



PhD School on QCD in Extreme Conditions

Lattice Field Theory for Extreme QCD

Maria Paola Lombardo

INFN Firenze lombardo@fi.infn.it



Lattice Field Theory for Extreme QCD - 1

Basics

From real to imaginary time - field theory thermodynamics

From continuum to the lattice and back

Importance sampling and basic observables

Symmetry and pattern of breaking at high T

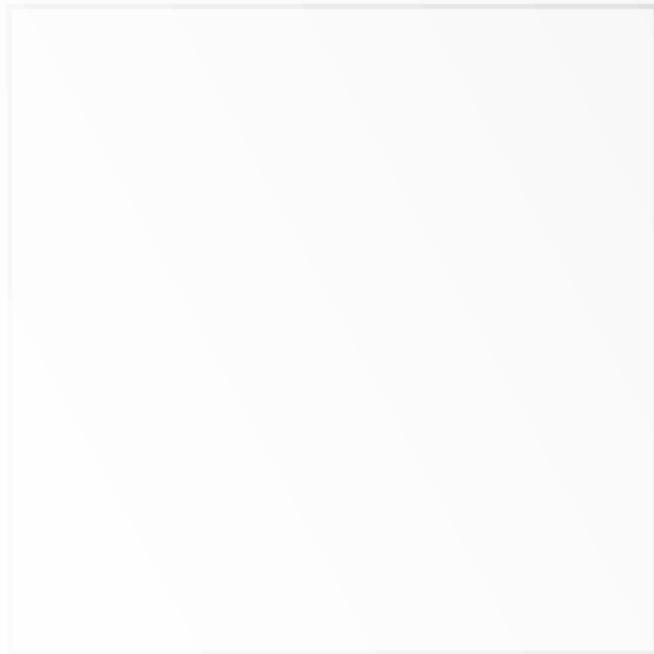
Yang Mills

Massless QCD - light quarks

Scaling window

Interplay of chiral symmetry and confinement ?

QCD - why Lattice Field Theory



QED vs QCD

- Photons do not carry charge
- Free electrons and free photons exist
- Interactions are strong at short distance - Coulomb force

A theory with only photons
Is free

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

- Gluons are charged
- Free quarks and gluons do not exist: confinement?
- Interactions are faible at short distance: asymptotic freedom

A theory with gluons only
is interacting and Interesting

$$F_{\mu\nu}^{(a)} = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - g_s f_{abc} A_\mu^b A_\nu^c$$

QED vs QCD vs Yang-Mills

- Photons do not carry charge
- Free electrons and free photons exist
- Interactions are strong at short distance - Coulomb force

A theory with only photons
Is free

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

- Gluons are charged
- Free quarks and gluons do not exist: confinement?
- Interactions are faible at short distance: asymptotic freedom

A theory with gluons only (Yang-Mills)
is interacting and Interesting

$$F_{\mu\nu}^{(a)} = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - g_s f_{abc} A_\mu^b A_\nu^c$$

From QED to Yang-Mills theories

Electrodynamics:

$$\mathcal{L}_{\text{QED}} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}(i\gamma^\mu\nabla_\mu - m)\psi$$

Infinite mass

$$\mathcal{L}_{\text{QED}} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}(i\gamma^\mu\nabla_\mu - m)\psi \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \quad \text{Free photons}$$

Yang-Mills

Gluons

$$\mathcal{L}_{\text{YM}} = -\frac{1}{4}F_{\mu\nu}^{(a)}F^{\mu\nu (a)}$$

$$F_{\mu\nu}^{(a)} = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - g_s f_{abc} A_\mu^b A_\nu^c$$

Self-interacting gluons

QCD : why Lattice Field Theory

Confinement: quarks and gluons are not observed as asymptotic states

Breaking of chiral symmetry: due to the coupling becoming large at large distance

Topological properties: non-existent at any order in perturbation theory

..why and where

Extreme QCD

Confinement: quarks and gluons are not observed as asymptotic states

Deconfinement : quark and gluon dynamics

Breaking of chiral symmetry: due to the coupling becoming large at large distance

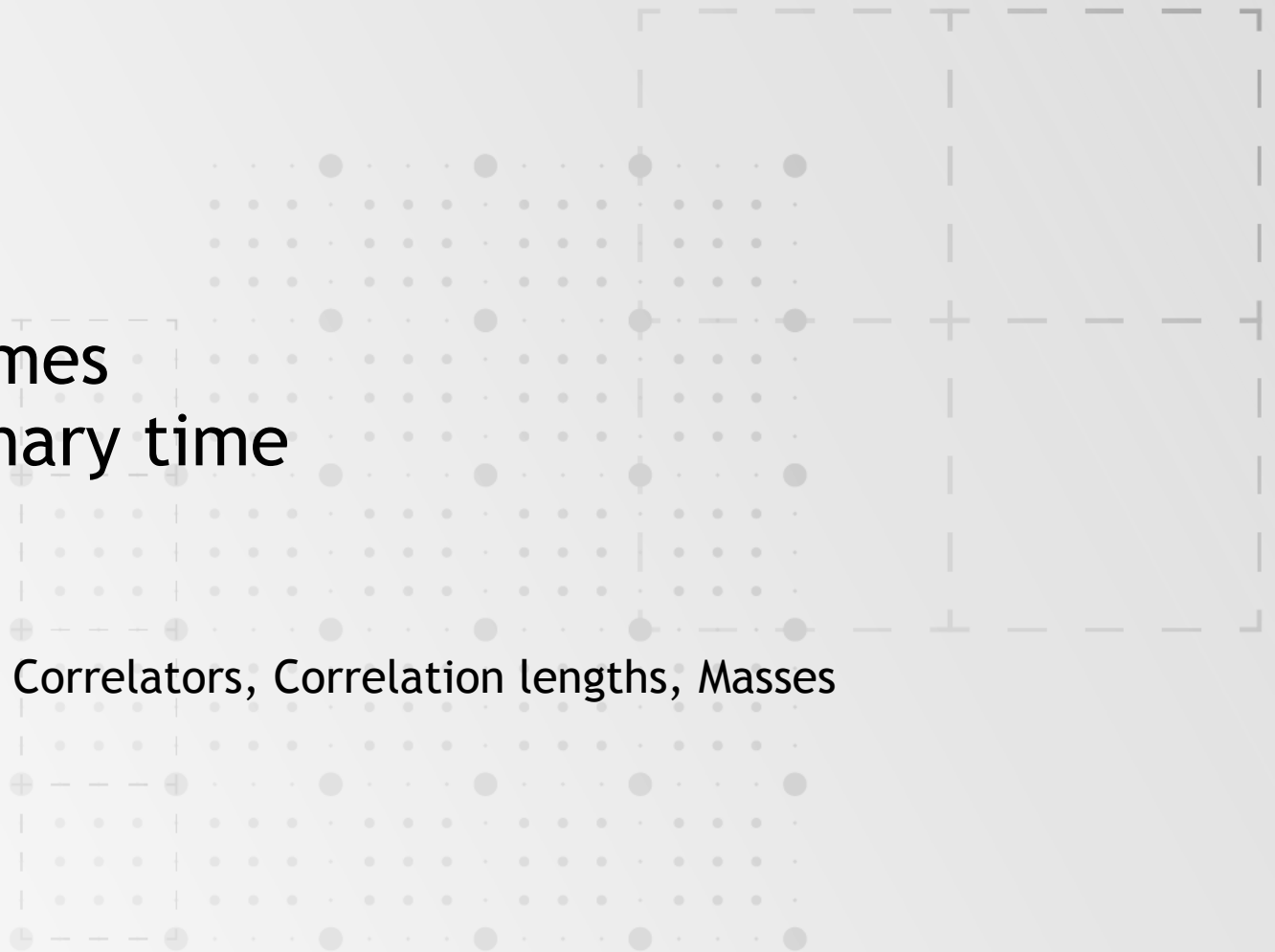
Coupling does not grow enough to break symmetry

Topological properties: non-existent at any order in perturbation theory

Topology becomes 'simpler'

Computational schemes from real to imaginary time

Correlators, Correlation lengths, Masses



General calculation scheme: Gran Canonical formalism

Rotate to imaginary time $x_0 \equiv t \rightarrow -ix_4 \equiv -i\tau$

GCPF \rightarrow $Z = \int \mathcal{D}A_\mu \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S}$ \leftarrow note: Euclidean space time

$$S = \int d^4x \left(\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \bar{\psi} M \psi \right) .$$

A RFT in d space dimensions becomes a statistical field theory in d+1 dimensions

Integrate out fermions

$$Z = \int \mathcal{D}A_\mu \det M e^{\int d^4x \left(-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \right)} .$$

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}A_\mu \mathcal{O} e^{-S} . \quad S = S_{gauge} + S_{quarks} = \int d^4x \left(\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \right) - \sum_i \log(\text{Det} M_i)$$

Minkowski \rightarrow Euclidean

Green functions \rightarrow Correlation functions

In many cases correlation functions decay exponentially at large distance:

$$\lim_{t \rightarrow \infty} \langle O(t) O(0) \rangle \propto e^{-t/t_0} \quad t_0 \quad \text{correlation length}$$

Back to Minkowski

$$\int dt e^{ip_0 t} \frac{e^{-t/t_0}}{2t_0} = \frac{1}{p_0^2 + \frac{1}{t_0^2}}$$

$$\rightarrow p_0 \rightarrow iE = \frac{1}{1/t_0^2 - E^2}$$

Mass = inverse correlation length

Minkowski \rightarrow Euclidean

Green functions \rightarrow Correlation functions

$$\lim_{t \rightarrow \infty} \langle O(t) O(0) \rangle \propto e^{-t M}$$

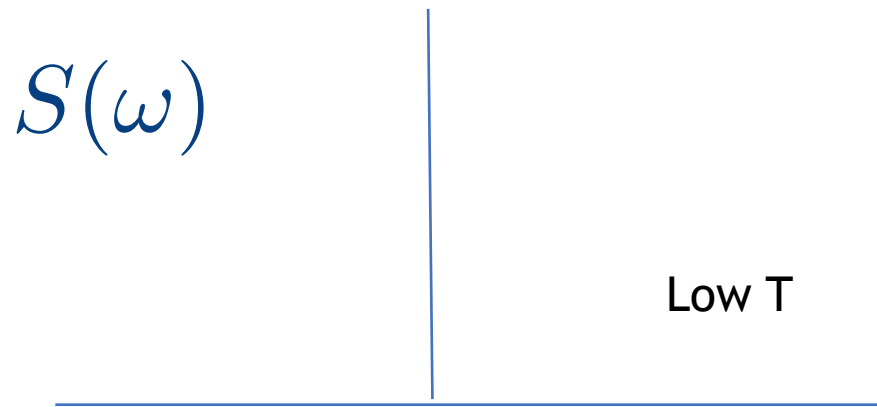
M = lowest excitation in the channel which couples to O

From real time to real frequency space:

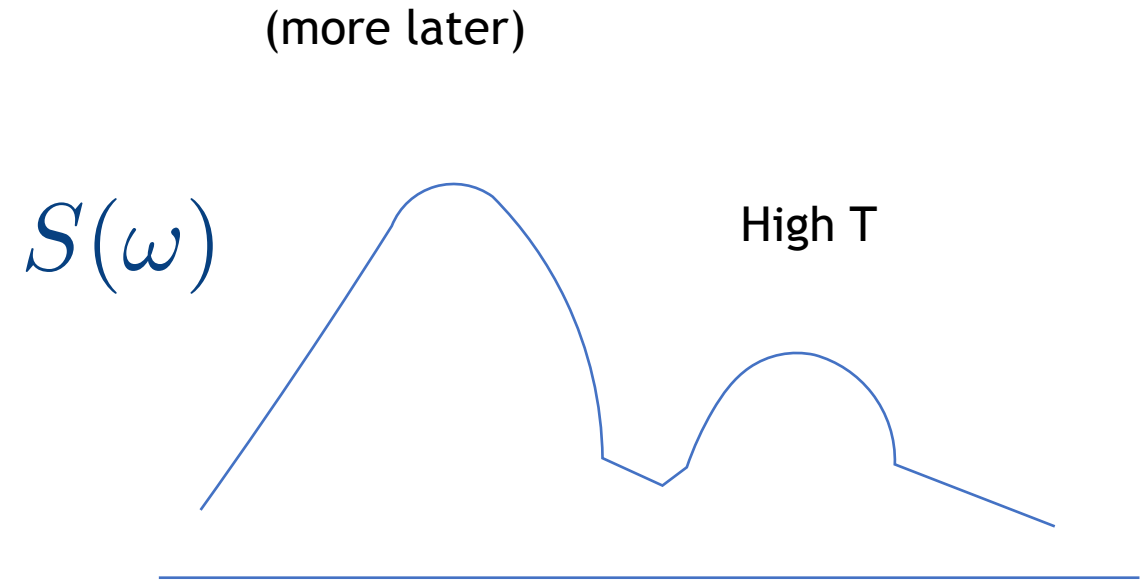
In imaginary time $G(t)$ $G(t) = \int \delta(M - \omega) e^{-\omega t} \propto e^{-Mt}$

In real frequency space: $\delta(M - \omega)$

Spectral functions and two point functions : a challenge for LFT

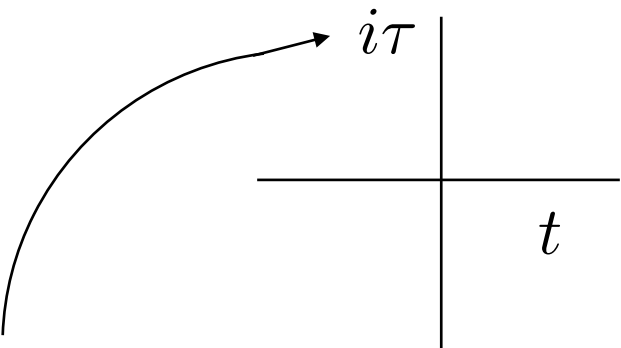


$$G(t) = \int \delta(M - \omega) e^{-\omega t} \propto e^{-Mt}$$

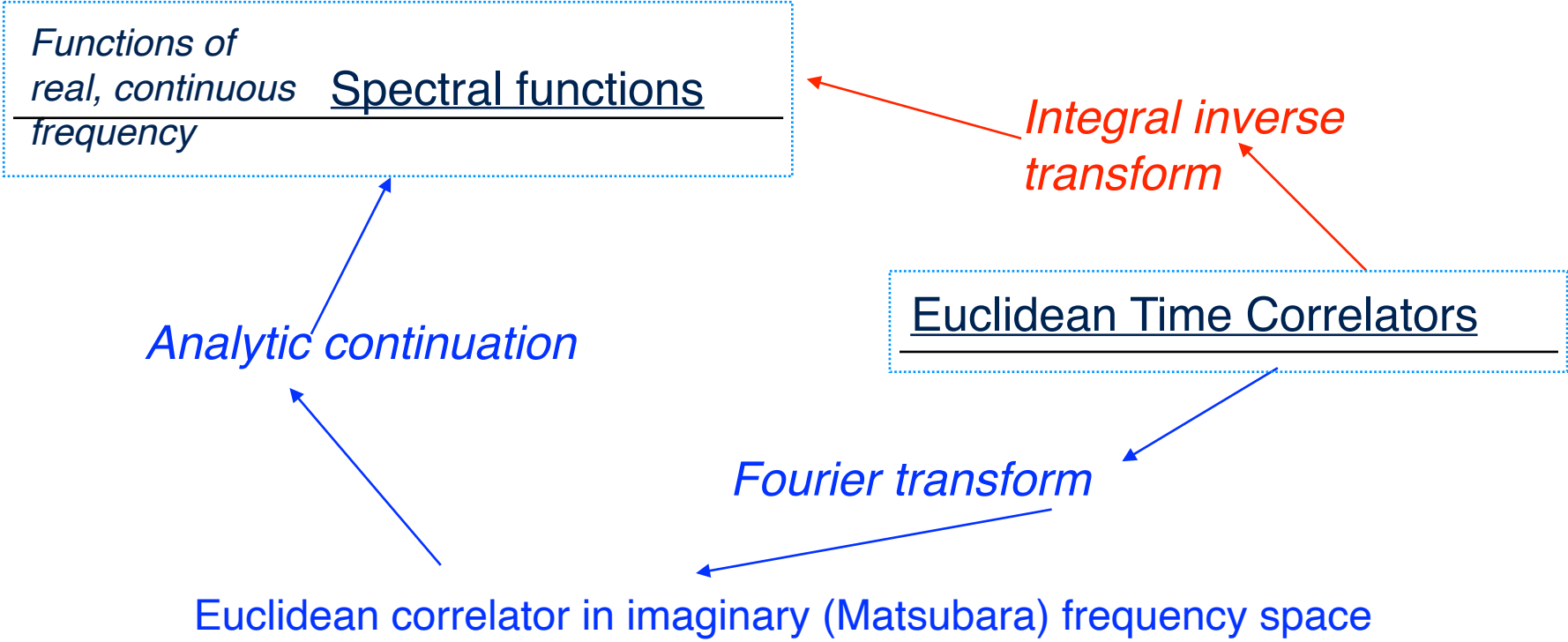


$$G(t) = \int S(\omega) e^{-\omega t}$$

Objects of interest: Spectral functions



Computed on the lattice: Euclidean (imaginary) Time Correlators



Field Theory in Euclidean space — summing up so far

Complete equivalence between Minkowski FT in d space dimension with statistical field theory in $d+1$ dimension

The Grand Canonical Partition Function defines all the observables of the theory

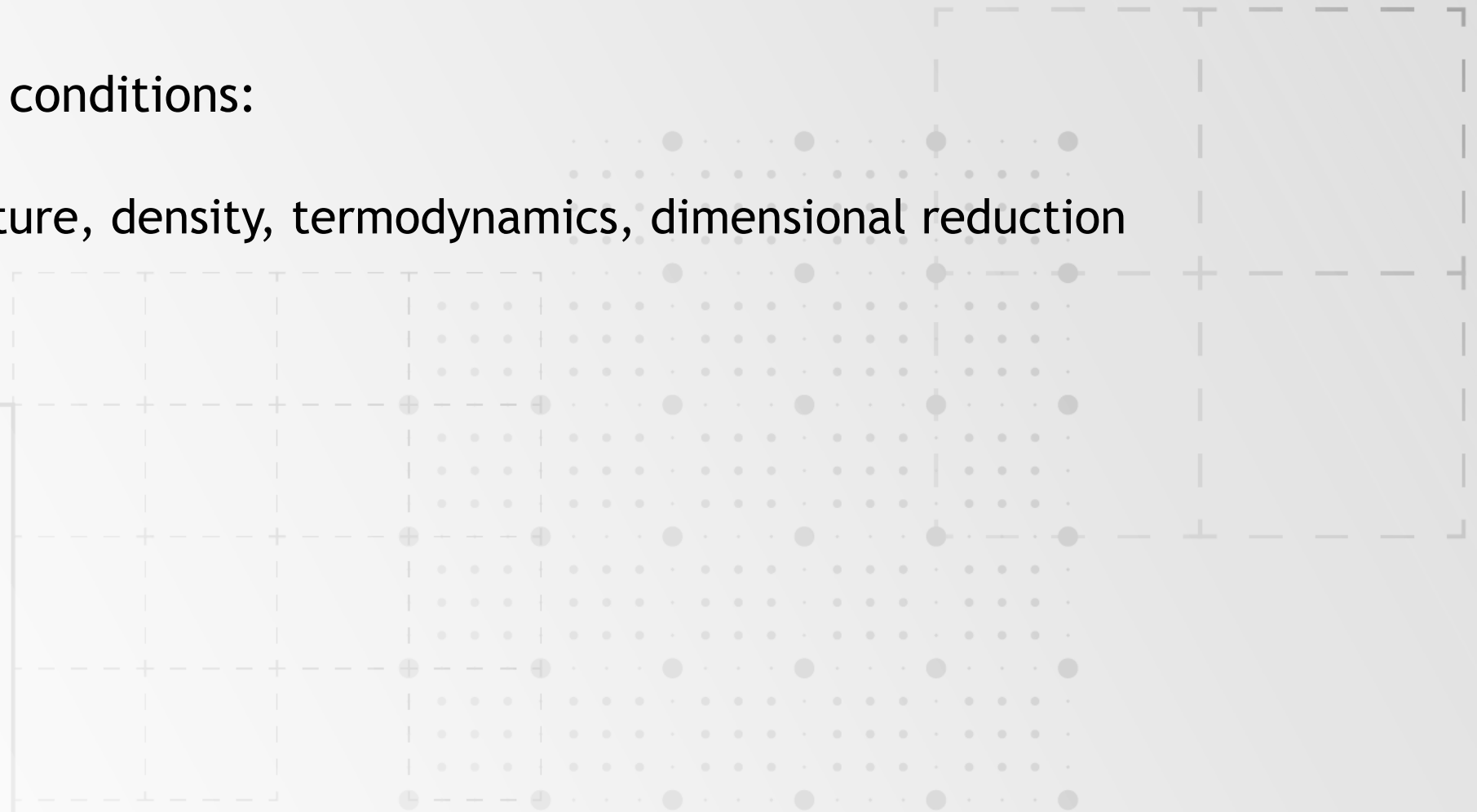
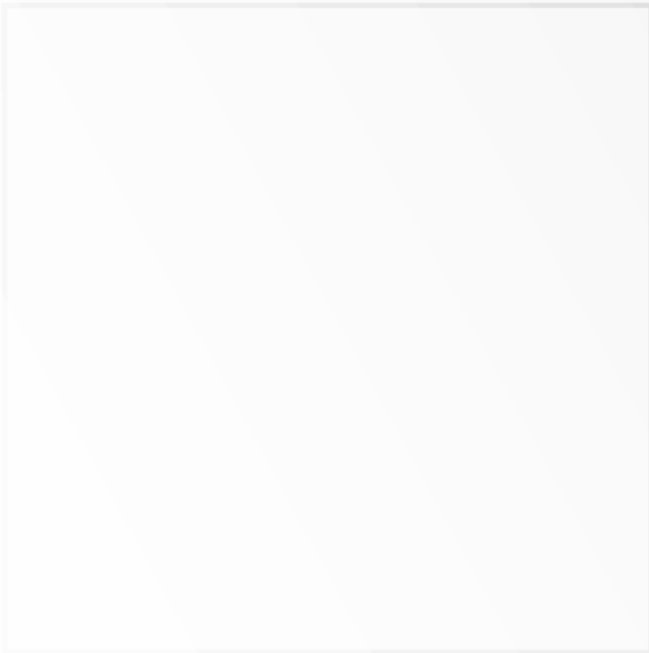
$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}A_\mu \mathcal{O} e^{-S}$$

Exponential decays of Euclidean two point functions \rightarrow mass of the lowest excitation in that channel

More general functional forms may appear, which require a dedicated analysis

Extreme conditions:

Temperature, density, thermodynamics, dimensional reduction



Euclidean Field Theory → Classical Statistical System

$$\langle \phi_a | e^{-iHt} | \phi_a \rangle = \int d\pi \int_{\phi(x,0)=\phi_a(x)}^{\phi(x,t)=\phi_a(x)} d\phi e^{i \int_0^t dt \int d^3x (\pi(\vec{x},t) \frac{\partial \phi(\vec{x},t)}{\partial t} - H(\pi, \phi))}$$

$$\mathcal{Z} = \text{Tr} e^{-\beta(H - \mu \hat{N})} = \int d\phi_a \langle \phi_a | e^{-\beta(H - \mu N)} | \phi_a \rangle$$

$$\beta \equiv \frac{1}{T} \rightarrow it$$

Temperature

Temperature and Density

Gran Canonical Formalism: introduce chemical potential for conserved charge

$$\mu J_0, \quad J_0 = \bar{\psi} \gamma_0 \psi$$

$$S_{QCD} = F_{\mu\nu} F_{\mu\nu} + \bar{\psi} (\not{\partial} + m + \mu \gamma_0) \psi = S_G + \bar{\psi} M \psi$$

$$\mathcal{Z}(\mu, T) = \int_0^{1/T} dt \int e^{S(\bar{\psi}, \psi, U)} d\bar{\psi} d\psi dU$$

$$\mathcal{Z}(T, \mu) = \int dU \det M e^{-S_G} = \int dU e^{-(S_g - \log(\det M))}$$

$$= S_{eff}$$

Boundary conditions for the fields

$$\mathcal{Z} = \int d\phi d\psi e^{-S(\phi, \psi)}$$

$$S(\phi, \psi) = \int_0^{1/T} dt \int d^d x \mathcal{L}(\phi, \psi)$$

Bosons : periodic

$$G_B(\vec{x}, \vec{y}; \tau, 0) = Tr\{\hat{\rho} T_\tau[\hat{\phi}(\vec{x}, \tau) \hat{\phi}(\vec{y}, 0)]\} / \mathcal{Z}$$

where T_τ is the imaginary time ordering operator:

$$T_\tau[\hat{\phi}(\tau_1) \hat{\phi}(\tau_2)] = \hat{\phi}(\tau_1) \hat{\phi}(\tau_2) \theta(\tau_1 - \tau_2) + \hat{\phi}(\tau_2) \hat{\phi}(\tau_1) \theta(\tau_2 - \tau_1)$$

Use now the commuting properties of the imaginary time ordering evolution and H:

$$[T_\tau, e^{-\beta H}] = 0$$

together with the Heisenberg time evolution

$$e^{\beta H} \phi(\vec{y}, 0) e^{-\beta H} = \phi(\vec{y}, \beta)$$

to get:

$$G_B(\vec{x}, \vec{y}; \tau, 0) = G_B(\vec{x}, \vec{y}; \tau, \beta)$$

Fermions

$$T_\tau[\hat{\psi}(\tau_1)\hat{\psi}(\tau_2)] = \hat{\psi}(\tau_1)\hat{\psi}(\tau_2)\theta(\tau_1 - \tau_2) - \hat{\psi}(\tau_2)\hat{\psi}(\tau_1)\theta(\tau_2 - \tau_1)$$

$$\hat{\psi}(\vec{x}, 0) = -\hat{\psi}(\vec{x}, \beta) \quad \text{Antiperiodic}$$

Fermions

$$T_\tau[\hat{\psi}(\tau_1)\hat{\psi}(\tau_2)] = \hat{\psi}(\tau_1)\hat{\psi}(\tau_2)\theta(\tau_1 - \tau_2) - \hat{\psi}(\tau_2)\hat{\psi}(\tau_1)\theta(\tau_2 - \tau_1)$$

$$\hat{\psi}(\vec{x}, 0) = -\hat{\psi}(\vec{x}, \beta) \quad \text{Antiperiodic}$$

Bosons

$$T_\tau[\hat{\phi}(\tau_1)\hat{\phi}(\tau_2)] = \hat{\phi}(\tau_1)\hat{\phi}(\tau_2)\theta(\tau_1 - \tau_2) + \hat{\phi}(\tau_2)\hat{\phi}(\tau_1)\theta(\tau_2 - \tau_1)$$

$$G_B(\vec{x}, \vec{y}; \tau, 0) = G_B(\vec{x}, \vec{y}; \tau, \beta) \quad \text{Periodic}$$

Thermodynamics

$$P = T \frac{\partial \ln \mathcal{Z}}{\partial V}$$

$$N = T \frac{\partial \ln \mathcal{Z}}{\partial \mu}$$

$$S = \frac{\partial T \ln \mathcal{Z}}{\partial T}$$

$$E = -PV + TS + \mu N$$

Dimensional Reduction

Imaginary time

and

Inverse
Temperature

d-dimensional space

+ coarse graining

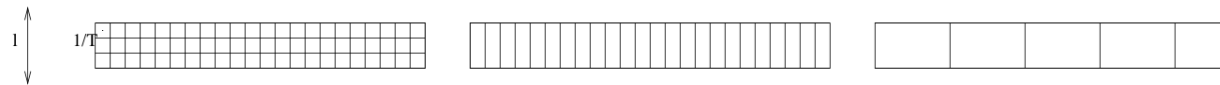


Figure 2: Sketchy view of the dimensional reduction from $d+1$ to d dimensions (from the leftmost to the middle picture) and subsequent coarse graining (from middle to rightmost)

Cases for Dimensional Reduction

- 1) $T \gg \text{any mass} \rightarrow \text{High T Electroweak transition}$
- 2) Diverging correlation length \rightarrow second order transition, basis for universality
High T QCD

Mode expansion and Decoupling

$$\phi(x, t) = \sum_{\omega_n=2n\pi T} e^{i\omega_n t} \phi_n(x) \quad \text{Bosons}$$

$$\psi(x, t) = \sum_{\omega_n=(2n+1)\pi T} e^{i\omega_n t} \psi_n(x) \quad \text{Fermions}$$

In the expression for the Action

$$S(\phi, \psi) = \int_0^{1/T} dt \int d^d x \mathcal{L}(\phi, \psi)$$

the integral over time can then be traded with a sum over modes, and we reach the conclusion that a $d+1$ statistical field theory at $T > 0$ is equivalent to a d -dimensional theory with an infinite number of fields.

When dimensional reduction is possible, only one boson field survives

Finite temperature at a glance

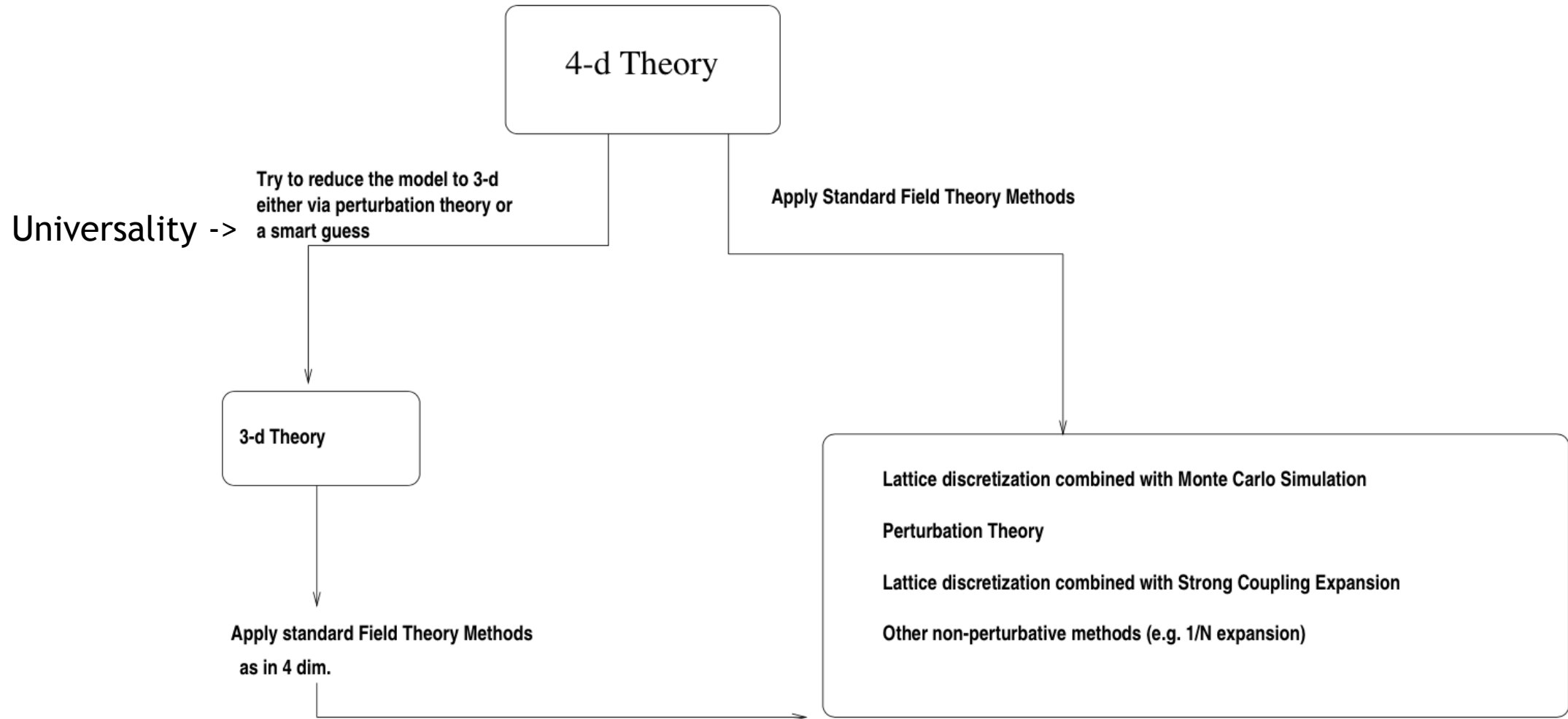
- The partition function \mathcal{Z} has the interpretation of the partition function of a statistical field theory in $d+1$ dimension, where the temperature has to be identified with the reciprocal of the (imaginary) time.
- The fields' boundary conditions follows from the Bose and Fermi s

$$\begin{aligned}\phi(t=0, \vec{x}) &= \phi(t=1/T, \vec{x}) \\ \psi(t=0, \vec{x}) &= -\psi(t=1/T, \vec{x})\end{aligned}$$

i.e. fermionic and bosonic fields obey antiperiodic and periodic boundary conditions in time.

- “Dimensional reduction”, when ‘true’ means that the system become effectively 3-dimensional. In this case only the Fourier component of each Bose field with vanishing Matsubara frequency will contribute to the dynamics, while Fermions would decouple.
- The scenario above is very plausible and physically well founded, but it is by no means a theorem. Ab initio calculations can confirm or disprove it.

Computational schemes at a glance



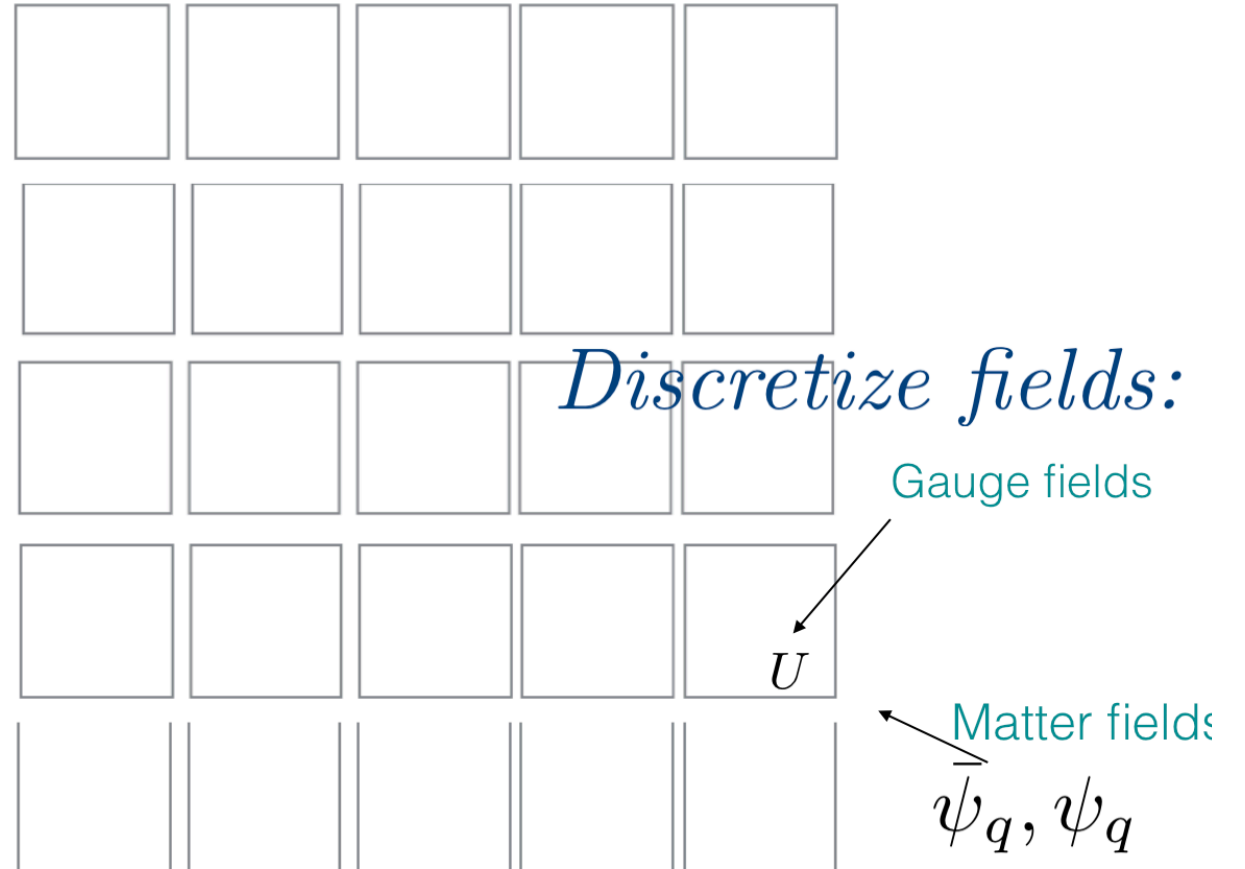
On the lattice - general issues



Computational Strategy:

1) Rotation to
imaginary time +
discretisation

Lattice Gauge Theory



Computational Strategy:

1) Rotation to imaginary time + discretisation

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}A_\mu \mathcal{O} e^{-S}$$

2) Monte Carlo Simulation

Performing the integration

$$\langle 0 | \mathcal{O} | 0 \rangle = \frac{\sum_{\alpha} \mathcal{O}_{\alpha} e^{-S_{\alpha}}}{\sum_{\alpha} e^{-S_{\alpha}}}.$$

Lattice Gauge Theory



Discretize fields:

Gauge fields

U

Matter fields

ψ_q, ψ_q

$$\rightarrow \frac{\sum_{i=1}^N \mathcal{O}_i}{N}$$

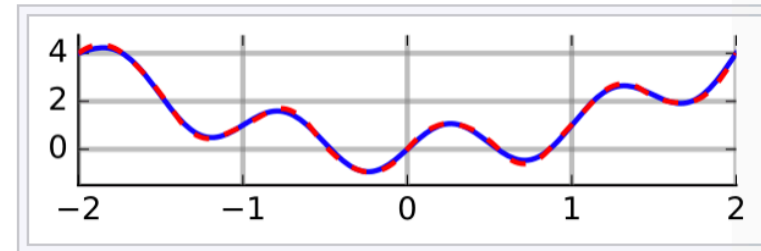
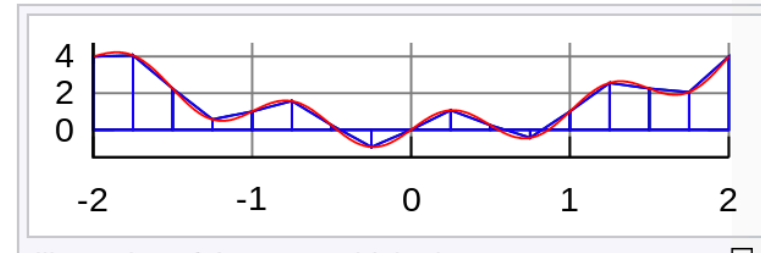
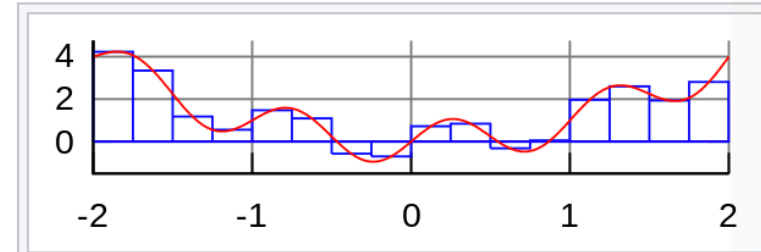
–Discretization: from continuum space to a grid

–Why? Two standard motivations:

1. Physical system intrinsically discrete (i.e. spin models)
2. **Make it amenable to a numerical study → QCD**

– Discretization is in principle trivial:

$$\int_a^b f(x) dx \approx \frac{b-a}{n} \left(\frac{f(a)}{2} + \sum_{k=1}^{n-1} f\left(a + k \frac{b-a}{n}\right) + \frac{f(b)}{2} \right)$$



e

Illustration of Simpson's rule.

– Already in this simple example:

.Strategies for improvement?

.How to check the ‘continuum limit?’

.Suppose $a, b \rightarrow \infty$

How to check **convergence to infinite volume?**

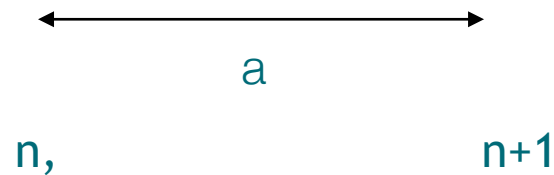
– Slightly more complicated: increase the dimensionality, make the function less smooth..

Computational costs??

Matter (scalar) fields: on sites

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)^2 + \frac{1}{2}m^2 \phi^2 + \lambda \phi^4.$$

$$S = \sum_n a^4 \left(\frac{1}{2} \sum_{\mu=1}^4 \left[\frac{\phi(n+1_\mu) - \phi(n-1_\mu)}{2a} \right]^2 + \frac{1}{2}m^2 \phi^2(n) + \lambda \phi^4(n) \right)$$



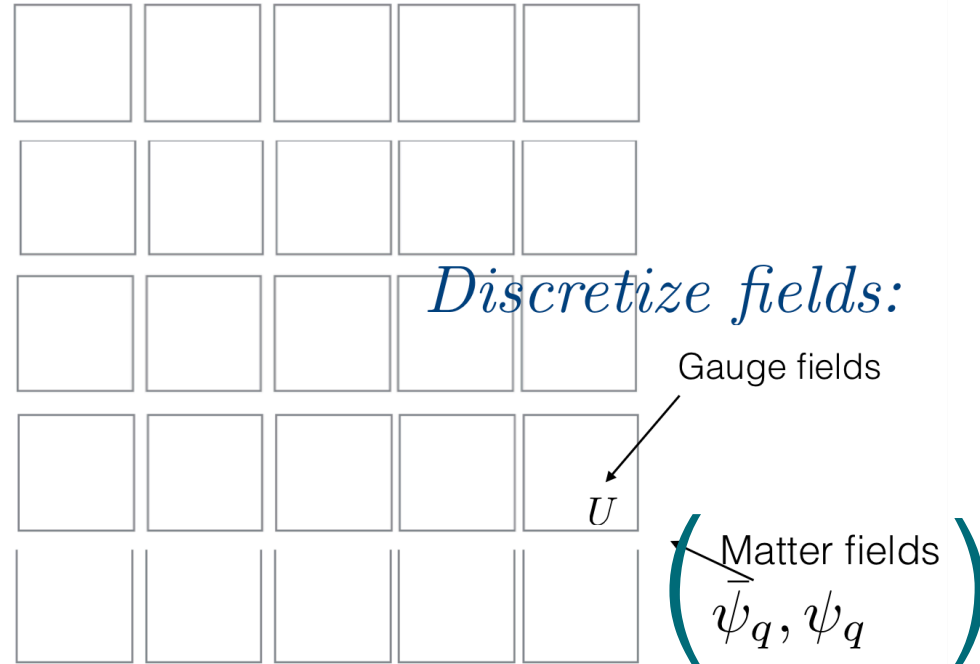
Gauge fields

$$\phi_s(y) \rightarrow P(\exp ig \int_s dx_\mu A_\mu) \phi(x) \equiv U(y, x) \phi(x)$$

$$U_\mu(n) = \exp(igaT^a A_\mu^a(n))$$

SU(3) Matrix

Parallel transport: Lattice Gauge Theory : gauge invariance ‘by fiat’



$$\text{Tr} \dots U_\mu(x) U_\mu(x + \hat{\mu}) \dots \rightarrow \text{Tr} \dots U_\mu(x) V^\dagger(x + \hat{\mu}) V(x + \hat{\mu}) U_\mu(x + \hat{\mu}) \dots$$

Gauge invariant

Build the Action ‘by guessing’..

$$S = \frac{2}{g^2} \sum_x \sum_{\mu > \nu} \text{Re Tr} (1 - U_{P\mu\nu}(x)). \quad ? \text{ Does it work?}$$

$$U_{P\mu\nu}(x) = U_\mu(x) U_\nu(x + \hat{\mu}a) U_\mu^\dagger(x + \hat{\nu}a) U_\nu^\dagger(x)$$

Check continuum limit $a \rightarrow 0$

$$A_\mu(x + \hat{\nu}a) = A_\mu(x) + a\partial_\nu A_\mu(x) + \dots$$

$$U_P(x) = 1 + ia^2 F_{\mu\nu} + \dots \quad \beta = 2N/g^2$$

Continuum limit OK

Continuum limit

Coming back to correlation functions:

$$\lim_{t \rightarrow \infty} \langle O(t)O(0) \rangle \propto e^{-tM}$$


M = dimensionless quantity, expressed in lattice units = $1/\xi$

$$M = M_{\text{phys}} * a = 1/\xi$$

$$a \rightarrow 0, \xi \rightarrow \infty$$

Continuum limit: singularity !

‘g’ in the Lattice Lagrangian is the coupling at the scale ‘a’

$$a\Lambda_L = \left(\frac{1}{b_0 g^2} \right)^{b_1/2b_0^2} e^{-1/2b_0 g^2}$$


Physical scale – dimensional transmutation

$$b_0 = \left(\frac{11}{3} N_c - \frac{2}{3} N_f \right) / 16\pi^2 \text{ and } b_1 = \left(\frac{34}{3} N_c^2 - \left(\frac{10}{3} N_c + \frac{N_c^2 - 1}{N_c} \right) N_f \right) / (16\pi^2)^2.$$

QCD Asymptotic freedom allows a rigorous continuum limit

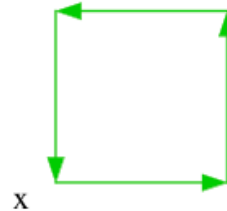
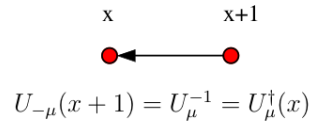
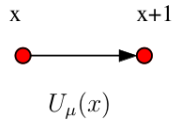
In perturbation theory, $a(g)$ is known.

Yang-Mills, continuum and lattice

$$S_{\text{cont}} = \int d^4x \frac{1}{4g^2} \text{Tr } F_{\mu\nu} F^{\mu\nu}$$

$$S_{\text{latt}} = \beta \sum_p \left(1 - \frac{1}{3} \text{Re} \{ \text{Tr } U_p \} \right); \quad \beta = \frac{6}{g^2}.$$

Not unique – improvement

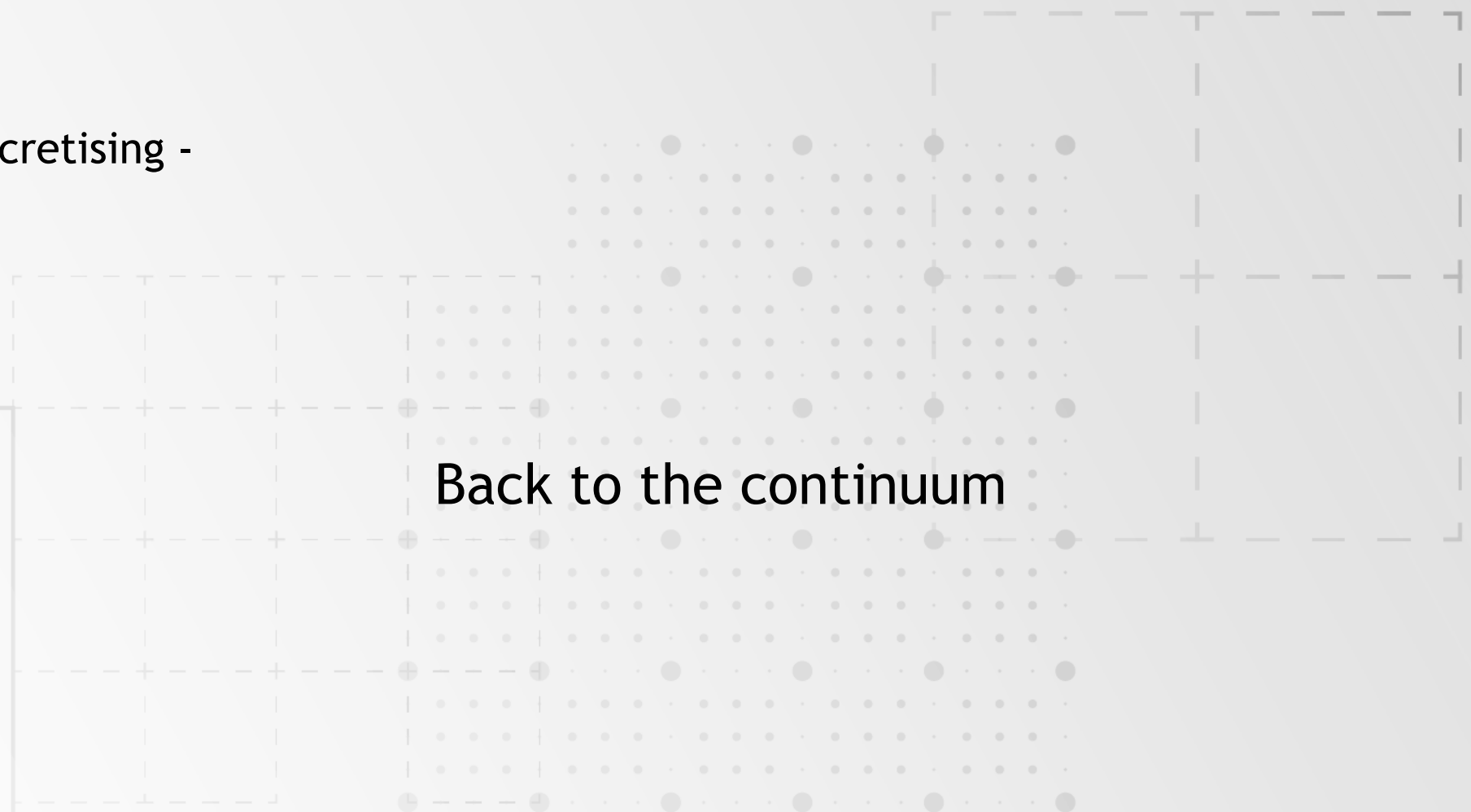
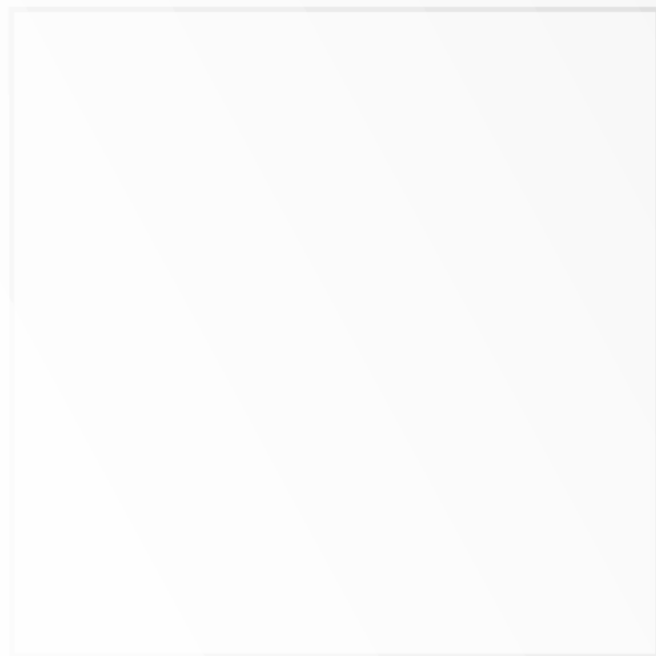


U : SU(3) matrix $\text{Det} = 1$
 $U^{-1} = U^*$

a : 0.1 fm? 0.003fm? 1cm???

g only parameter. \rightarrow where is the spacing?

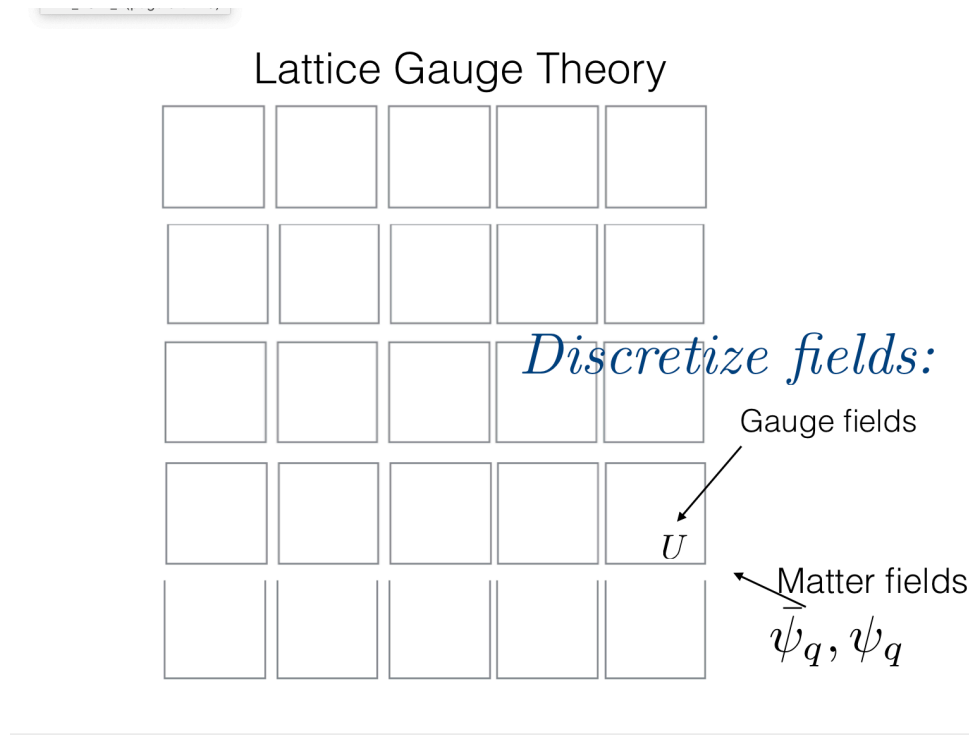
After discretising -



Back to the continuum

Planning a simulation

Parameters: N_σ, N_τ, g



Assume we have the lattice results for some masses

$M_{1\text{Lat}}$

$M_{2\text{Lat}}$

$M_{3\text{Lat}}$

How do we get results in physical units?

Issues

- Scale setting : one physical value needed as input!
- Scaling : how strong are the discretisation effects?
- Asymptotic scaling : are we sensitive to the $g=0$ singularity?

Scaling : repeat for different couplings and check consistencies of results -
or, which is the same, check that dimensionless ratios do not depend on g

Asymptotic scaling : repeat for different couplings, and check consistency with the two-loop universal scaling — implies scaling, but much harder to get

$$a\Lambda_L = \left(\frac{1}{b_0 g^2} \right)^{b_1/2b_0^2} e^{-1/2b_0 g^2}$$

Improvement: in general, a program aimed at controlling lattice artifacts, so to reach faster and with more confidence scaling (hence continuum limit)

The functional integral

Sampling the phase space



Task:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}A_\mu \mathcal{O} e^{-S}$$

from Mike Creutz:

$$J = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}U$$

A direct evaluation of such an integral has pitfalls. At first sight, the basic size of the calculation is overwhelming. Considering a 10^4 lattice, small by today standards, there are 40,000 links. For each is an $SU(3)$ matrix, parametrized by 8 numbers. Thus we have a $10^4 \times 4 \times 8 = 320,000$ dimensional integral. One might try to replace this with a discrete sum over values of the integrand. If we make the extreme approximation of using only two points per dimension, this gives a sum with

$$2^{320,000} = 3.8 \times 10^{96,329} \quad (6)$$

terms! Of course, computers are getting pretty fast, but one should remember that the age of universe is only $\sim 10^{27}$ nanoseconds.

!!!

Monte Carlo methods:

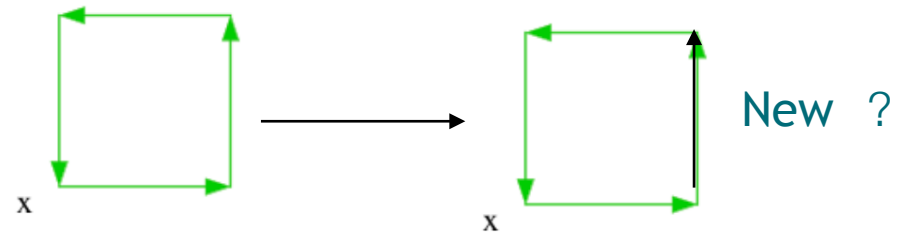
Create a sample of configurations distributed according to

$$e^{-S}$$

The functional integral may then be traded with an average over configurations

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}A_\mu \mathcal{O} e^{-S} \quad \rightarrow \quad \frac{\sum_{i=1}^N \mathcal{O}_i}{N}$$

Monte Carlo time 'evolution'



Different methods use different strategies for choosing the new link

Crucial point: positive Action!

1. Metropolis

$$\Delta S = S(\hat{U}_{ji}) - S(U_{ji}) \text{ (all other variables kept fixed) .}$$

If $\Delta S \leq 0$ the move is accepted

Otherwise: pick random number r $0 < r < 1$ and accept if

$$r \leq e^{-\Delta S} .$$

Maximise distance between configurations, at the price of high rejection rate

2. Heath Bath

Choose new U with the appropriate weight:

$$\exp\{-\bar{S}(U_{ji}')\}$$

Accept step always satisfied by construction

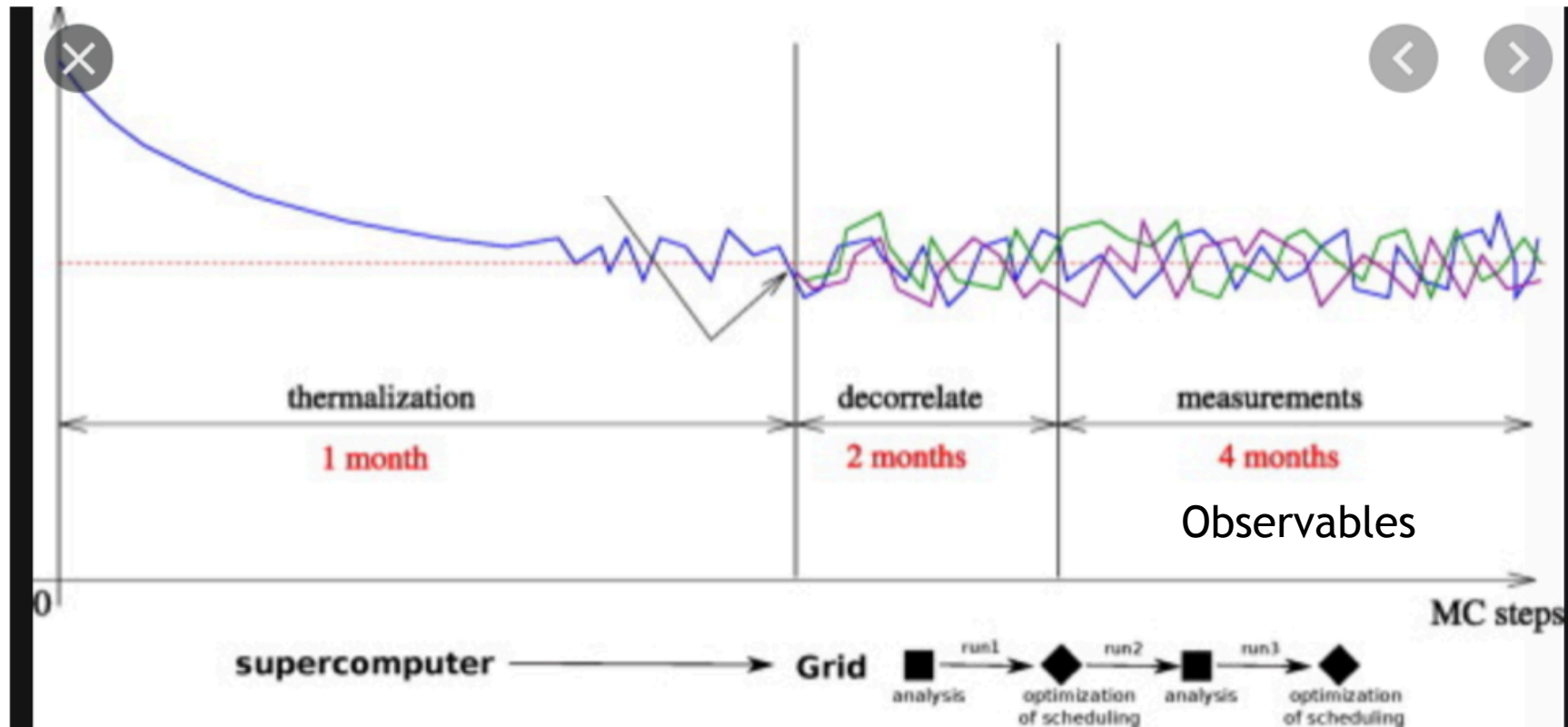
It may be expensive

3. Modified Metropolis

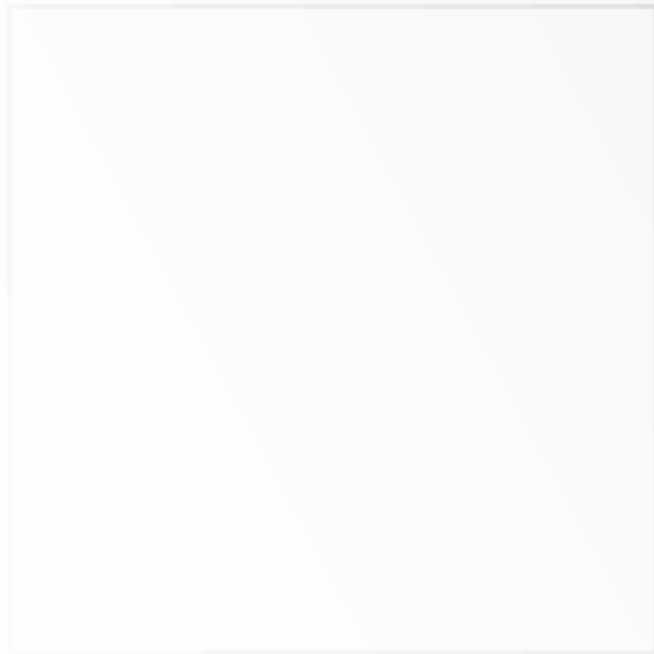
Same as Metropolis, but make several hits
with the same link :
“n upgrading per step”

It ‘interpolates’ between the two previous cases - optimal n to be determined

A typical Monte Carlo simulation:



Basic observables



Thinking in abstract terms - i.e. let us consider the discretised theory as a statistical system in $d+1$ dimension – these are basic measurable quantities:

1) Wilson loops

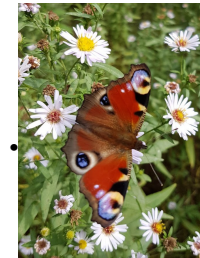


2) Polyakov loop



3) Topological charge

Difficult to draw 'butterfly operator' .



$F \tilde{F}$ In the continuum
(more later)

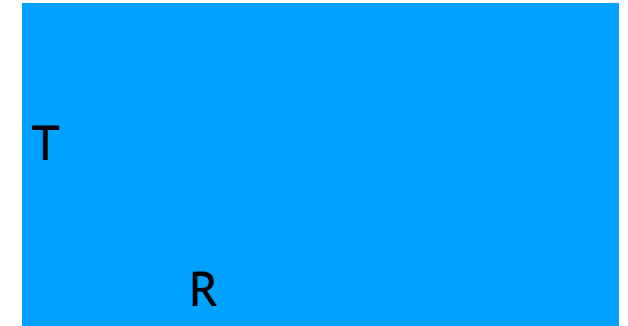
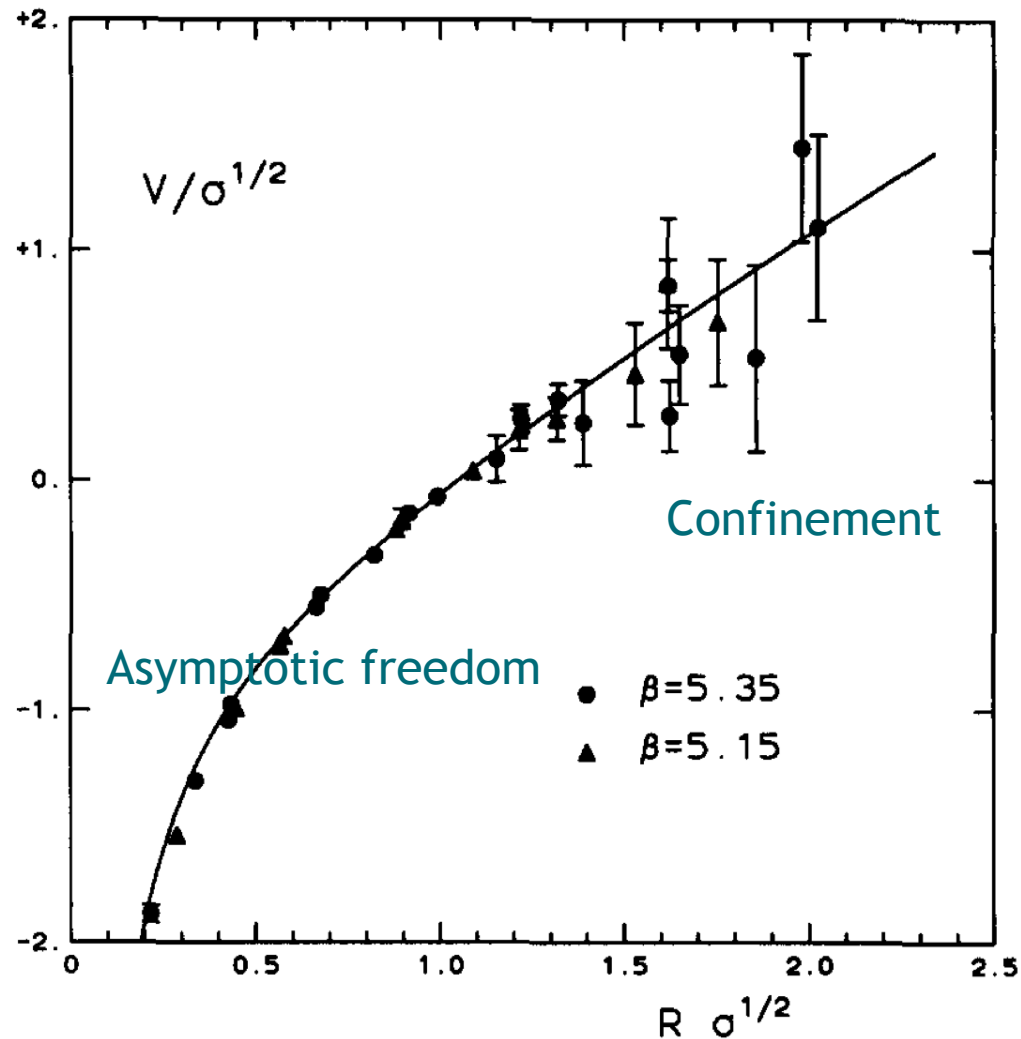
4) Two point functions of any of the above

5) Two point functions of composite fermion operators

Wilson loop

String tension - Interquark potential

$$V(R) = - \lim_{T \rightarrow \infty} \frac{1}{T} \ln W(R, T)$$



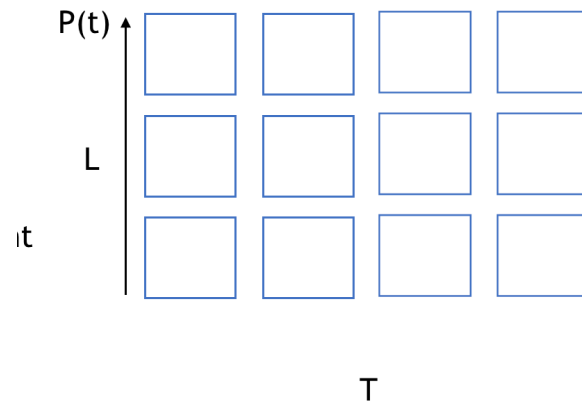
$$V_l(R) = c_0 - \frac{e}{R} + \sigma R \quad \text{Cornell form}$$

String tension $\sqrt{\sigma} = 420 \text{ MeV}$, Physical value

Fig. 1. The interquark potential measured for two values $\beta = 5.15$ and $\beta = 5.35$ and mapped onto each other by setting the scale from the fitted string tension.

Two point functions of Polyakov loop: alternative extraction of the potential

$$e^{-V(R,T)/T} \propto \langle P(\vec{0}) P^\dagger(\vec{R}) \rangle \xrightarrow{R \rightarrow \infty} \propto e^{-\sigma R}$$



Parametro d'ordine per $Z(N_c)$.

→ Confinement as a symmetry

For two colours: $Z(2)$: Ising model!!

→ Universality

‘Build’ Polyakov loop system: it is a cube of spins!!

→ dimensional reduction at T_c

Checking the universality class of Yang Mills

Order parameter : L Analogous to magnetisation In 3D

$$M = \begin{cases} A \left(\frac{T_c^0 - T}{T_c^0} \right)^\beta, & T < T_c^0 \\ 0 & T \geq T_c^0 \end{cases}$$

Note: high and low temperatures interchanged

Some references:

Basics, from QCD to lattice:

Thomas Schaefer <https://arxiv.org/pdf/1608.05459.pdf>

Lattice pedagogical reviews:

Christine Davies, <https://arxiv.org/pdf/hep-ph/0205181.pdf>

Tom de Grand <https://arxiv.org/pdf/1907.02988.pdf>

Martin Luescher <https://arxiv.org/pdf/hep-lat/9802029.pdf>

Michael Creutz <https://arxiv.org/pdf/hep-lat/0406007.pdf>