Hartree approximations have  $\Sigma^F = \Sigma^\rho \equiv 0$ ,  
i.e. quantum  $\equiv$  classical)

$\rightsquigarrow$  *sufficient* condition for classical evolution:

$$|F(t, t'; \mathbf{q})F(t, t'; \mathbf{k})| \gg \frac{3}{4} |\rho(t, t'; \mathbf{q})\rho(t, t'; \mathbf{k})|$$

Estimate in terms of nonequilibrium 'quasi-particle' number:

$$\overline{F^2}(t, t'; \mathbf{p}) \equiv \frac{\omega_{\mathbf{p}}}{2\pi} \int_{t-2\pi/\omega_{\mathbf{p}}}^t dt' F^2(t, t'; \mathbf{p}) \rightsquigarrow \frac{(n_{\mathbf{p}}(t) + 1/2)^2}{2\omega_{\mathbf{p}}^2(t)}$$

and for time-averaged spectral function:  $\overline{\rho^2}(t, t'; \mathbf{p}) \rightsquigarrow 1/2\omega_{\mathbf{p}}^2(t)$

$$\rightsquigarrow \left[ n_{\mathbf{p}}(t) + \frac{1}{2} \right]^2 \gg \frac{3}{4} \quad \text{or} \quad n_{\mathbf{p}}(t) \gg 0.37$$

2. For the source-dependent matrix element one has in complete analogy to the vacuum/equilibrium case:

$$\begin{aligned}
 & \langle \varphi^{(2)} | T e^{i \left( \int_x J(x) \Phi(x) + \frac{1}{2} \int_{xy} R(x,y) \Phi(x) \Phi(y) \right)} | \varphi^{(1)} \rangle \\
 &= \int \mathcal{D}'\varphi e^{i \left( S[\varphi] + \int_x J(x) \varphi(x) + \frac{1}{2} \int_{xy} R(x,y) \varphi(x) \varphi(y) \right)} \\
 & \quad \varphi(0^+, \mathbf{x}) = \varphi^{(1)}(\mathbf{x}) \\
 & \quad \varphi(0^-, \mathbf{x}) = \varphi^{(2)}(\mathbf{x})
 \end{aligned}$$

3. In contrast to the equilibrium case the density matrix,  $\mathcal{D}(0) \not\sim e^{-\beta H}$ , cannot be interpreted as an evolution operator in imaginary time!

Example: the most general *Gaussian* density matrix can be written as

$$\begin{aligned}
 & \langle \varphi^{(1)} | \mathcal{D}(0) | \varphi^{(2)} \rangle = \\
 & \frac{1}{\sqrt{2\pi\xi^2}} \exp \left\{ i\dot{\phi}_0 (\varphi^{(1)} - \varphi^{(2)}) - \frac{\sigma^2 + 1}{8\xi^2} \left[ (\varphi^{(1)} - \phi_0)^2 + (\varphi^{(2)} - \phi_0)^2 \right] \right. \\
 & \left. + i \frac{\eta}{2\xi} \left[ (\varphi^{(1)} - \phi_0)^2 - (\varphi^{(2)} - \phi_0)^2 \right] + \frac{\sigma^2 - 1}{4\xi^2} (\varphi^{(1)} - \phi_0)(\varphi^{(2)} - \phi_0) \right\}
 \end{aligned}$$

... where we neglect the spatial dependencies for a moment.

The density matrix is equivalent to the set of *initial conditions*:

$$\phi_0 \equiv \phi(t)|_{t=0} = \text{Tr} \{ \mathcal{D}(0) \Phi(t) \} |_{t=0}$$

$$\dot{\phi}_0 \equiv \partial_t \phi(t)|_{t=0}$$

$$\xi^2 \equiv G(t, t')|_{t=t'=0} = [\text{Tr} \{ \mathcal{D}(0) \Phi(t) \Phi(t') \} - \phi(t) \phi(t')] |_{t=t'=0}$$

$$\xi \eta \equiv \frac{1}{2} [\partial_t G(t, t') + \partial_{t'} G(t, t')] |_{t=t'=0}$$

$$\eta^2 + \frac{\sigma^2}{4\xi^2} \equiv \partial_t \partial_{t'} G(t, t') |_{t=t'=0}$$

The equivalence between initial density matrix and initial conditions can be checked explicitly:

$$\begin{aligned} \text{Tr} \mathcal{D}(0) &= \int_{-\infty}^{\infty} d\varphi \langle \varphi | \mathcal{D}(0) | \varphi \rangle \\ &= \frac{1}{\sqrt{2\pi\xi^2}} \int_{-\infty}^{\infty} d\varphi \exp \left\{ -\frac{1}{2\xi^2} (\varphi - \phi_0)^2 \right\} = 1 \end{aligned}$$

$$\text{Tr} \{ \mathcal{D}(0) \Phi(0) \} = \frac{1}{\sqrt{2\pi\xi^2}} \int_{-\infty}^{\infty} d\varphi \varphi \exp \left\{ -\frac{1}{2\xi^2} (\varphi - \phi_0)^2 \right\} \stackrel{\varphi \rightarrow \varphi + \phi_0}{=} \phi_0$$

etc.

Similarly one finds

$$\text{Tr} \mathcal{D}^2(0) = \int_{-\infty}^{\infty} d\varphi \int_{-\infty}^{\infty} d\varphi' \langle \varphi | \mathcal{D}(0) | \varphi' \rangle \langle \varphi' | \mathcal{D}(0) | \varphi \rangle = \frac{1}{\sigma}$$

$\rightsquigarrow$  for  $\sigma > 1$  the initial conditions with  $\eta^2 + \frac{\sigma^2}{4\xi^2} \equiv \partial_t \partial_{t'} G(t, t')|_{t=t'=0}$  describe a *mixed state*. For  $\sigma = 1$  the “mixing term” in  $\mathcal{D}(0)$  is absent and one obtains a pure-state density matrix.





## HEidelberg Linux Cluster System



- 512 AMD Athlon MP processors (~1 Teraflops)
- 2 Gbit Myrinet
- MPI-Standard