

Lattice Simulations of Non-Equilibrium Dynamics

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Lattice

- non-perturbative as much as possible: computers
 1. classical approximations
 2. 2PI approximations & topological 'defects'

Initial-value problem

scalar field $\phi(x)$

observable $O(x)$, e.g. $T^{\mu\nu}(x) = \partial^\mu\phi(x)\partial^\nu\phi(x) + \dots$

e.o.m. for Heisenberg fields

$$\partial_t\hat{\phi} = \hat{\pi}, \quad \partial_t\hat{\pi} - \nabla^2\hat{\phi} + \mu^2\hat{\phi} + \lambda\hat{\phi}^3 = 0$$

state described by density operator $\hat{\rho}$

$$\langle\hat{O}(x)\rangle = \text{Tr}\hat{O}(x)\hat{\rho}, \quad \langle\hat{O}(x)\hat{O}(y)\rangle = \text{Tr}\hat{O}(x)\hat{O}(y)\hat{\rho}, \quad \dots$$

operator $\hat{\phi}(x) \approx$ infinite-dimensional matrix

- need to truncate/approximate in relation to $\hat{\rho}$ and \hat{O}

- Langevin?

classical approximation

$$\hat{\phi}(x) \rightarrow \phi(x), \quad \hat{\pi}(x) \rightarrow \pi(x)$$

classical fields, solns of classical e.o.m. with initial values

$$\phi_i(\mathbf{x}), \pi_i(\mathbf{x})$$

$$\hat{\rho} \rightarrow \rho_c = \rho_c[\phi_i, \pi_i], \quad \hat{O}(x) \rightarrow O[\phi_i, \pi_i; x]$$

classical average over initial values

$$\langle O(x) \rangle = \int D\phi_i D\pi_i \rho_c[\phi_i, \pi_i] O[\phi_i, \pi_i, x], \quad \dots$$

discretize space-time on a lattice, spacings $a, a_t \ll a$

1. draw initial values from ρ_c ensemble
2. solve field equations on computer
3. evaluate averages over ρ_c ensemble

when applicable?

intuition: large occupation numbers

define $n_{\mathbf{k}}$ and $\tilde{n}_{\mathbf{k}}$ from two-point correlators at $t = t_i$

$$C_{\mathbf{k}}^{\phi\phi} = \langle \phi_{\mathbf{k}} \phi_{-\mathbf{k}} \rangle - \langle \phi_{\mathbf{k}} \rangle \langle \phi_{-\mathbf{k}} \rangle \equiv \left(n_{\mathbf{k}} + \frac{1}{2} \right) \frac{1}{\omega_{\mathbf{k}}}$$

$$C_{\mathbf{k}}^{\phi\pi} = \langle \phi_{\mathbf{k}} \pi_{-\mathbf{k}} \rangle - \langle \phi_{\mathbf{k}} \rangle \langle \pi_{-\mathbf{k}} \rangle \equiv \tilde{n}_{\mathbf{k}} + \frac{1}{2} i$$

$$C_{\mathbf{k}}^{\pi\pi} = \langle \pi_{\mathbf{k}} \pi_{-\mathbf{k}} \rangle - \langle \pi_{\mathbf{k}} \rangle \langle \pi_{-\mathbf{k}} \rangle \equiv \left(n_{\mathbf{k}} + \frac{1}{2} \right) \omega_{\mathbf{k}}$$

free field:

$$n_{\mathbf{k}} = \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle, \quad \tilde{n}_{\mathbf{k}} = \text{Im} \langle a_{\mathbf{k}} a_{-\mathbf{k}} \rangle$$

in case $n_{\mathbf{k}} \gg 1$: expect classical approximation to be good for observables dominated by these \mathbf{k} -modes

in case of weak coupling, can study classical approximation in perturbation theory*

*Aarts, JS, PLB 393 (1997) 395; NPB 511 (1998) 451; Aarts, Nauta, van Weert, PRD 61 (2000) 105002; Van der Meulen, JS, JCAP 023(2007)0711

initial conditions

gaussian: determine/choose

$$\bar{\pi} = \langle \hat{\phi} \rangle, \bar{\pi} = \langle \hat{\pi} \rangle, C^{\phi\phi}, C^{\{\phi,\pi\}} = \frac{1}{2}(C^{\phi\pi} + C^{\pi\phi}), C^{\pi\pi}$$

probability distribution for the fluctuations

$$\phi' = \phi - \bar{\phi} \quad \pi' = \pi - \bar{\pi}$$

$$\begin{aligned} P &\propto \exp \left[-\frac{1}{2} (\phi' \quad \pi') C^{-1} \begin{pmatrix} \phi' \\ \pi' \end{pmatrix} \right] \\ &= \exp \left[-\frac{1}{2} \sum_{\mathbf{k}} \left(\frac{|\xi_{\mathbf{k}}^+|^2}{n_{\mathbf{k}} + 1/2 + \tilde{n}_{\mathbf{k}}} + \frac{|\xi_{\mathbf{k}}^-|^2}{n_{\mathbf{k}} + 1/2 - \tilde{n}_{\mathbf{k}}} \right) \right] \end{aligned}$$

$$\xi_{\mathbf{k}}^{\pm} = \frac{1}{\sqrt{2\omega_{\mathbf{k}}}} (\omega_{\mathbf{k}} \phi'_{\mathbf{k}} \pm \pi'_{\mathbf{k}})$$

(assumed homogeneous ensemble)

draw initial ϕ', π' from P , add mean fields to get initial

$$\phi_i = \bar{\phi}_i + \phi'_i, \quad \pi_i = \bar{\pi}_i + \pi'_i$$

two schemes:

1. initialize only modes with $n_{\mathbf{k}} > 1/2$

no power in the UV, typically $|\mathbf{k}| < k_{\max} \ll 1/a$

good for sensitive observables with many derivatives, e.g. $F\tilde{F}$, winding number densities

2. initialize all modes*

power in the UV, need renormalization & matching

however, non-local UV divergencies require finite a

*E.g. [Khlebnikov, Tkachev, PRL 77 \(1966\) 219](#)

beyond gaussian initial conditions

- $\rho = Z^{-1} e^{-H/T}$

need finite $1/a = \mathcal{O}(T)$, matching to quantum theory, 'power in the UV',

add 'HTL particles' in case of large separation of scales

examples: sphaleron rate*, correlators in SU(2)-Higgs model**

- recent studies of plasma instabilities (cf. this meeting)

*Ambjørn, Krasnitz, PLB 362 (1995) 97, NPB 506 (1997) 387; Tang, JS, NPB 482 (1996) 265; Arnold, Son, Yaffe, PRD 55 (1997) 6264; Arnold, PRD 55 (1997) 7781; Moore, Rummukainen, PRD 61 (2000) 105008; Bödeker, Moore, Rummukainen, PRD 61 (2000) 056003

**Tang, JS, NPB 510 (1998) 401; Arnold, Yaffe PRD 57 (1998) 1178

- quantum?

$$\text{Tr} e^{-\hat{H}/T} = \int D\phi e^{-S}$$

sample (MC) ϕ_i, π_i from two imaginary-time slices

QCD two-point functions: large occupation numbers in the vacuum?

fermions

always quantum

classical approximation for Bose fields gives linear Dirac equation; use mode functions*

$$\hat{\psi}(x) = \sum_{\alpha} w_{\alpha}(x) \hat{\psi}_{\alpha}$$

$$0 = [\gamma^{\mu} \partial_{\mu} - igA_{\mu}(x)] w_{\alpha}(x)$$

$$0 = \partial_{\mu} F^{\mu\nu}(x) + g \sum_{\alpha, \beta} \langle \hat{\psi}_{\alpha}^{\dagger} \hat{\psi}_{\beta} \rangle \bar{w}_{\alpha}(x) i\gamma^{\nu} w_{\beta}(x)$$

fermion doubling**

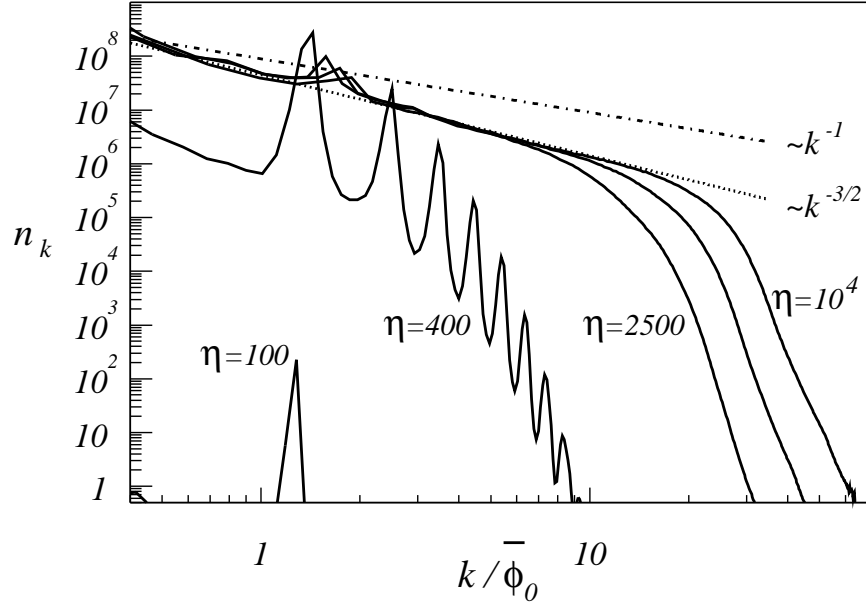
*Aarts, JS, NPB555 (1999) 355; PRD61 (2000) 025002

**avoidable? cf. Yukawa model Berges, Borsányi, Serreau, NPB 660 (2003) 51

Example: cascade to the UV

- has self similar features, turbulence*

*Son, PRD 54 (1996) 3745; Micha, Tkachev PRD 70 (2004) 043538, Boyanovsky, Destri, De Vega, PRD 69 (2004) 045003; Destri, De Vega, PRD 73 (2006) 025014; Díaz-Gil, García-Bellido, González-Arroyo, Pérez, POS Lat2005 (2005) 242



'cascade' to higher momenta: n_k vs $k/\bar{\Phi}_0$ ($\bar{\Phi}_0 =$ amplitude of zero-mode oscillations) at various conformal times η (Micha & Tkachev)

Example: cold electroweak transition*

inflaton χ , Higgs doublet φ

after EW-scale inflation: universe is cold

χ -energy transferred to other d.o.f.

$$V(\chi, \dots) = V(\chi) + (\lambda_{\chi\varphi}\chi^2 - \mu^2)\varphi^\dagger\varphi + \dots$$

time-dependent effective φ -mass

$$\mu_{\text{eff}}^2 = -\mu^2 + \lambda_{\chi\varphi}\chi^2$$

$\mu_{\text{eff}}^2 < 0 \rightarrow$ tachyonic instability, large occupation numbers in χ and φ in limited momentum range: preheating

*scenario for baryogenesis, [García-Bellido, Grigoriev, Kusenko, Shaposhnikov, PRD 60 \(1999\) 123504](#); [García-Bellido, García-Pérez, González-Arroyo, PRD 67 \(2003\) 03501](#); [PRD 69 \(2004\) 023504](#); [Tranberg, JS, JHEP 12 \(2002\) 020](#), [JHEP 0311 \(2003\) 016](#); [JHEP 08 \(2006\) 012](#); [Tranberg, Hindmarsh, JS, JHEP 01 \(2007\) 034](#)

tachyonic transition at $t = t_c$, $\mu_{\text{eff}}(t_c) = 0$

gaussian approximation:

$$\ddot{\phi}_{\mathbf{k}} + (\mu_{\text{eff}}^2 + k^2)\phi_{\mathbf{k}} = 0$$

shortly after t_c :

$$\mu_{\text{eff}}^2 = -M^3(t - t_c),$$

or consider a quench:

$$\begin{aligned}\mu_{\text{eff}}^2 &= +\mu^2, \quad t < t_c, \\ &= -\mu^2, \quad t > t_c\end{aligned}$$

for $k < k_{\max}$: n_k and \tilde{n}_k grow \approx exponentially

$$n_k + 1/2 - \tilde{n}_k \rightarrow 0$$

$$\begin{aligned} k_{\max} &= \sqrt{M^3(t - t_c)} \\ &= \mu, \quad \text{for the quench} \end{aligned}$$

initial distribution for classical approximation:

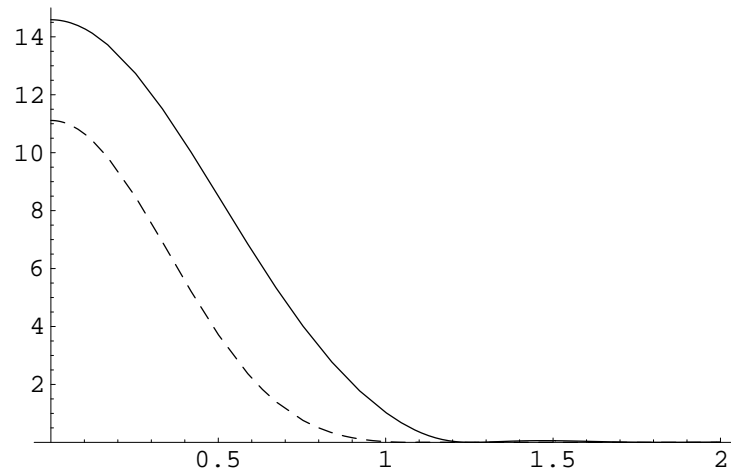
- at time $t_i > t_c$, when $n_k \gg 1$ and non-linear terms in e.o.m. still small

or

- at $t_i = t_c$, 'just the half'

1. $k < k_{\max}$

2. all modes initialized



n_k versus k/μ in 1+1 D at time $t_s = 2.05 \mu^{-1}$ (full)
 $10^{-2} n_k$ vs k/μ in 3+1 D at time $t_s = 4.2 \mu^{-1}$ (dashed)

initial quench ($t_c = 0$)

t_s = spinodal time at which back reaction becomes important

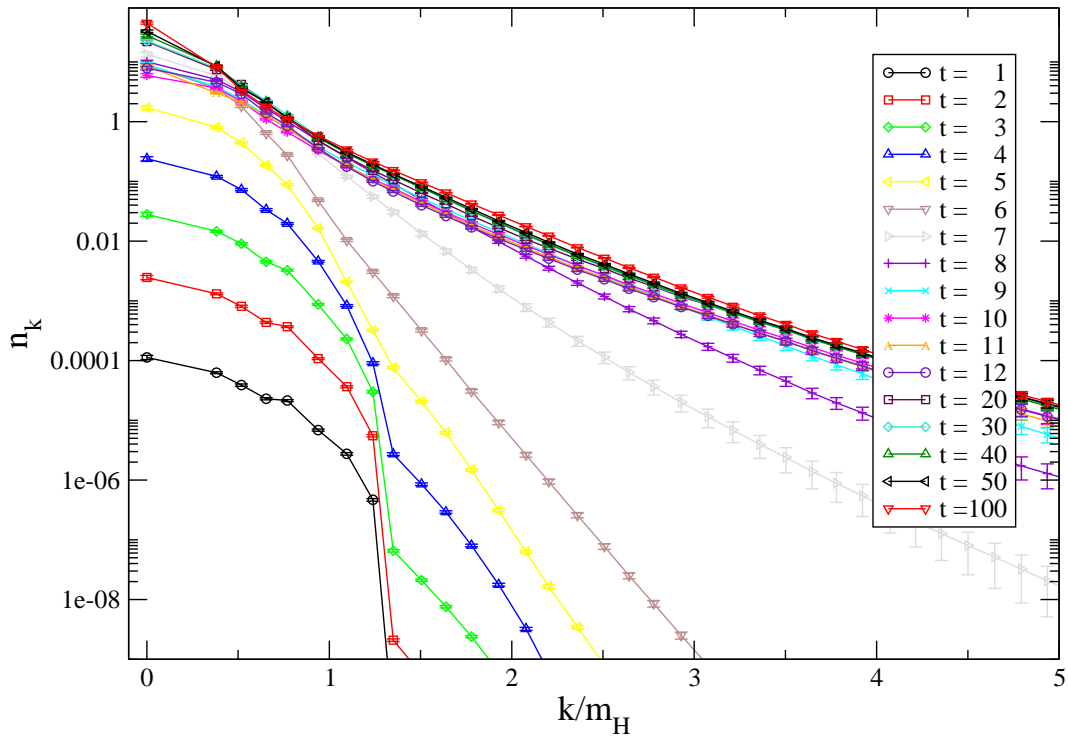
particle numbers in the SU(2)-Higgs model*

$$-\mathcal{L} = \frac{1}{2g^2} \text{tr} F_{\mu\nu} F^{\mu\nu} + (D_\mu \varphi)^\dagger D^\mu \varphi - \mu^2 \varphi^\dagger \varphi + \lambda (\varphi^\dagger \varphi)^2$$

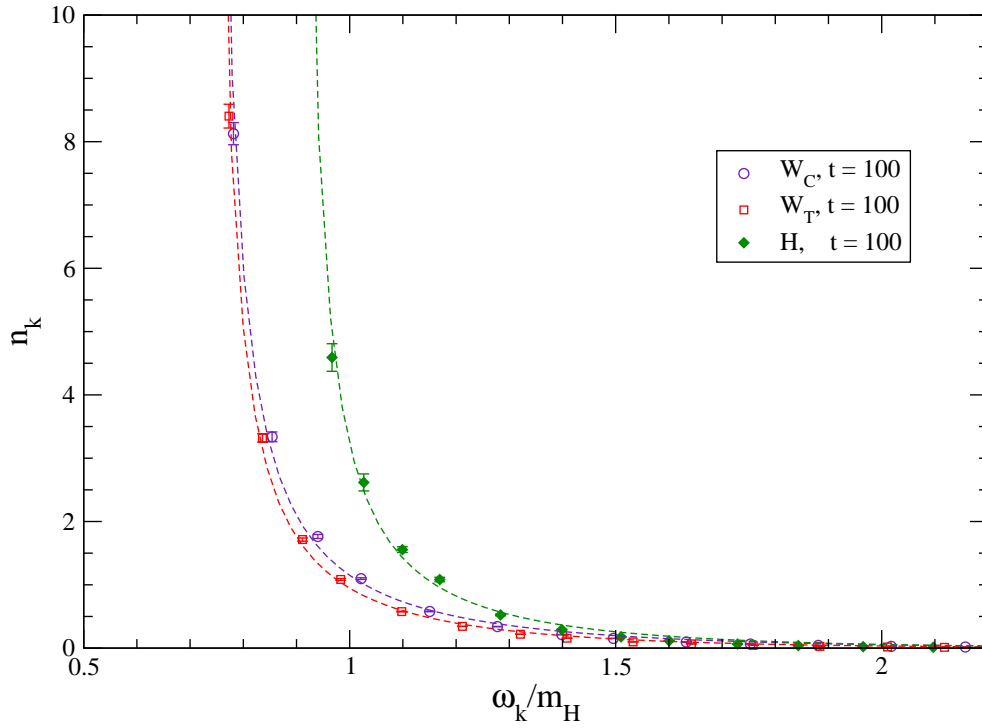
quench, 'just the half', $k_{\text{max}} = \mu$

$\mathbf{A}_{\text{init}} = 0$, $A_0 = 0$, Gauss' law

*Skullerud, JS, Tranberg, JHEP 0308 (2003) 045



Coulomb-gauge W-particle numbers as a function of momentum, time in units of m_H^{-1}



Higgs- and W-particle numbers at time $t = 100 m_H^{-1}$; W_C : Coulomb gauge; W_T : unitary gauge, transverse; H: unitary gauge Higgs

approx. gauge-independence of transverse n_k^W (Coulomb- and unitary-gauge) after $t = 50 m_H^{-1}$ not much happens in $50 \lesssim tm_H < 100$

temperature $T \approx 0.4 m_H$

chemical potential $\mu_{\text{ch}} \approx 0.7(0.9)m_H$ for W(H)

low temperature, but still many $n_k \gg 1$ because of chemical potential

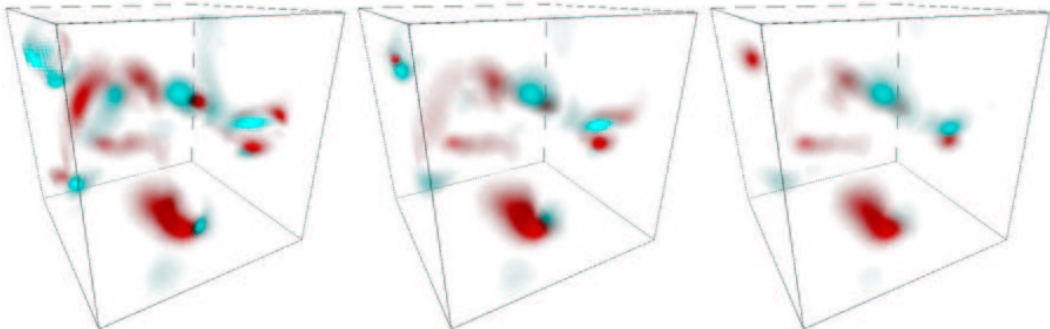
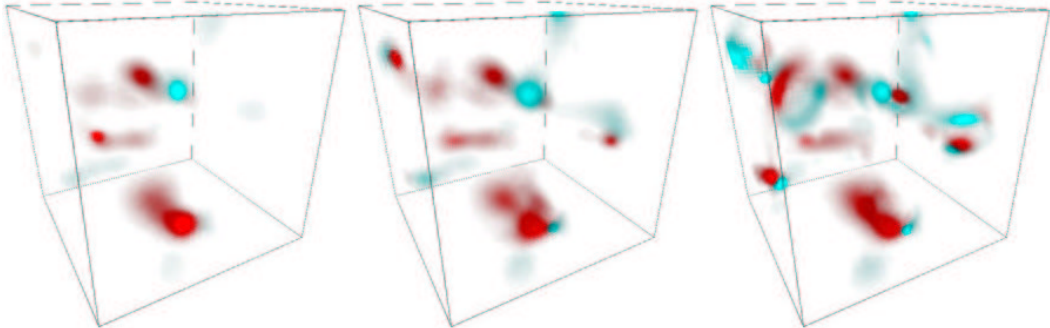
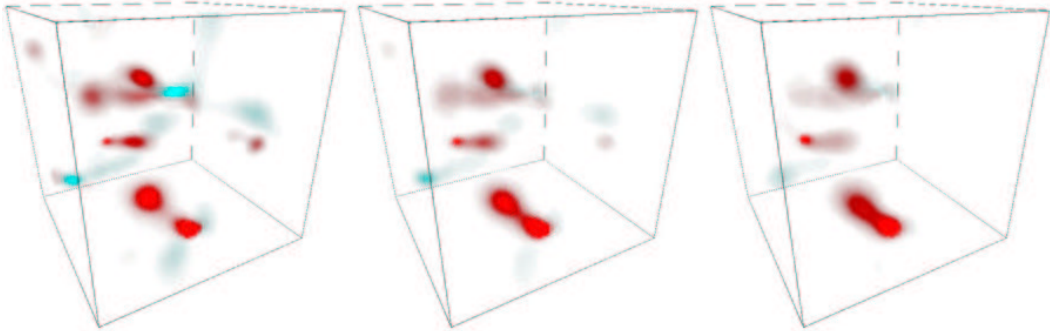
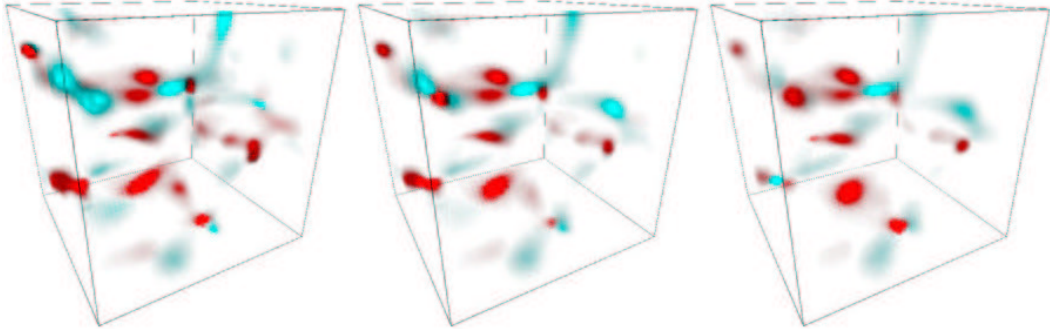
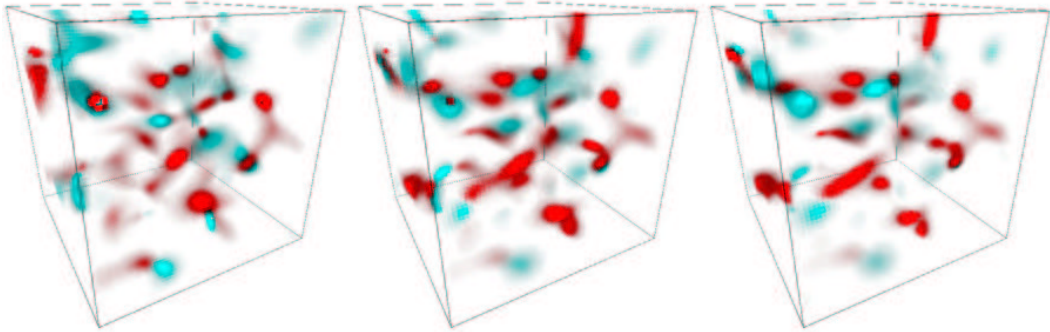
longitudinal modes settle at slower rate

winding-number density of the Higgs field

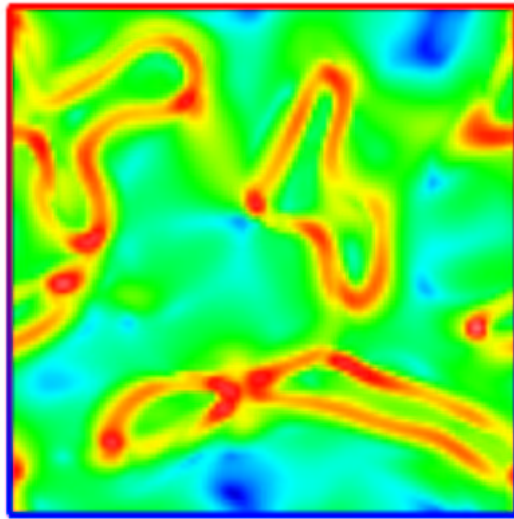
for $t m_H = 1, \dots, 15$

study of generation of Chern-Simons number in cold
electroweak baryogenesis*

*[Van der Meulen, Sexty, JS, Tranberg, JHEP02\(2006\)029](#)



primordial magnetic field in $U(1) \times SU(2)$ Higgs model*



2D contour plot of magnetic field flux tubes at $t_\mu = 15$

*Díaz-Gil, García-Bellido, García Pérez, González-Arroyo, [arXiv:0712.4263](https://arxiv.org/abs/0712.4263)

classical approximation

good:

- gauge fields no problem
- topological defects naturally included

not so good:

- limited time, 'cascade' to the UV leads to $n_{\mathbf{k}} < 1$
- lattice artefacts in case $1/a$ is physical scale (e.g. T)

Quantum: 2PI approximation

Effective action

$$\Gamma[\phi, G] = S[\phi] - \frac{i}{2} \text{Tr} \ln G + \frac{i}{2} \text{Tr} \frac{\delta^2 S[\phi]}{\delta \phi \delta \phi} G + \Phi[\phi, G]$$

with

$$i \Phi = \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} + \begin{array}{c} \text{---} \\ \text{---} \end{array} + \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} + \dots$$

$$\dots = \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} + \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} + \dots$$

The diagrams represent Feynman diagrams for the effective action. The first row shows the expansion of $i\Phi$ as a sum of diagrams: two circles connected at a point, a circle with a horizontal line through its center, and a circle with two horizontal lines through its center, followed by an ellipsis. The second row shows the expansion of the ellipsis from the first row as a sum of diagrams: a circle with two curved lines meeting at a point on the left, and a circle with three lines meeting at a central point, followed by an ellipsis.

presumably diagrammatic series does not converge, asymptotic series

each vertex $\rightarrow \int dx^0 \int d^3x \Rightarrow$ numerically expensive

use $1/N$ to sum diagrams when applicable*
($1/N$ exp. also asymptotic)

truncate $\Phi \Rightarrow \Phi$ -derivable approximation

*Berges, NPA 699 (2002) 847

$\bar{\phi} = \langle \hat{\phi} \rangle$ and $\bar{G} = \langle \hat{\phi}\hat{\phi} \rangle - \langle \hat{\phi} \rangle \langle \hat{\phi} \rangle$ determined by solving

$$\frac{\delta\Gamma[\bar{\phi}, \bar{G}]}{\delta\bar{\phi}} = 0, \quad \frac{\delta\Gamma[\bar{\phi}, \bar{G}]}{\delta\bar{G}} = 0$$

on the closed-time-path

\Rightarrow e.o.m. for

$$F(x, y) = \frac{1}{2} \langle \hat{\phi}(x)\hat{\phi}(y) + \hat{\phi}(y)\hat{\phi}(x) \rangle - \langle \hat{\phi}(x) \rangle \langle \hat{\phi}(y) \rangle$$

$$\rho(x, y) = i \langle [\hat{\phi}(x), \hat{\phi}(y)] \rangle$$

initial conditions as for classical, plus

$$\langle [\hat{\phi}_{\mathbf{k}}, \hat{\phi}_{-\mathbf{k}}] \rangle = 0, \quad \langle [\hat{\phi}_{\mathbf{k}}, \hat{\pi}_{-\mathbf{k}}] \rangle = i$$

Note: classical $\phi \equiv \bar{\phi} + \phi' \neq \bar{\phi}$

'memory kernels'

ϕ^4 model:

$$[\partial_0^2 - \nabla^2 + M^2(x)]F(x, y) = \int_0^{x^0} dz^0 \int d^3z \Sigma_\rho(x, z)F(z, y) - \int_0^{y^0} dz^0 \int d^3z \Sigma_F(x, z)\rho(z, y)$$

$$[\partial_0^2 - \nabla^2 + M^2(x)]\rho(x, y) = \int_{y^0}^{x^0} dz^0 \int d^3z \Sigma_\rho(x, z)\rho(z, y)$$

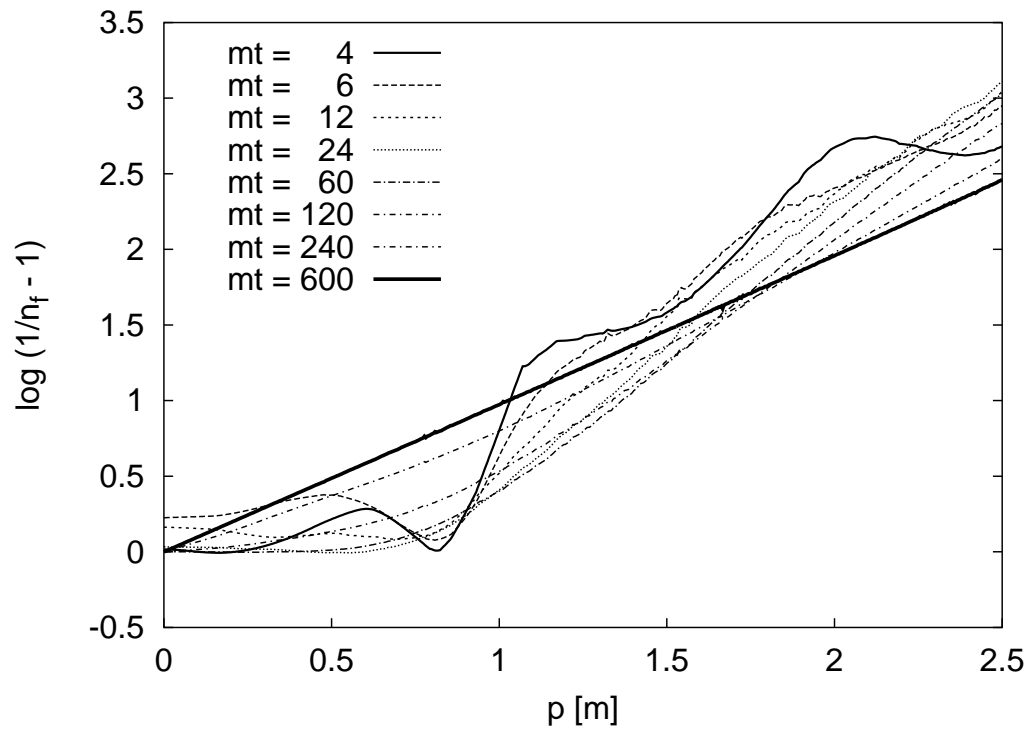
$$M^2(x) = m^2 + \frac{1}{2} \lambda \bar{\phi}^2(x) + \frac{1}{2} \lambda F(x, x)$$

$$0 = [\partial_0^2 - \nabla^2 + m^2 + \frac{1}{6} \lambda F(x, x)] \bar{\phi}(x) + \frac{1}{6} \lambda \bar{\phi}(x)^3 + \int_0^{x^0} dz^0 \int d^3z \tilde{\Sigma}_\rho(x, z) \bar{\phi}(z)$$

$$\begin{aligned}\Sigma_F(x, y) &= \frac{1}{2}\lambda^2\bar{\phi}(x)\bar{\phi}(y) [F(x, y)^2 - \frac{1}{4}\rho(x, y)^2] \\ &\quad + \lambda^2 [\frac{1}{6}F(x, y)^3 - \frac{3}{24}F(x, y)\rho(x, y)^2] \\ &\quad + \dots\end{aligned}$$

$$\Sigma_\rho(x, y) = \lambda^2\bar{\phi}(x)\bar{\phi}(y)F(x, y)\rho(x, y) + \tilde{\Sigma}_\rho(x, y)$$

$$\begin{aligned}\tilde{\Sigma}_\rho(x, y) &= \lambda^2 [\frac{1}{2}F(x, y)^2\rho(x, y) - \frac{1}{24}\rho(x, y)^3] \\ &\quad + \dots\end{aligned}$$



thermalization: $\ln(-1 + 1/n_p) \rightarrow p/T$, Fermi-Dirac
 $1/\gamma_F^{\text{therm}} \approx 95 m^{-1}$, $g = 1$

good:

- large times OK
- lots of physics included by 'self consistent' resummation, e.g. quantum equilibration à la BE and FD

not so good:

- instabilities at large (effective) couplings $(\lambda n_{\mathbf{k}})^*$
- RG β -function wrong at low orders
- gauge theory: gauge-fixing dependence; some 3-loop contributions to Φ numerically too expensive
- topological defects?

*however, see [Garny, Müller, poster at this meeting](#)

defects and other creatures

domain walls, strings, textures, monopoles, Q-balls, I-balls, oscillons, half knots, Chern-Simons numbers, . . .

homogeneous ensemble:

$$\langle \hat{\phi}(x) \rangle = \bar{\phi}(x^0), \quad F(x, y) = F(\mathbf{x} - \mathbf{y}; x^0, y^0), \quad \text{etc.}$$

finite volume: $\bar{\phi} = 0$

defects are expected to contribute to the 2-point correlators

can truncated 2PI action Φ incorporate 'defects' ?

Example: $O(N)$ model

$$-\mathcal{L} = (1/2)\partial_\mu\phi_a\partial^\mu\phi_a - (\mu^2/2)\phi_a\phi_a + (\lambda/4)(\phi_a\phi_a)^2$$

$$a = 1, \dots, N, \lambda \propto 1/N$$

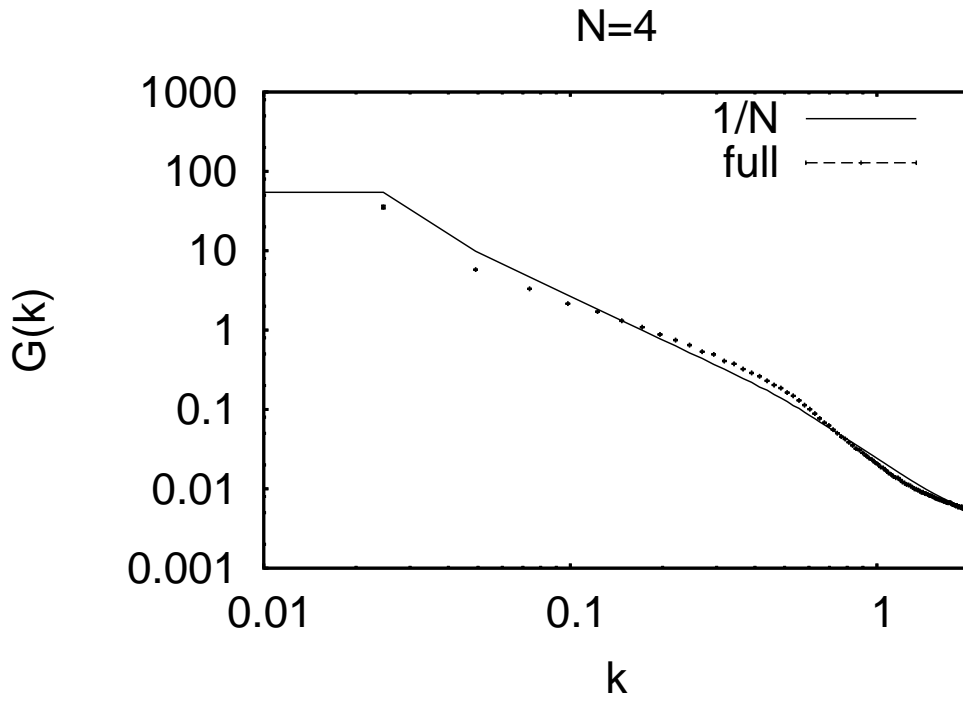
kinks and textures in 1+1 D*:

$$N = 1: \text{kinks } \phi(x) = v \tanh(\mu x/\sqrt{2}), \quad L\mu \gg 1$$

$$N = 2: \text{textures } \phi_1(x) + i\phi_2(x) = v e^{i2\pi N_w x/L}$$

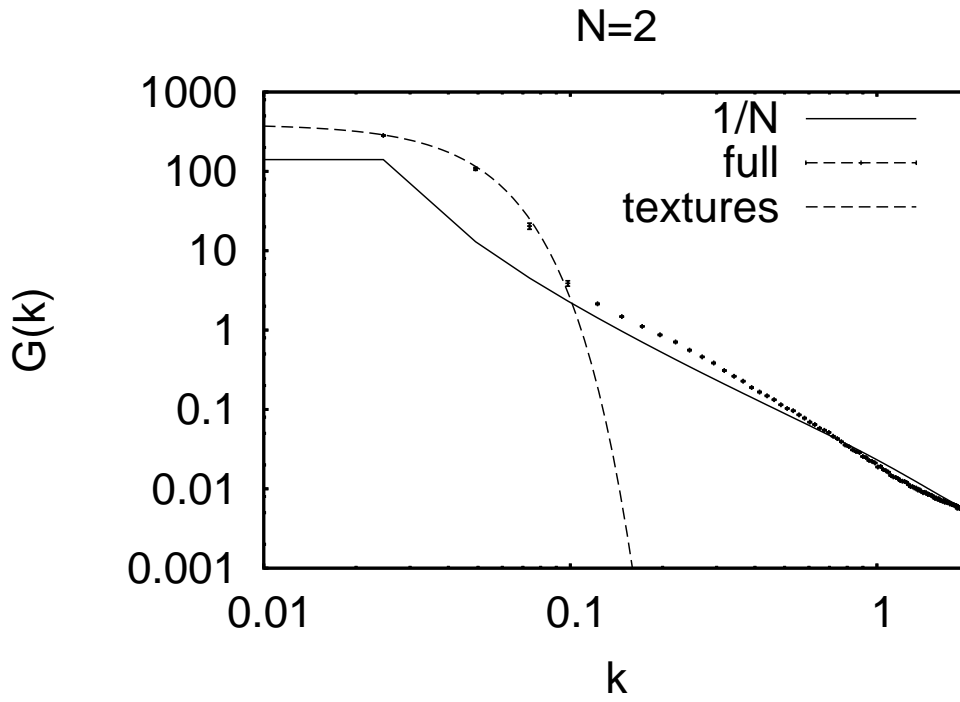
damping added* to relax initial randomized state to low energy

*Rajantie, Tranberg, JHEP11 (2006)020



full: equal-time F correlator at late time in 2PI-NLO large N , $N = 4$

dotted: classical



similar, $N = 2$;

dashed: fit to expected form due to textures

cold electroweak quench in 3+1 D*

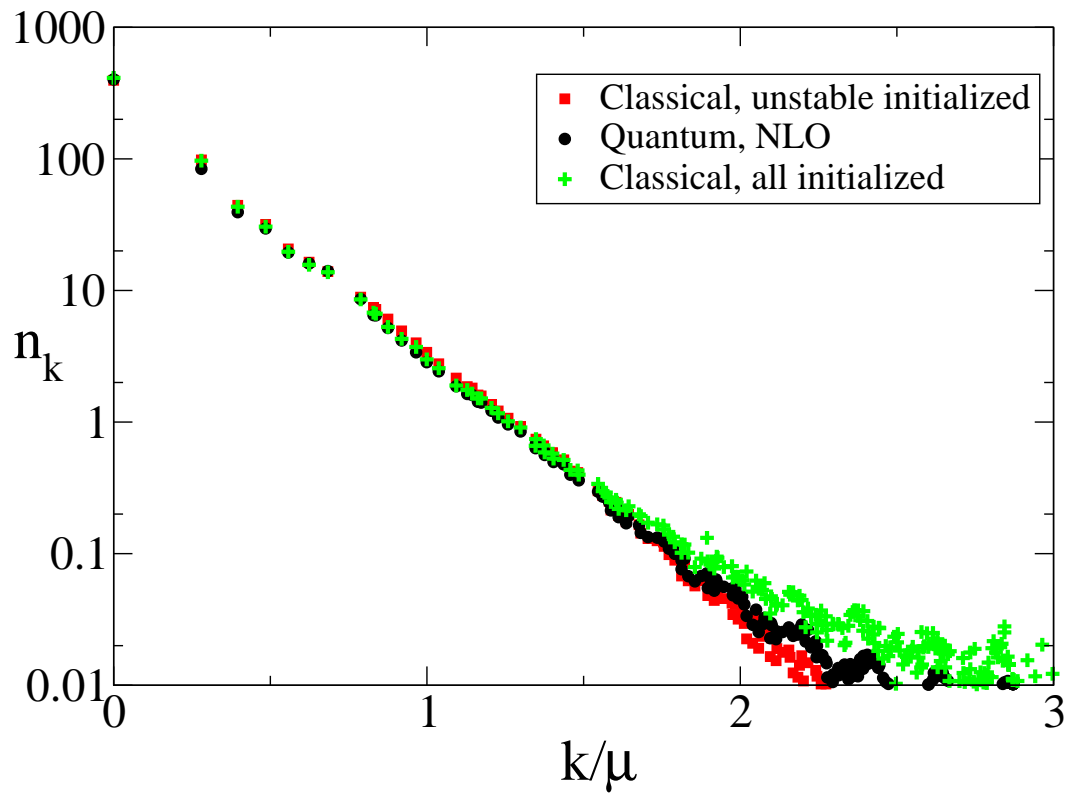
$$N = 4$$

next three slides:

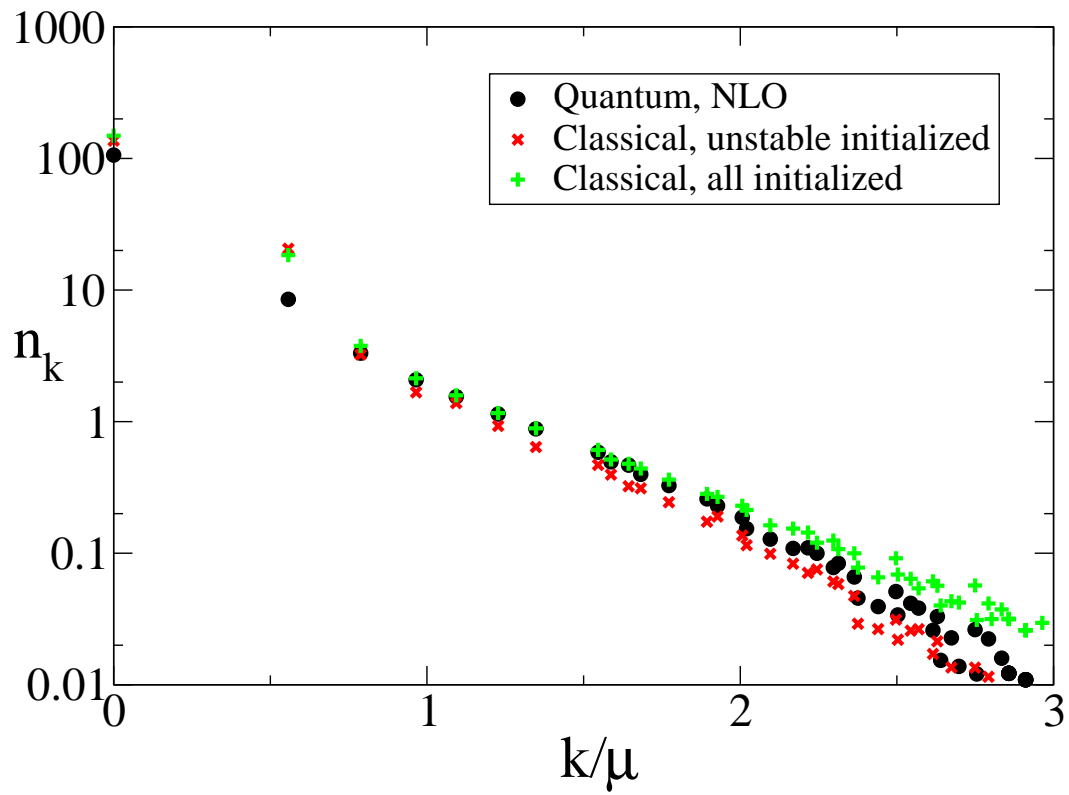
comparison of n_k in NLO $1/N$ with two 'just the half' classical approximations:

1. only unstable modes initialized ($k_{\max} = \mu$)
2. all modes initialized

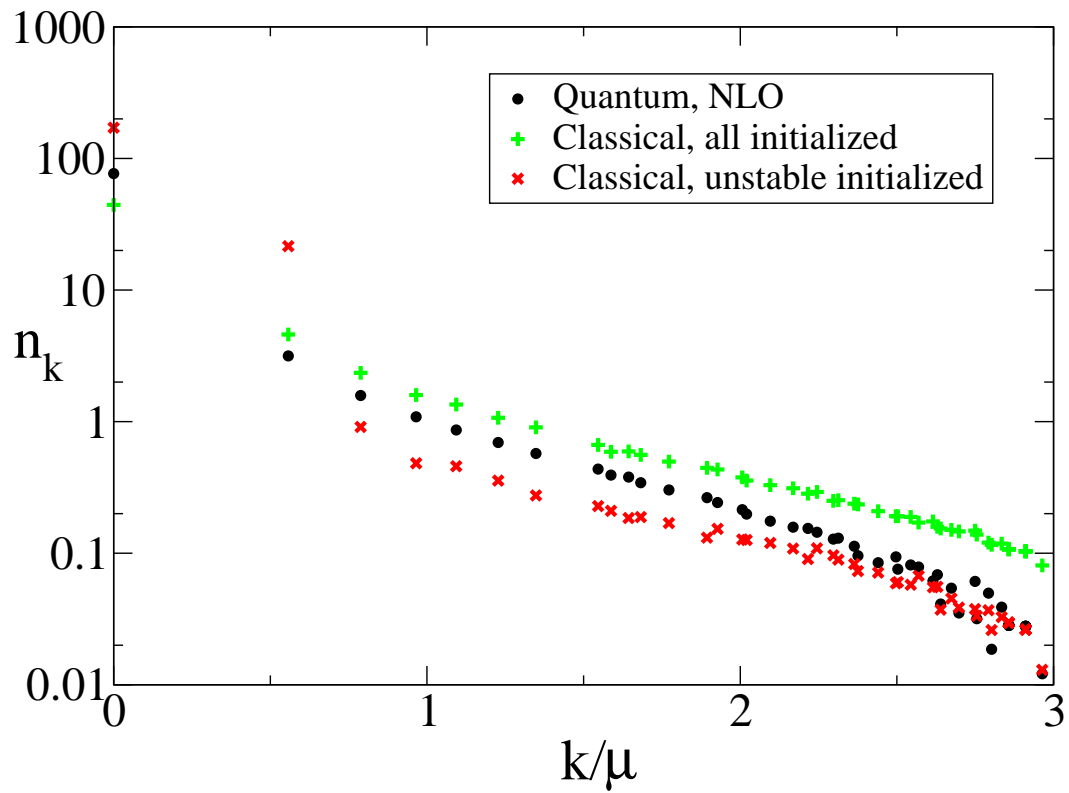
*[Arrizabalaga, JS, Tranberg, JHEP 0410 \(2004\) 017](#)



particle numbers at time $t\mu = 14$; $\lambda = 1/24$, $L\mu = 22.4$



particle numbers at time $t\mu = 100$
 $\lambda = 1/4$ ($m_H = 174$ GeV), $L\mu = 11.2$



similar, time $t\mu = 700$

differences at $k/\mu \approx 0.5$ for $t \gtrsim 100 \mu^{-1}$ due to textures?

sample quantum mean field

$$\hat{\rho} = \int D\phi D\pi \rho_q(\phi, \pi) |\phi, \pi\rangle\langle\phi, \pi|$$

representation in terms of coherent states $|\phi, \pi\rangle$

$\hat{\rho}$ homogeneous, $\langle\phi, \pi|\hat{\phi}(x)|\phi, \pi\rangle$ *in*-homogeneous

'Hartree ensemble approximation'*

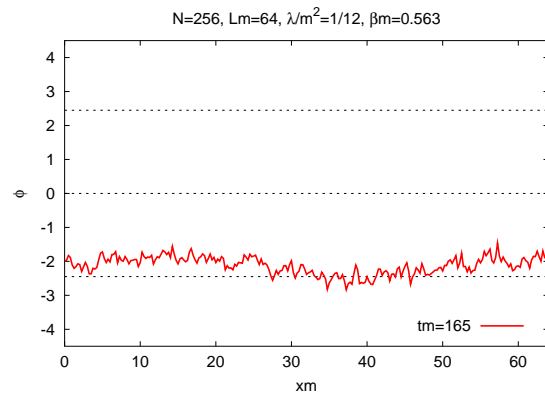
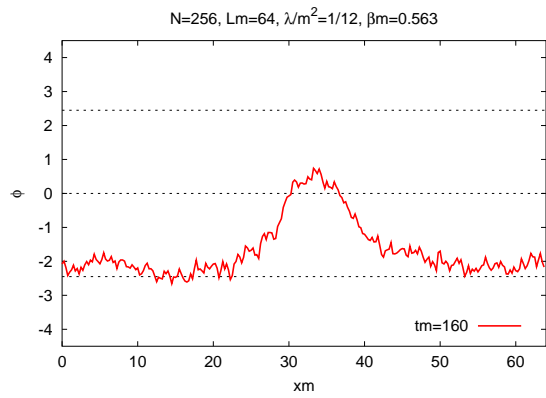
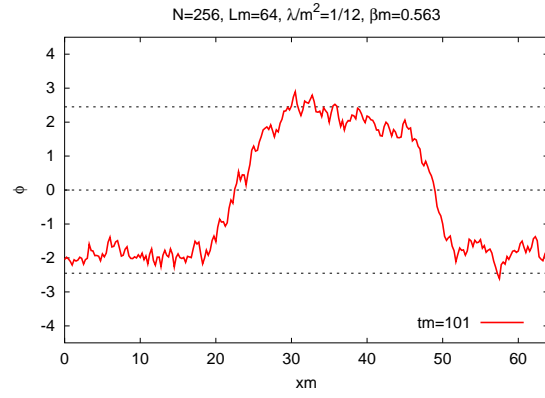
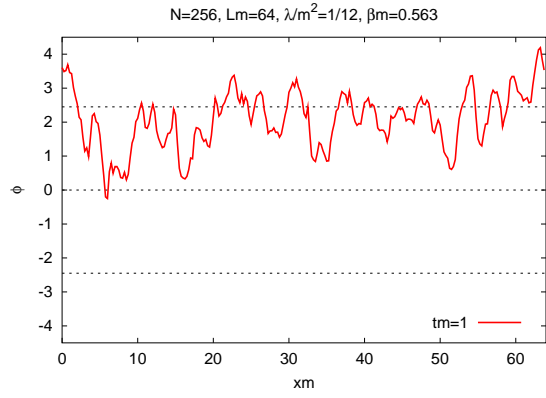
next slide:

Thermal kink-antikink cleation and annihilation

snapshots of a realization of an initial BE ensemble**

*Salle, JS, Vink, PRD 64 (2001) 025016; PRD 76 (2003) 116006

**Salle, PRD 69 (2004) 025005



outlook

- classical approximation powerful, develop further
- more work comparing classical and Φ -derivable
- Φ -derivable for gauge fields

$N = 4$ texture in 3+1 D

$$\vec{(\phi, \phi_4)} = v (\hat{x} \sin \chi(r), \cos \chi(r))$$

$$\mathbf{x} = r \hat{x}, \chi(r) = \pi(1 - e^{-r/d})$$