Introduction to Lattice QCD
and
some applications to Nuclear and Hadronic physics

…. in two Lectures

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Plan of First Lecture (1h)

Praeludium

Some basic points in QFT

- LSZ
- QCD Lagrangian
- Euclidean formulation
- Basic models in euclidean
- Euclidean Correlators

The set up of Lattice QCD

Gluonic action

- Pure glue numerical simulations
- Wilson and Polyakov loops
- Quark-antiquark potential

Fermionic action

Numerical simulations with full QCD

Computing observables

Finite temperature

Prelude

The solution of a QFT in the non perturbative regime is a hopeless task.
It would require the knowledge of a four-dimensional continuum of singular operators $\Phi(t,x)$ (operateor-valued distributions) satisfying (anti)commutation relations at diferent space points

$$[\phi(x), \Pi(y)] = i\delta(\vec{x} - \vec{y})$$

It has however been possible to obtain the solutions of a wide class of QFT problems (not all) by following a protocol suggested by K. Wilson in the 70's, in the framework of QCD.
It consists in using the Feynmann path-integral formulation of the theory in a discretized Euclidean space-time lattice $V=L^3xT$ and Monte Carlo integration techniques.
It is known as « Lattice Calculations », in particular « Lattice QCD calculations » **(LQCD)** although the method is in principle applicable to any QFT.

In the LQCD context, all Nuclear and Hadronic Physics can be (should be) obtained by **solving *ab-initio* a fundamental theory** which depends – essentially - on **two parameters**:

β which controls the lattice spacing **a**

$\mathbf{m_q}$ the bare quark mass $m_q=m_u=m_d$

That makes the **strong interaction world as simple as atomic physics**… except in practice !

This lecture aims to shortly describe this fantastic intellectual adventure which, after many troubles, is nowadays reaching a maturity era.

Some basics of QFT

The link betwen QFT and the formal objects manipulated in LQCD is the LSZ reduction formula
It states that the **S-matrix elements of a theory can be obtained by the time-ordered correlations functions.**
In the simplest case of $q_1+q_2 \rightarrow p_1+p_2$ process in a scalar theory Φ, e.g., it reads

$$\int d^4x_1 e^{ip_1x_1} \int d^4x_2 e^{ip_2x_2} \int d^4y_1 e^{-iq_1y_1} \int d^4y_2 e^{-q_2y_2} \langle 0 \mid T\left\{\hat{\phi}(x_1)\hat{\phi}(x_2)\hat{\phi}(y_1)\hat{\phi}(y_2)\right\} \mid 0\rangle$$
$$= \frac{i\sqrt{Z}}{p_1 - m^2 + i\epsilon} \frac{i\sqrt{Z}}{p_2 - m^2 + i\epsilon} \frac{i\sqrt{Z}}{q_1 - m^2 + i\epsilon} \frac{i\sqrt{Z}}{q_2 - m^2 + i\epsilon} \langle p_1 p_2; out \mid q_1 q_2; in\rangle$$

Everything can be computed in terms of time-ordered correlations functions, the **LQCD bricks**
Not need to know $\Phi(x)$ but only vacuum expectation values (vev) of products of $\Phi(x)$

How to compute them ?

Feynman path integral formulation:

$$\langle 0 \mid \hat{O}[\hat{\phi}(x)] \mid 0\rangle = \int [d\phi]\; O[\phi(x)]\; e^{iS[\phi]} \qquad S = \int d^4x\; \mathcal{L}[\phi(x)]$$

?☆★ش

A **quite a tricky** approach, handable only on a **discretized euclidean world**.

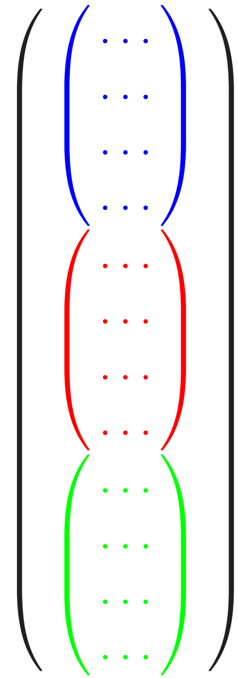
All we need is a (classical) lagrangian density…

I. The QCD Lagrangian

Ensemble of N_f=6 spin ½ quarks (u,d,c,s,t,b)
Eeach q is represented by a color triplet of spinor fields

$$\mathcal{L}(x) = \sum_{f=1}^{6} \bar{q}_f(x)\,(i\gamma_\mu \partial^\mu - m_f)\,q_f(x)$$

$$q^c_\alpha(x) = \begin{pmatrix} q^b_\alpha(x) \\ q^r_\alpha((x) \\ q^v_\alpha((x) \end{pmatrix}$$



If one impose **gauge invariance** in color space

$$\begin{array}{lll} q(x) & \rightarrow & q'(x) = G(x)q(x) \\ \bar{q}(x) & \rightarrow & \bar{q}'(x) = \bar{q}(x)G^\dagger(x) \end{array} \qquad \begin{array}{l} G(x) \in SU(3) \\ G(x)G^\dagger(x) = 1 \end{array}$$

a vector field $A_\mu(x)$ is required, inducing an interaction between quarks

$$\mathcal{L}(x) = \sum_{f=1}^{6} \bar{q}^f(x)\,(i\gamma_\mu D^\mu - m_i)\,q^f(x) \qquad D_\mu = \partial_\mu + igA_\mu$$

The QCD Lagrangian is completed by fixing the $A_\mu(x)$ dynamics

$$\mathcal{L}_{QCD}(x) = \sum_{f=1}^{6} \bar{q}^f(x)\,(i\gamma_\mu D^\mu - m_i)\,q^f(x) - \frac{1}{2}\mathrm{Tr}\,\{F_{\mu\nu}(x)F_{\mu\nu}(x)\}$$

with $g\;F_{\mu\nu} = i[D_\mu, D_\nu]$

In a gauge transform

$$A_\mu \rightarrow A'_\mu = GA_\mu G^\dagger + \frac{i}{g}(\partial_\mu G)G^\dagger$$

$$F_{\mu\nu}(x) \rightarrow F'_{\mu\nu}(x) = G(x)F_{\mu\nu}(x)G^\dagger(x)$$

Everything relies on « gauge invariance »

II. Euclidean formulation

It consists in an analytic continuation (imaginary time) of normal QFT

New set of coordinates $x_M^\mu = (x^0, x^1, x^2, x^3) \rightarrow x_E^\mu = (x^1, x^2, x^3, x^4) = x_\mu^E$

With
$$\begin{aligned} x^4 &= +ix^0 \\ x^0 &= -ix^4 \end{aligned} \quad \Leftrightarrow \quad \begin{aligned} p^4 &= -ip^0 \\ p^0 &= +ip^4 \end{aligned}$$

and $d^4x_M = -id^4x_E$

and $x_M.y_M \equiv x^0y^0 - x^1y^1 - x^2y^2 - x^3y^3 = -x^1y^1 - x^2y^2 - x^3y^3 - x^4y^4 \equiv -x_E.y_E$

Euclidean metric $\delta_{\mu\nu}$

Dirac matrices $[\gamma_\mu, \gamma_\mu]_+ = 2\delta_{\mu\nu}$

Choice (Montvay) $\vec{\gamma}_E = -i\vec{\gamma}_M \qquad \gamma_E^4 = \gamma_M^0$

$$\gamma_E^4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \vec{\gamma}_E = \begin{pmatrix} 0 & -i\vec{\sigma} \\ i\vec{\sigma} & 0 \end{pmatrix} \qquad \gamma^5 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

$$\gamma_E^1 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \quad \gamma_E^2 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \quad \gamma_E^3 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix} \quad \gamma_E^5 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

an inexhaustible source source of confusion and numerical errors …

III. Some basic models in euclidean

Exemple 1: Klein Gordon

$$\mathcal{L}_M^{KG} = +\frac{1}{2}\left\{\partial_0^2 - \partial_x^2 - m^2\right\}\phi = -\frac{1}{2}\left\{\partial_4^2 + \partial_x^2 + m^2\right\}\phi \qquad \partial_0^2 = -\partial_4^2$$

$$\mathcal{L}_M^{KG} = -\mathcal{L}_E^{KG} \qquad \mathcal{L}_E^{KG} = \frac{1}{2}\left\{\partial_4^2 + \partial_x^2 + m^2\right\}\phi$$

$$S_M = \int d^4x_M\, \mathcal{L}_M^{KG}(x) = i\int d^4x_E\, \mathcal{L}_E^{KG}(x) = iS_E \qquad S_E = \int d^4x_E\, \mathcal{L}_E^{KG}(x)$$

$$e^{iS_M} = e^{-S_E} \qquad S_E > 0$$

Exemple 1: Dirac

$$\mathcal{L}_M^D = \bar{\Psi}(x)\left[i\gamma_M^\mu \partial_\mu^M - m\right]\Psi(x)$$

$$i\gamma_M^0\partial_0 + i\gamma_M^1\partial_1 = -\gamma_M^0\partial_4 + i\gamma_M^1\partial_1 = -\gamma_E^4\partial_4 - \gamma_E^1\partial_1$$

since $\begin{array}{rcl} \gamma_E^4 & = & \gamma_M^0 \\ \gamma_E^k & = & -i\gamma_M^k \end{array}$

$$\mathcal{L}_M^D = -\mathcal{L}_E^D \qquad \mathcal{L}_E^D = \bar{\Psi}(x)\left[\gamma_E^\mu \partial_\mu^E + m\right]\Psi(x)$$

$$S_M^D = \int d^4x_M\, \mathcal{L}_M^D = -i\int d^4x_E\, \mathcal{L}_E^D = iS_E^D$$

with $S_E^D = \int d^4x_E\, \mathcal{L}_E^D$

$$e^{iS_M^D} = e^{-S_E^D} \qquad S_E^D > 0$$

(not obvious !)

IV. Euclidean correlators

Vacuum expectation value (VEV) of a product of two operators at different (euclidean) times

$$< 0 \mid O_1(t) O_2(0) \mid 0 >$$

Is a central quantity in LQCD computations.

On one hand it has a simple physical interpretation in terms of interesting physical quantities
One can show that:

$$< 0 \mid O_1(t) O_2(0) \mid 0 >= \sum_k < 0 \mid O_1 \mid k >< k \mid O_2 \mid 0 > e^{-(E_k - E_0)t}$$

We use for that (Heisenberg picture)

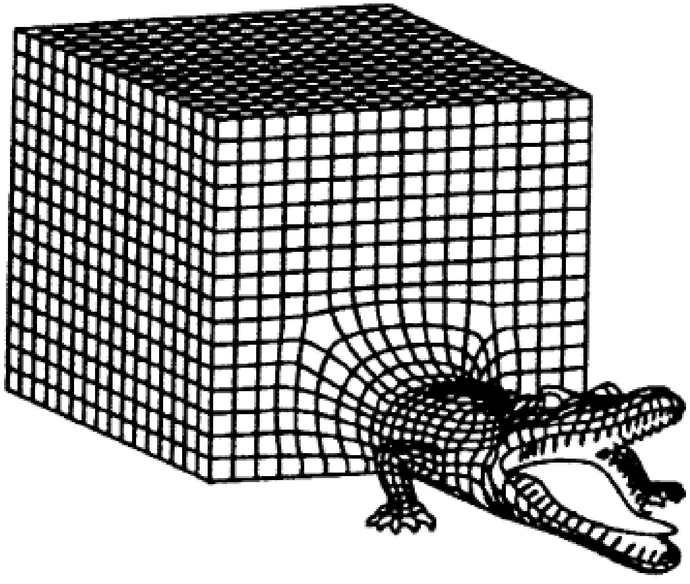
$$O_H(t) = e^{Ht} O(0) e^{-Ht}$$

and introdcue a complet set of H eigenstate:

$$H \mid n >= E_n \mid n > \qquad 1 = \sum_n \mid n >< n \mid$$

On the other hand it is accessible in the numerical simulations of euclidean QFT
(as any VEV)

The setup of Lattice QCD



LQCD : Gluonic part

Ingredients

8 gluon vector fields $$A^a_\mu(x) = \{A^1_\mu, A^2_\mu, A^3_\mu, \dots, A^8_\mu\}$$

1 « color-matrix» gluon field

λ=Gell-Mann SU(3) matrices

$$\left[\lambda^a, \lambda^b\right] = 2i f_{abc}\, \lambda^c$$

$$Tr\{\lambda_a \lambda_b\} = 2\delta_{ab}$$

$$A_\mu(x) = \frac{1}{2}\sum_{a=1}^{8} \lambda_a A^a_\mu(x) = \begin{pmatrix} A^{11}_\mu & A^{12}_\mu & A^{13}_\mu \\ A^{21}_\mu & A^{22}_\mu & A^{23}_\mu \\ A^{31}_\mu & A^{32}_\mu & A^{33}_\mu \end{pmatrix}$$

10x8 tensor fields $$F^a_{\mu\nu}(x) = \partial_\mu A^a_\nu(x) - \partial_\nu A^a_\mu(x) + g\sum_{\beta\gamma} f^a_{\beta\gamma} A^\beta_\mu(x) A^\gamma_\nu(x)$$

10 « color tensor » fields $$F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) + ig[A_\mu(x), A_\nu(x)]$$

$$F^{cc'}_{\mu\nu}(x) = \frac{1}{2}\sum_a \lambda^{cc'}_a F^a_{\mu\nu}(x) = \partial_\mu A^{cc'}_\nu(x) - \partial_\nu A^{cc'}_\mu(x) + g\sum_{a\beta\gamma} \lambda^{cc'}_a\ f^a_{\beta\gamma}\ A^\beta_\mu(x) A^\gamma_\nu(x)$$

Gluonic action $$\mathcal{S}_g(x) = \frac{1}{2}\int d^4x\ \mathrm{Tr}\left[F_{\mu\nu}F_{\mu\nu}(x)\right]$$

Show : $\mathcal{L}_g = \frac{1}{4} F^a_{\mu\nu} F^a_{\mu\nu}$

it is gauge invariant since $F_{\mu\nu}(x) \to F'_{\mu\nu} = G(x) F_{\mu\nu}(x) G^\dagger(x)$

LQCD : Gluonic part

Discretization

« Natural » procedure:

1. Replace derivative by finite differences with lattice spacing **a**

$$\begin{array}{rcl} 2a\,\partial_\mu A_\nu(x) & = & A_\nu(x+\mu) - A_\nu(x-\mu) + o(a^3) \\ 2a\,\partial_\nu A_\mu(x) & = & A_\mu(x+\nu) - A_\mu(x-\nu) + o(a^3) \end{array}$$

$$2a\,F_{\mu\nu}(x) = A_\nu(x+\mu) - A_\nu(x-\mu) - A_\mu(x+\nu) + A_\mu(x-\nu) + 2iag[A_\mu(x), A_\nu(x)] + o(a^3)$$

2. Insert it in a discret sum over lattice sites

$$S_g = \frac{a^4}{2}\sum_x F_{\mu\nu}(x)F_{\mu\nu}(x)$$

It does not work !
Gauge invariance is lost for a non zero value of **a**

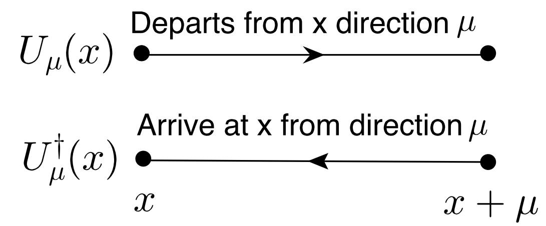
K.G. Wilson overcame this problem in 74 (Phys Rev D10, 2445)
thus giving the starting point of LQCD

LQCD : Gluonic part

Wilson action : consider the « Wilson line » along a « link »

$$U_\mu(x) = \exp\left\{ig \int_x^{x+\mu} dz_\mu A_\mu(z)\right\} = e^{igaA_\mu(x)}$$

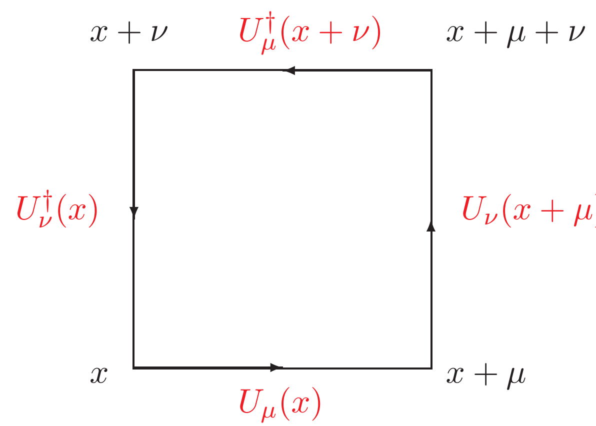
$$U_\mu^\dagger(x) = \exp\left\{ig \int_{x+\mu}^{x} dz_\mu A_\mu(z)\right\} = e^{-igaA_\mu(x)}$$



Not Gauge Invariant but « good » transformations $U_\mu(x) \to G(x) U_\mu(x) G^\dagger(x+\mu)$

Consider product of 4 link variables along a « plaquette »

$$U_{\mu\nu}(x) = U_\mu(x)\, U_\nu(x+\mu)\, U_\mu^\dagger(x+\nu) U_\nu^\dagger(x)$$



Show that: $U_{\mu\nu}(x) = e^{ia^2 F_{\mu\nu}(x)}$

GREAT !!!

Since by expaning: $\mathrm{Re}\,\mathrm{Tr}\,\{1 - U_{\mu\nu}(x)\} = \dfrac{a^4}{2}\,\mathrm{Tr}\,\{F_{\mu\nu}(x) F_{\mu\nu}(x)\} + o(a^6)$

and finally:

$$\boxed{S_g = \frac{\beta}{3} \sum_x \sum_{\mu<\nu} \mathrm{Re}\,\mathrm{Tr}\,\{1 - U_{\mu\nu}(x)\} = \frac{\beta}{3} \sum_x \sum_{\mu<\nu} P_{\mu\nu}(x) \qquad \beta = \frac{6}{g^2}}$$

All kind of improvements: Luscher-Weisz, Iwasaki,…

Pure glue numerical simulations

The Feynman path-integral fromulation for a VEV of any operator

$$< 0 \mid \hat{O}[U] \mid 0 >= \frac{1}{Z} \int [dU] \; \hat{O}[U] \; e^{-S_g[U]} \qquad Z = \int [dU] \; e^{-S_g[U]}$$

Becomes on a lattice V=L^{3}T $\quad < 0 \mid \hat{O}[U] \mid 0 >= \frac{1}{N} \sum_{i=1}^{N} \hat{O}[\{U\}_i] \; + \; O\left(\frac{1}{\sqrt{N}}\right)$

i.e. an aritmetic average of O(U) over an **statistical sample of N configurations**

$$\{U\}_i = \left\{ U_\mu^{(i)}(x_1), U_\mu^{(i)}(x_2), \ldots, U_\mu^{(i)}(x_V) \right\} \qquad \{U\}_i \sim \rho[U] = e^{-S_g[U]}$$

distributed according to a probability law ρ

How to generate such an ensemble ?

Metropolis algortim:

Start with a more or less arbitrary configuration U_0 (e.g. $U = 1$ or $U = ran$)

1. For any link variable $U_\mu(x)$ propose random change according to some "democratic" criterion

$$U_\mu(x) \to U'_\mu(x)$$

2. Compute the resulting modification in the total action

$$\Delta S = S_g(U') - S_g(U)$$

3. Generate a random number $r \in [0,1]$. If $r \leq e^{-\Delta S}$ accept the change, otherwise keep $U_\mu(x)$

4. Go to 1 untill all links are examined

QM is here !

At the end we obtain a new configuration

$$U_n \to U_{n+1}$$

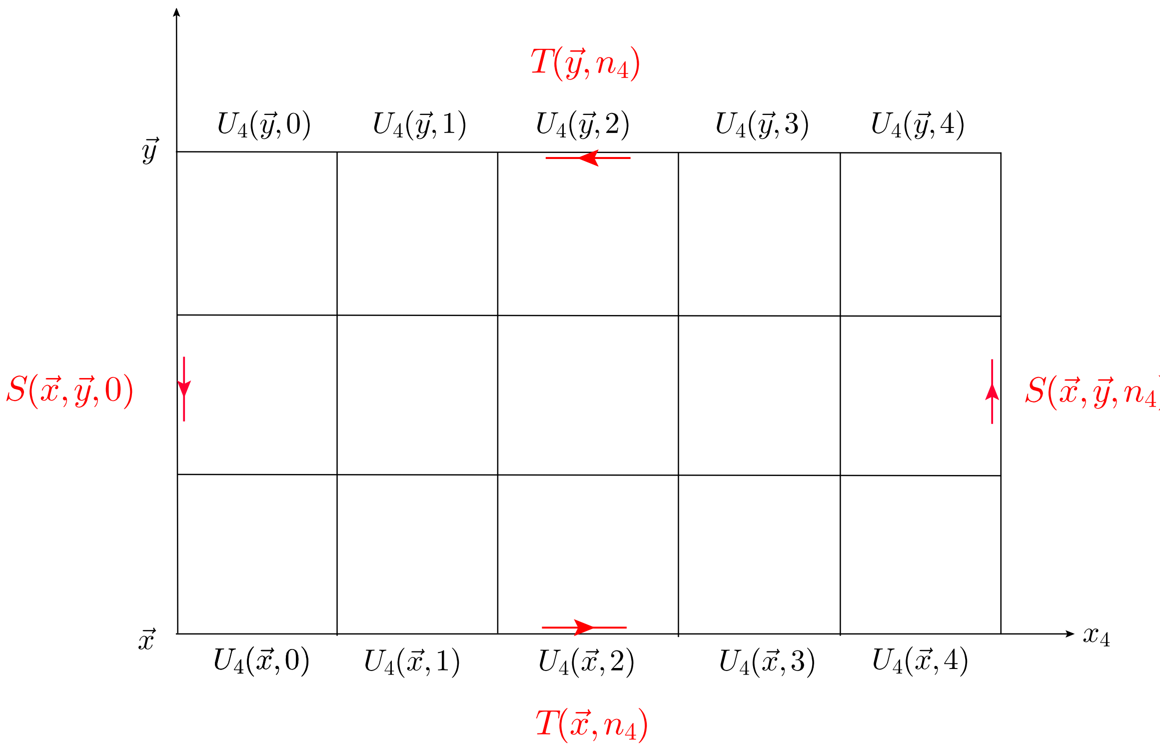
One generates this way a Markov chain reaching a statistical equilibrium.

$$U_0, U_1, \ldots, U_i, U_{i+1}, \ldots$$

Once this is achieved, a series of uncorrelated N measurements can be done.

This seminal method is however not very efficient, specially for gauge theories.
More efficient algorithms exists: Heat bath, overrelaxation, Hybrid Monte Carlo (HMC), ...

A first application: the $q\bar{q}$ potential



Consider Wilson loop $$W(\vec{x},\vec{y},n_4) = \mathrm{Tr}\left\{S(\vec{x},\vec{y},n_4)\; T^\dagger(\vec{y},n_4)\; S^\dagger(\vec{x},\vec{y},0)\; T(\vec{x},n_4)\right\}$$

where, e.g. $$T(\vec{x},n_4) = U_4(\vec{x},0)U_4(\vec{x},1)U_4(\vec{x},2)\ldots U_4(\vec{x},n_4-1)$$

Compute Its VEV in a « temporal gauge » U_4=0 (since gauge invariant!)

$$<0\mid W(\vec{x},\vec{y},n_4)\mid 0> = <0\mid \mathrm{Tr}\left\{S(\vec{x},\vec{y},n_4)\; S^\dagger(\vec{x},\vec{y},0)\right\}\mid 0>$$

It s an Euclidean correlator between t=0 and t=n_t, and so

$$<0\mid W(\vec{x},\vec{y},n_4)\mid 0> = \sum_k \sum_{ij} <0\mid S_{ij}(\vec{x},\vec{y},n_4)\mid k><k\mid S^\dagger_{ji}(\vec{x},\vec{y},0)\mid 0>\, e^{-(E_k-E_0)n_4 a}$$

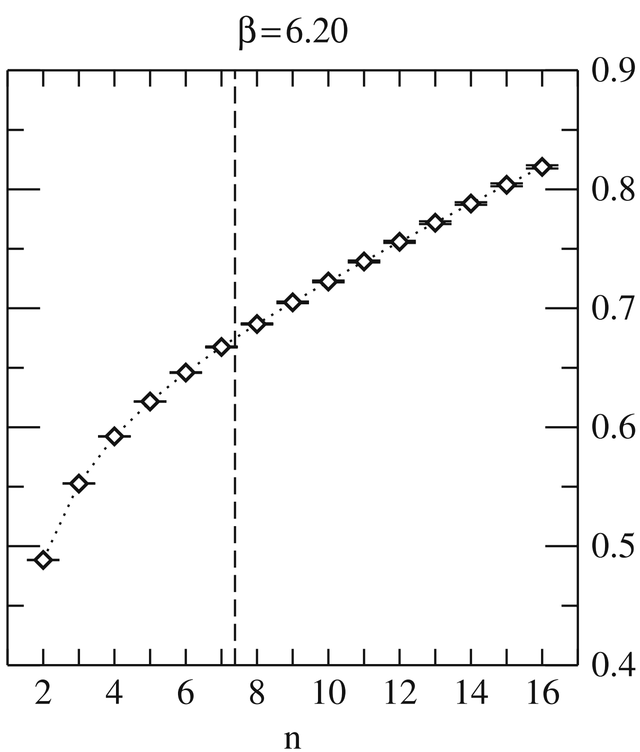
The excitation energy with respect to vacuum state E_0 is interpreted (not arbitrarily!!!) as the $\bar{q}q$ excitation energy (potential) at the respectives positions x and y

$$(E_1 - E_0) \equiv V_{q\bar{q}}(r) \qquad r = a\,|\,\vec{x} - \vec{y}\,|$$

The VEV of the Wilson Loop provides a Lattice measurement of the $\bar{q}q$ potential

$$< 0\,|\,W(\vec{x}, \vec{y}, n4)\,|\,0 > \sim e^{-V(r)\,n_4 a} = e^{-V(r)\,t}$$

It can be numerically computed by the techniques just described (Good exercise!)



It displays the expected « Cornell » form

$$V(r) = A + \frac{B}{r} + \sigma\, r$$

The string is « broken » in more elaborate (unquenched) simulations

Polyakov loops

It is a temporal Wilson line over all the lattice t-extend with periodic boundary conditions (so a loop!)

$$P(\vec{x}) = \mathrm{Tr}\left\{U_4(\vec{x},0)U_4(\vec{x},1)U_4(\vec{x},2)\dots U_4(\vec{x},T-1)\right\} \qquad U_4(\vec{x},0) = U_4(\vec{x},T)$$

Abandon the « temportal gauge » !

Used to obtain the $\bar{q}q$ potential independently, since

$$< 0 \mid P(\vec{x})\ P^\dagger(\vec{y}) \mid 0 > \sim\ e^{-V(r)\ aT}$$

The single loop is also used as order parameter in the deconfinement transition of gluonic matter at finite T

$$\eta =< 0 \mid P(\vec{x}) \mid 0 >$$

All these things are easy-to-compute (even from scratch) and very rich !

LQCD : Fermionic Action

« Naive » discretization

Free fermion action $$\mathcal{L}_D = \bar{\Psi}(x)(\gamma_\mu \partial_\mu + m)\Psi(x)$$

Discretizing derivative $$2a\ \partial_\mu \Psi(x) = \Psi(x+\mu) - \Psi(x-\mu)$$

Leads to the discret action $$S_F = \frac{a^3}{2} \sum_x \bar{\Psi}_x \sum_\mu \gamma_\mu \left[\Psi_{x+\hat{\mu}} - \Psi_{x-\hat{\mu}}\right] + Ma^4 \sum_x \bar{\Psi}_x \Psi_x$$

Local term is gauge invariant but non local ones not !

$$\bar{\Psi}_x \Psi_{x+\hat{\mu}} \longrightarrow \bar{\Psi}'_x \Psi'_{x+\hat{\mu}} = \bar{\Psi}_x G^\dagger(x) G(x+\mu) \Psi_{x+\mu}$$

Gauge invariance is restored buy inserting « link operators » in forward and backward derivatives

$$\begin{array}{lcl} \bar{\Psi}_x \Psi_{x+\hat{\mu}} & \longrightarrow & \bar{\Psi}_x \ U_\mu(x) \ \Psi_{x+\hat{\mu}} \\ \bar{\Psi}_x \Psi_{x-\hat{\mu}} & \longrightarrow & \bar{\Psi}_x \ U_{-\mu}(x) \ \Psi_{x-\hat{\mu}} \end{array}$$

One obtains this way a « naive » , gauge invariant, fermionic action action

$$S_F = \frac{a^3}{2} \sum_x \bar{\Psi}_x \sum_\mu \gamma_\mu \left[U_\mu(x)\Psi_{x+\hat{\mu}} - U_\mu^\dagger(x-\mu)\Psi_{x-\hat{\mu}}\right] + Ma^4 \sum_x \bar{\Psi}_x \Psi_x$$

It use to be writen as a bilinear form in terms of the **Dirac operator D, a key ingredienty in LQCD**

$$S_F = a^4 \sum_{x,y} \bar{\Psi}_x D_{xy} \Psi_y \qquad D_{xy} = M\delta_{xy} + \frac{1}{2a} \sum_\mu \gamma_\mu \left[U_\mu(x)\delta_{x+\mu,y} - U_\mu^\dagger(x-\mu)\delta_{x-\mu,y}\right]$$

(color and spinor indexs are implicit)

But we are not done yet ….

The « doubling » problem and the « Wilson action »

When inspecting S_F, one can see* that it actually represents 16 fermion propagating on the lattice!

Wilson proposed a way to remove 15 unwanted poles.
Technically this is done by adding an additional Laplacian term to D

$$D^W_{xy} = D_{xy} - \frac{a}{2}\Delta_{xy} \qquad \Delta_{xy} = \frac{1}{a^2}\sum_{\mu=1}^{4} U_\mu(x)\delta_{x+\mu,y} - 2\delta_{xy} + U^\dagger_\mu(x-\mu)\delta_{x-\mu,y}$$

Putting all together

$$D^W_{xy} = \left(M + \frac{4}{a}\right)\delta_{xy} + \frac{1}{2a}\sum_\mu \left[(1-\gamma_\mu)U_\mu(x)\delta_{x+\mu,y} - (1+\gamma_\mu)U^\dagger_\mu(x-\mu)\delta_{x-\mu,y}\right]$$

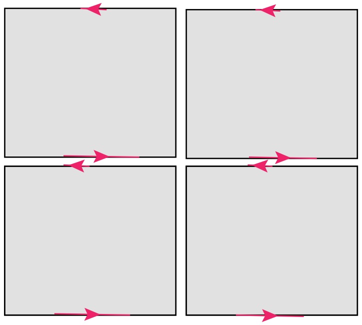
(*)The fermion propagator is given by the invers of D.

This is the first (and simplest) example of a long series of discretized « fermionic actions »

Wilson - « Clover » (Sheikholeslami-Whoelert 1985)

Add a term to the Wilson action $\mathcal{L}_C(x) = \sigma_{\mu\nu} C_{\mu\nu}(x)$

$$\sigma_{\mu\nu} = -\frac{i}{2}[\gamma_\mu, \gamma_\nu]$$
$$8iC_{\mu\nu}(x) = f_{\mu\nu}(x) - f^\dagger_{\mu\nu}(x)$$

$f_{\mu\nu}(x)$ 

Staggered fermions (Kogut Suskind)

Split 1 component in 4 « tastes » distributed in the lattice.
To recover the initial fields one use the « det$^{1/4}$ trick ».
Unclear but very fast simulations

$$S = \sum_x \Psi[D+m]\Psi = \sum_x \sum_{i=1}^{4} \chi_i[f(x)D+m]\chi_i$$

Domain-Wall (Kaplan 1992): Introducing a 5th dimension

Ginsparg-Wilson Overlap: Neuberger
As a solution to Ginzparg-Wilson equation $[D,\gamma_5]_+ = aD\gamma_5 d$ to get good chiral properties

$$D = \frac{1}{a}\left(1 - \gamma_5 \frac{A}{\sqrt{A^2}}\right) \qquad A = \gamma_5 D_W$$

The very best… but numerically very expensive !

Twisted-mass fermions (Frezzoti, Rossi, Sint, Papinutto,..)

Introduce an imaginary mass in a isospin doublet
In the « γ_5 direction »

$$D_{tw} = D_W + i\mu\gamma_5\tau_3$$

Numerical simulation with Full LQCD

Whatever the particular choice of discretization one has $$S_{QCD} = S_q[\bar{q}, q, U] + S_g[U]$$

with
$$S_g = a^4 \sum_x ....$$
$$S_q = a^4 \sum_{xy} \bar{q}_x D_{xy}[U] q_y$$

One aims to compute
$$<| \hat{O}(q, \bar{q}, U) |>= \frac{1}{Z} \int [dU][d\bar{q}](dq]\ O(q, \bar{q}, U)\ e^{-S_q - S_g}$$
$$Z = \int [dU][d\bar{q}](dq]\ e^{-S_q - S_g}$$

Integrals over fermionic fields (Grassmann variables) are performed analytically: **THE LQCD MIRACLE !**

- for Z
$$Z = \int [dU] \left\{ \int [d\bar{q}](dq]\ e^{-S_q[\bar{q},q,U]} \right\}\ e^{-S_g[U]} = \int [dU]\ Z_F[U]\ e^{-S_g[U]}$$
$$Z_F[U] = \int [d\bar{q}][dq] e^{-S_q[\bar{q},q,U]} = \det\ [D(U)]$$

- for fermion propagator
$$<| q_\alpha(x)\bar{q}_\beta(y) |>= \frac{1}{Z} \int [dU] \left\{ \int [d\bar{q}](dq]\ q_\alpha(x)\bar{q}_\beta(y)\ e^{-S_q[\bar{q},q,U]} \right\} e^{S_g[U]} = \frac{1}{Z} \int [dU]\ O_F[U]\ e^{S_g[U]}$$
$$O_F[U] = \int [d\bar{q}](dq]\ q_\alpha(x)\bar{q}_\beta(y)\ e^{-S_q[\bar{q},q,U]} = \left[D^{-1}\right]_{\alpha x, \beta y} \det\ [D(U)]$$

finally $$<| q_\alpha(x)\bar{q}_\beta(y) |>= \frac{1}{Z} \int [dU]\ \left[D^{-1}\right]_{\alpha x, \beta y} \det\ [D(U)]\ e^{S_g[U]}$$

In the discretized version

$$S_{\alpha\beta}(x,y) = <| q_\alpha(x)\bar{q}_\beta(y) |> = \frac{1}{N}\sum_{i=1}^{N}\left[D^{-1}[U_i]\right]_{\alpha x,\beta y}$$

with U_i distributed according to a probability law

$$\rho(U) = \frac{1}{Z}\det\left[D(U)\right] e^{S_g[U]}$$

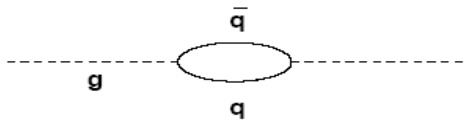
Contrary to scalar and glue case, calculations require:

- Invert huge matrices ! (Iterative processes D*X)
- Compute determinant in generating gauge configurations (HMC)
  Never « brut force » but introducing additional fields and using

$$\det(A) = \frac{1}{Z}\int d\phi\; e^{-\phi^\dagger (AA^\dagger)^{-1/2}\phi}$$

« Quenched » and « uquenched » (dynamical) simulations

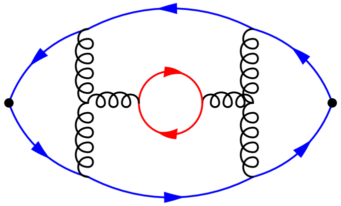
Det(D) accounts for the $\bar{q}q$ loops from gluons propagators (not trivial!)



If q_1 and q_2 det(D)=det(D_1) x Det(D_2)

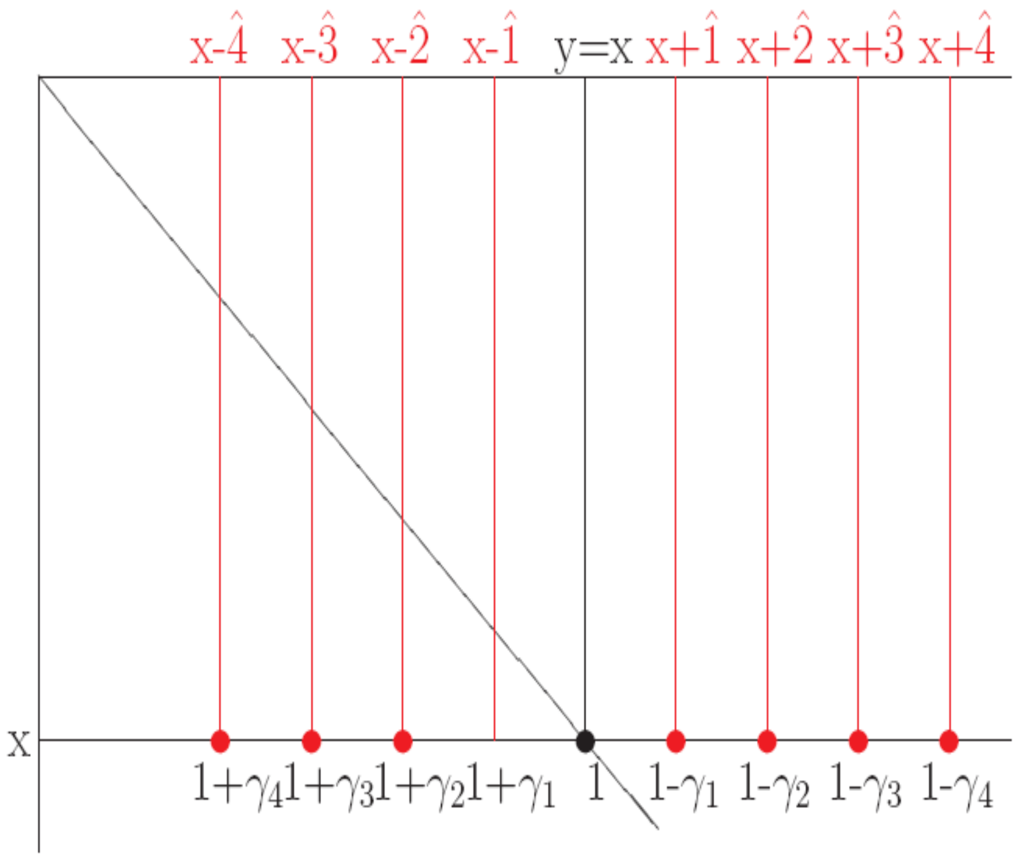
One talks about dynamical calculations with n_f=0, 2(u,d), 2+1(u,d,s), 2+1+1(u,d,c,s)

The case n_f=0 corresponds to det(D)=1 is called « quenched »
… and things are much easier !!!



Dirac matrice in practice

All numerics in “Lattice” consists essentially in solving linear systems   D*x=b
with D=Dirac operator,
That is, with an almost empty matrix… but very large



1 on diagonal

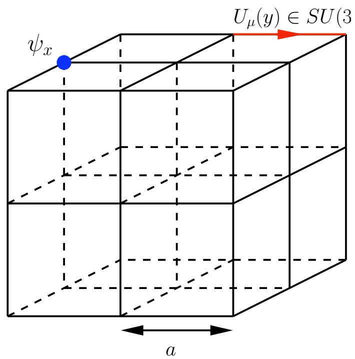
8 Dirac matrices x U outside

This explain the almost perfect scalability in parallel supercomputers (BGQ 400 000 CPU)

SUMMARY

LQCD: Many discretized QCD action

$$\mathcal{L}_{QCD} = \sum_{s=1}^{6} \bar{q}_s D(U) q_s + \mathcal{L}_g(U)$$



On each « link »
4 SU(3) matrices

(gluons)

$$U_\mu(x) = \exp\left\{ \frac{iag}{2} \sum_{c=1}^{8} \int_0^1 d\tau A_\mu^c(x + a\tau\mu)\lambda^c \right\} \in SU(3)$$

On each site
3 x 4 x N_f complex « fields »

(quarks)

$$q_f(x) = \begin{pmatrix} q_f^b(x) \\ q_f^r(x) \\ q_f^v(x) \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} \cdots \\ \cdots \\ \cdots \\ \cdots \end{pmatrix} \\ \begin{pmatrix} \cdots \\ \cdots \\ \cdots \\ \cdots \end{pmatrix} \\ \begin{pmatrix} \cdots \\ \cdots \\ \cdots \\ \cdots \end{pmatrix} \end{pmatrix}$$

L	T	V
24	48	660 000
32	64	2 100 000
48	96	10 600 000
64	128	32 200 000
96	192	169 600 000

Parameters:

- "bare" quark masses $\mathbf{m_l}$ $=m_u=m_d$, m_s , ...

  To control the "physical value" of m_l , one computes m_π (m_π^2=B m_q)

  If m_π=140 MeV… m_l is the right one ! But it is almost never he case !!!

- one parameter $\boldsymbol{\beta}$ that controls the "lattice spacing"

  one goes down to a=0.05 fm (**Errors** due to discretisation: o(a), o(a2),…)

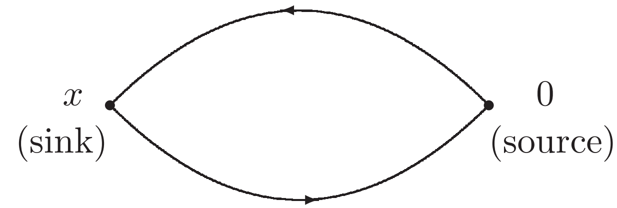
- Lattice **L** (**Errors** due to "finite volume" L x a fm)

- $\mathbf{n_f}$ = number of quarks in the loops in unquenched calculations ($\mathbf{n_f}$=0,2,2+1,2+1+1,…)

COMPUTING OBSERVABLES

Each observable requires an specific approach.
My aim in what follows is to illustrate with some detail two particular cases:

Meson masses



Consider space-time propagation of $\bar{q}q$

Compute correlator between currents J

$$C(t) = \sum_{\vec{x}} < 0 \mid J(x) J^\dagger(0) \mid 0 >$$

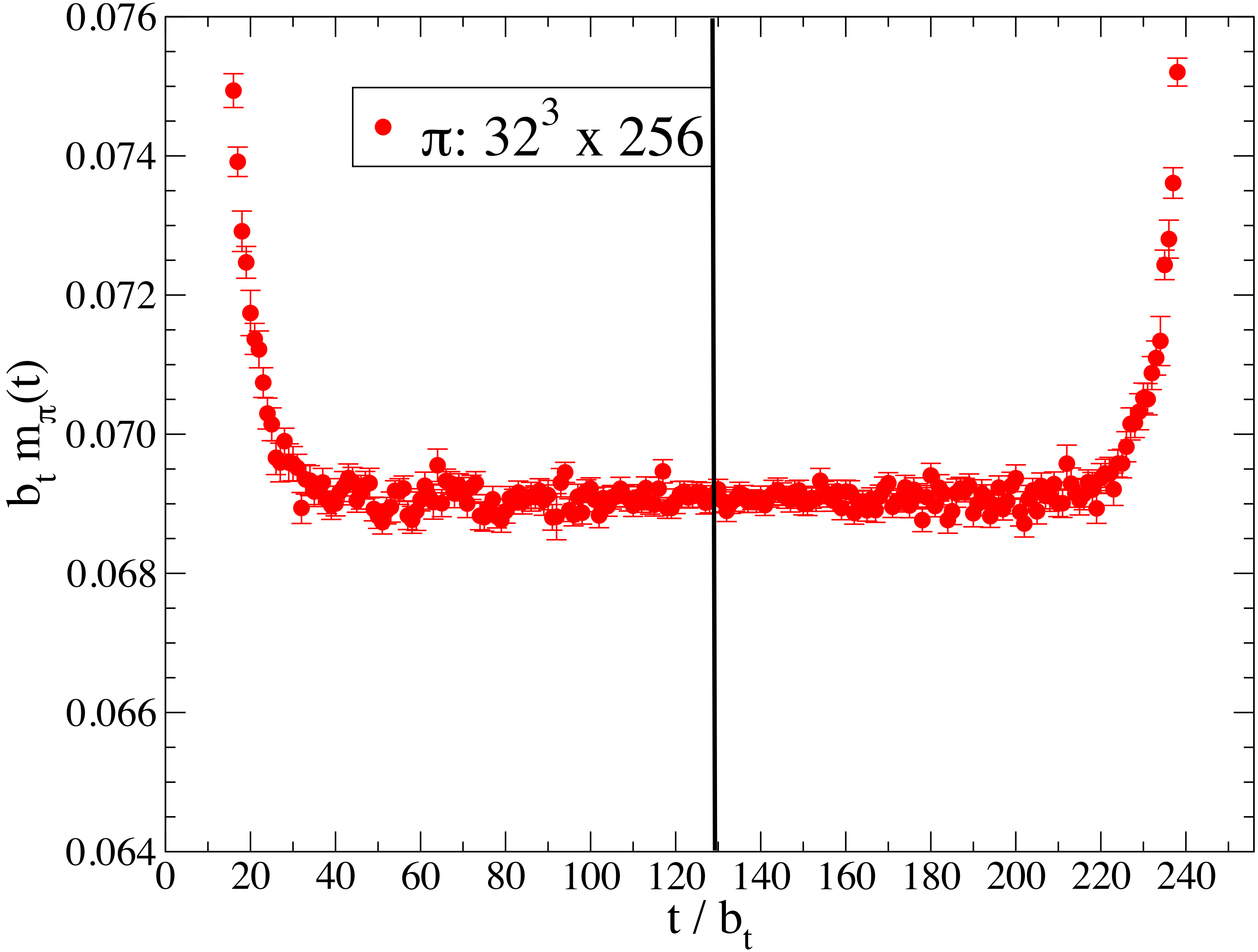
Simplest case $\quad J(x) = \bar{u}(x) d(x)$

$$\begin{aligned} C(t) &= \sum_{\vec{x}} < 0 \mid \bar{u}(x) d(x) \bar{d}(0) u(0) \mid 0 > \\ &= -\sum_{\vec{x}} < 0 \mid d(x) \bar{d}(0) \mid 0 >< 0 \mid u(0) \bar{u}(x) \mid 0 > \\ &= -\sum_{\vec{x}} \mathrm{Tr}\left[S_d(x,0) S_u(0,x)\right] \\ &= -\sum_{\vec{x}} \mathrm{Tr}\left[S_d(x,0)\gamma_5 S_u^\dagger(x,0)\gamma_5\right] \end{aligned}$$

Exo: $J_P(x) = i\bar{u}(x)\gamma_5 d(x) \qquad C_P(t) = \sum_{\vec{x}} \mathrm{Tr}\left\{\left[\gamma_5 S_d(x,0)\right]\left[\gamma_5 S_u(x,0)\right]^\dagger\right\}$

On another hand $\quad < 0 \mid O_1(t) O_2(0) \mid 0 >= \sum_n < 0 \mid O_1 \mid n >< n \mid O_2 \mid 0 > e^{-E_n t} \sim e^{-E_0 t}$

This provides an effcient way to compute meson masses $\qquad aM_{eff}(t) = \log \dfrac{C(t)}{C(t+1)}$



0.076
0.074
0.072
0.070
0.068
0.066
0.064
0
20
40
60
80
100
120
140
160
180
200
220
240
$b_t m_\pi(t)$
t / b_t
π: 32^3 x 256

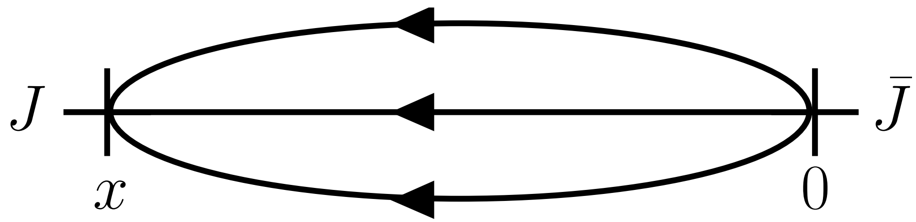
Baryon masses (N)

First step: "built " a N (in fact a $J^\pi=1/2^+$ state) by combining 3 q fields

Create N at y=0

Propagate N from y→x

Annihilate N at x



$$N_a \equiv \bar{\epsilon}^{ijk}(u^i C\gamma_5 d^j)u^k_a \qquad \overline{N}_a \equiv \epsilon^{ijk}(\bar{u}^i C\gamma_5 \bar{d}^j)\bar{u}^k_a$$

$$C_{\alpha\beta}(x,y) = \langle 0 \mid N_\alpha(x)\bar{N}_\beta(y) \mid 0\rangle = \sum C^{abcd}_{\alpha\beta}\langle 0 \mid q_\alpha(x)q_a(x)q_b(x)\bar{q}_\beta(y)\bar{q}_c(y)\bar{q}_d(y) \mid 0\rangle$$

It is a v.e.v. of a product of 6 quark fields q(x)

Wick Th: sum of products of **q propagators** ("contractions")

$$S^{cc'}_{ss'}(x) =< 0|q^c_s(x)\bar{q}^{c'}_{s'}(0)|0 > \qquad D^{c'c}_{s's}(x,y)\; S^{cc"}_{ss"}(y) = \delta^{c'c"}\delta^{s's"}\delta(x)$$

N mass is extracted from matrix elements of this correlator 4x4 (y=0)

$$\mathrm{Tr}\left[C_{\alpha\beta}(t)\right] = \mathrm{Tr}\left[\sum_{\vec{x}} C_{\alpha\beta}(\vec{x},t)\right] \sim e^{-aM_N t}$$

The method can be extended to (6A) q fields and access to A-baryon system

Things becomes quickly complicated

$$\begin{aligned}\chi^p(x) &= \epsilon^{abc}[u^{Ta}(x)C\,\gamma_5 d^b(x)]u^c(x)\\ \chi^n(x) &= \epsilon^{abc}[d^{Ta}(x)C\,\gamma_5 u^b(x)]d^c(x)\end{aligned}$$

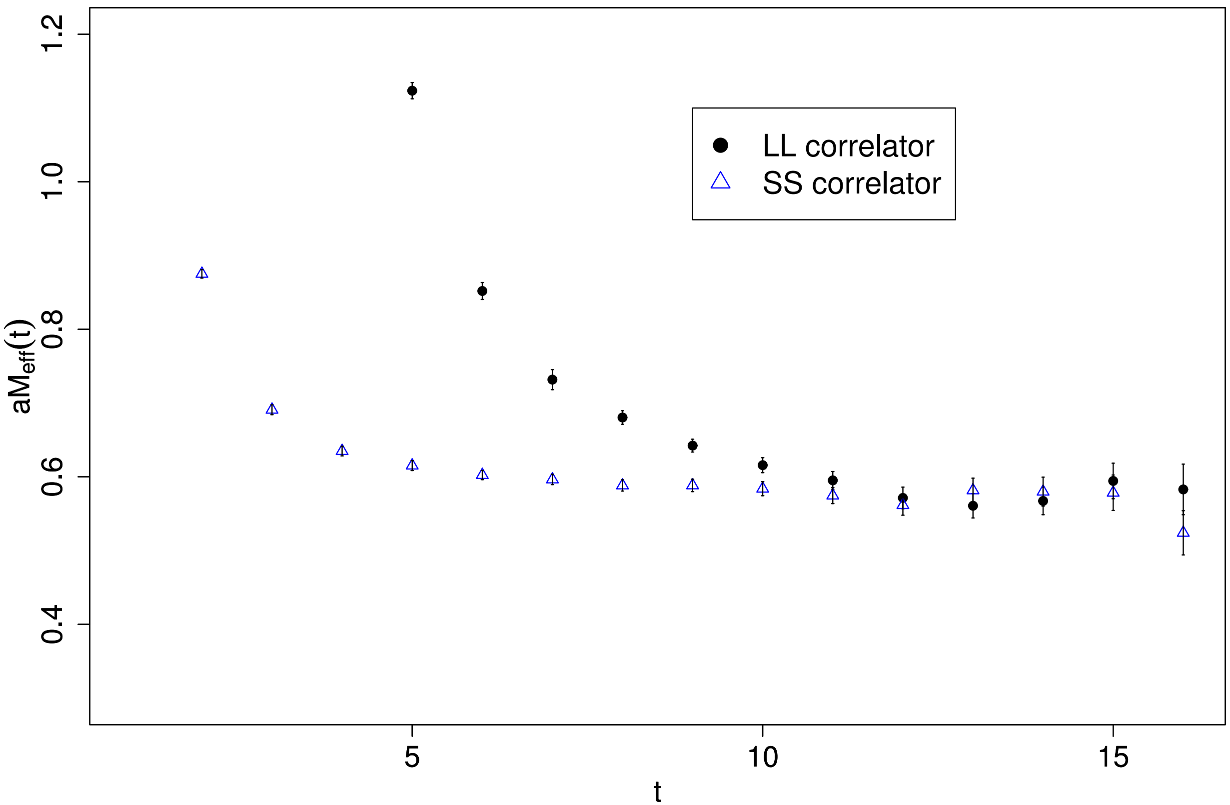
$$C = \gamma_0\gamma_2$$

$$C^p_{ss'}(x) = -\epsilon^{abc}\epsilon^{a'b'c'}\left\{-S_u^{cc'}\,[\Gamma^N S_d^{bb'}\tilde{\Gamma}^N]^T S_u^{aa'} + S_u^{ca'}\,\mathrm{Tr}(S_u^{ac'}[\Gamma^N S_d^{bb'}\tilde{\Gamma}^N]^T)\right\}$$

$$\Gamma^N = C\gamma_5$$

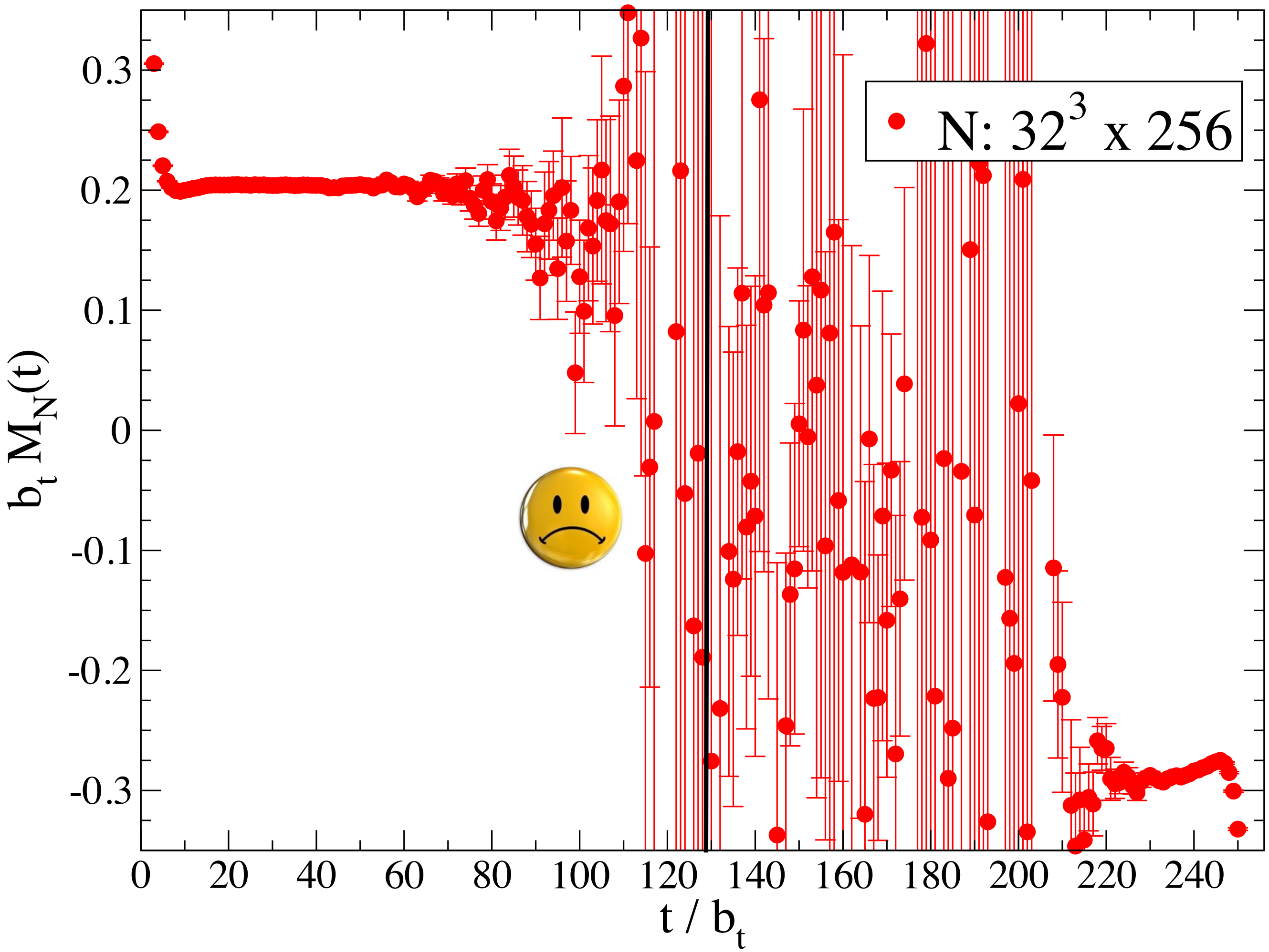
Example: N

$$aM_{eff}(t) = \log \frac{C(t)}{C(t+1)}$$



Same quality for other baryons (ground state !)

Signal to noise $\sim e^{-\left(M_N - \frac{3}{2} M_\pi\right)t}$



Finite Temperature

There is a close formal analogy between

Statistical Mechanics

$$< O > = \frac{1}{Z} \sum_{[c]} O([c]) e^{-\beta H[s]} \qquad Z = \sum_{[c]} e^{-\beta H[s]}$$

$$\beta = \frac{1}{T} \qquad < \hat{O} > = \frac{1}{Z} \mathrm{Tr} \left[\hat{O} \, e^{-\beta \hat{H}} \right] \qquad Z = \mathrm{Tr} \left[e^{-\beta \hat{H}} \right]$$

Lattice Field Theories

$$< \hat{O} > = \frac{1}{Z} \int [d\phi] O[\phi] e^{-S_E[\phi]} \qquad Z = \int [d\phi] \, e^{-S_E[\phi]}$$

Temperature is introduced by limiting the temporal extend in the action

$$S_E(\beta, \Phi) = \int_0^\beta dt \int_{R^3} d^3x \mathcal{L}_E(\Phi, \partial_\mu \Phi)$$

identifying $aN_T \equiv \beta = \frac{1}{T}$

The limiting case $aN_T \to \infty$ corresponds to T=0

Polyakov loops as order parameter

Let us consider a Polyakov loop at some spatial point

$$P(\vec{x}) = \mathrm{Tr}\left\{U_4(\vec{x},0)U_4(\vec{x},1)U_4(\vec{x},2)\ldots U_4(\vec{x},T-1)\right\} \qquad U_4(\vec{x},0) = U_4(\vec{x},T)$$

and average over the spatial lattice $P = \frac{1}{L^3}\sum_x P(\vec{x})$

One can show that its VEV $< P >= \frac{1}{L^3}\sum_x < 0 \mid P(\vec{x}) \mid 0 >$

is related to the **free energy of a static color charge F_q**

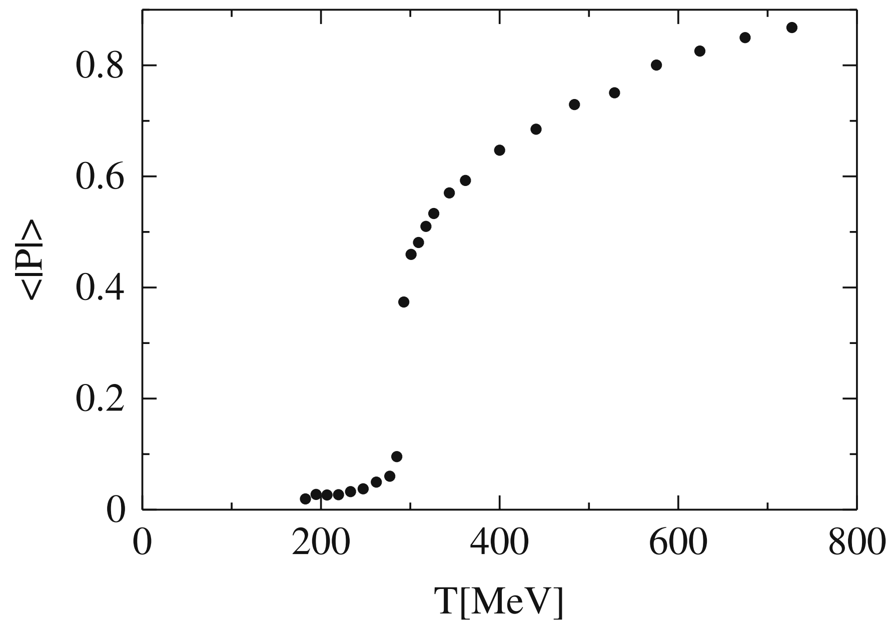
$$< P > \sim \; e^{\beta F_q}$$

It is an **order parameter** for the confinement/deconfinement transition as a function of T

The case **<P>=0** correpsonds to an **infinite value of F_q** ➔ **Confined Phase**

The case **<P>#0** correpsonds to a **finite value of F_q** ➔ **Deconfined Phase**

“Quenched” calculations $T_c \approx 270$ MeV



In the unquenched case the result change dramatically: T_c (n_f=2+1) ≈150 MeV !

The simple picture of Polyakov order parameter fails and other P are required

Chiral condensate $< \bar{q}q >$ or susceptibility $\chi_{ud} = \frac{\partial}{\partial m_{ud}} \langle \bar{\psi}\psi \rangle_{ud}$
display a phase transition at T very close to T_c

Is $T^{chiral}_c = T^{confinement}_c$?

Nobody has prove it: big debate (hotQCD and Wuppertal/Budapest) !

Thermodynamics and equation of state

Knowing Z(T,V,m_q,…) we can acces to usual thermodynamical quantities

Energy density
$$\epsilon = -\frac{1}{V}\frac{\partial \log Z}{\partial \beta} = \frac{T^2}{V}\frac{\partial \log Z}{\partial T}$$

Pression
$$p = T\frac{\partial \log Z}{\partial V}$$

Chiral condensate
$$\Sigma_i = \frac{\partial \log Z}{\partial m_i}$$

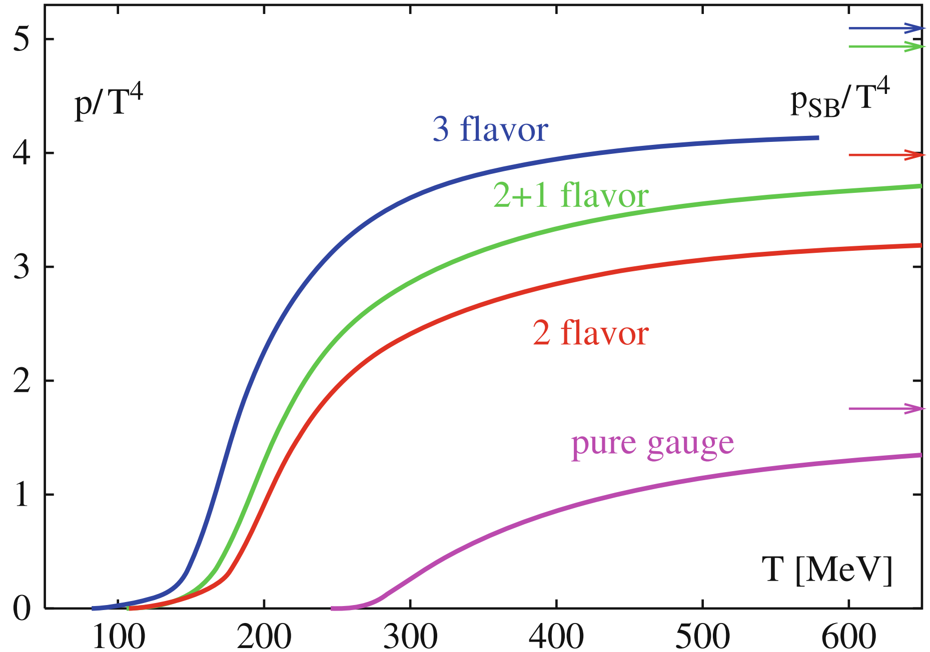
From what one can get the "equation of state" ε(p)

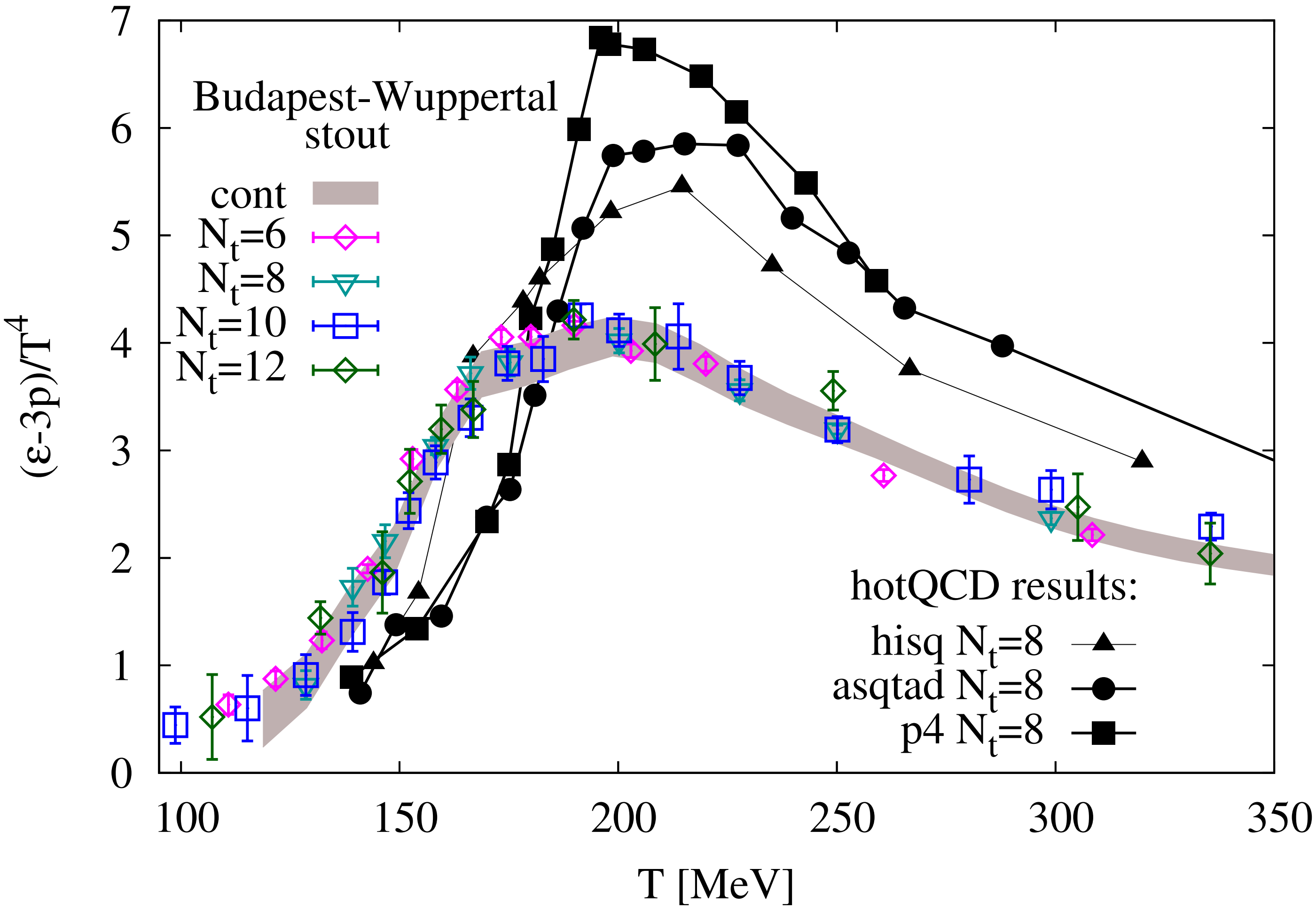
For a relativistic non interacting gas of q and g
$$p(T) = \frac{\pi^2}{45}\left(8 + \frac{21}{4}N_f\right)\ T^4$$
$$\epsilon(p) = 3p$$

The "tradition" is to plot rather
$$\frac{p(T)}{T^4} = f(T)$$

or the "Interaction measure" I=ε(p)-p
$$\frac{\epsilon(p) - p}{T^4} = f(T)$$

Zero baryon number (pure glue)




Budapest-Wuppertal
stout
cont
N_t=6
N_t=8
N_t=10
N_t=12
hotQCD results:
hisq N_t=8
asqtad N_t=8
p4 N_t=8
(ε-3p)/T^4
T [MeV]
0
1
2
3
4
5
6
7
100
150
200
250
300
350

Thermodynamics and equation of state

This can be generalized to non zero baryonic number by introducing a quark chemical potential and the grand canonical ensemble.

$$Z(T,\mu) = \mathrm{Tr}\,\left[e^{-\beta(\hat{H}-\mu_q \hat{N}_q)}\right]$$

μ_q = quark chemical potential $\quad (\mu_B = 3\mu_q)$

N_q = quark number operator $\quad (\hat{N}_B = 3\hat{N}_q)$