LATTICE 4 BEGINNERS

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May 14th, 2012

LATTICE REMAINING QUESTIONS

What's wrong with the classical action?

There's nothing wrong. There's no typo. It's correct if you change t = -it. I double checked this with Joe Kiskis and I added a link to a pdf on page 10.

How do you recover the units at the end of the day?

Basically you don't. Everything is in units of the lattice spacing. All that can be calculated are dimensionless ratios of physical quantities. (Joe Kiskis)

QCD GENERAL

QCD – Gauge theory of the strong interaction

- Lagrangian: formulated in terms of quarks and gluons

$$\mathcal{L}_{\mathrm{QCD}} = -\tfrac{1}{4} F^a_{\mu\nu} F^{a\,\mu\nu} + \sum_f \overline{\psi}_f \left(i\gamma^\mu D_\mu - m_f\right) \psi_f, \quad f = u, d, s, c, b, t$$

$$D_\mu = \partial_\mu - ig(\tfrac{1}{2}\lambda^a) A^a_\mu$$

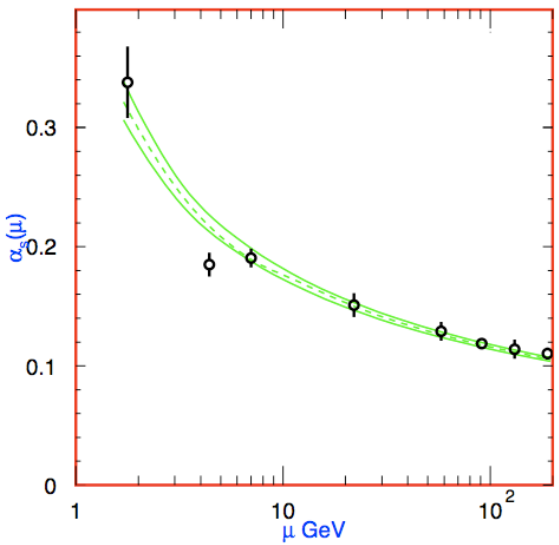
Harald Fritzsch

Murray Gell-Mann

Heinrich Leutwyler

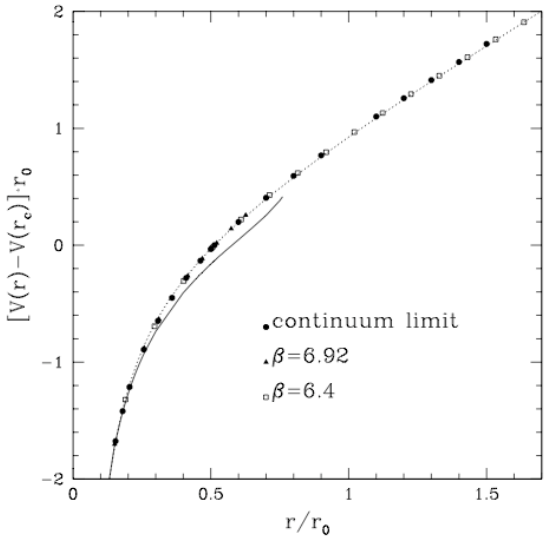
QCD GENERAL

Asymptotic freedom: $g(\mu)$



[Yao et al., PDG 2006]

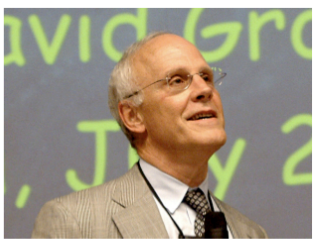
Confinement



[Necco & Sommer, Nucl Phys B622 (2002) 328]

Nobel Prize in Physics 2004

"...for the discovery of asymptotic freedom in the theory of the strong interaction"



David Gross

Frank Wilczek

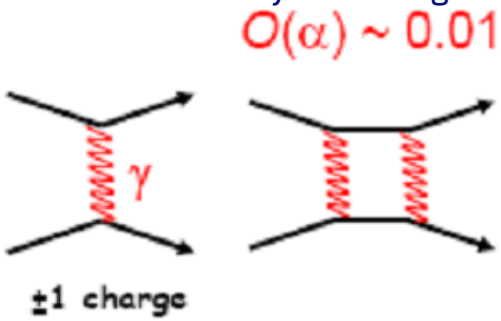
David Politzer

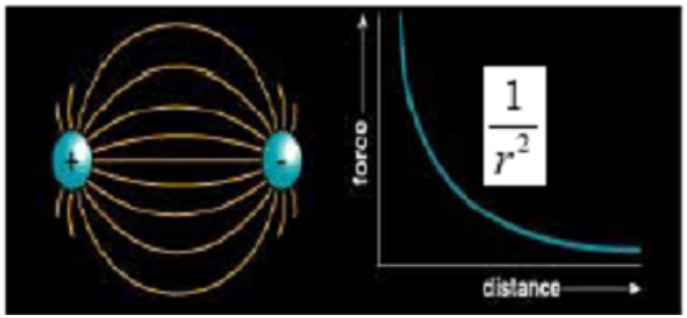
QCD vs QED

QCD versus QED

Quantum Electrodynamics (QED): The interaction is due to the exchange of photons. Every time there is an exchange of a photon there is a correction in the interaction of the order of 0.01.

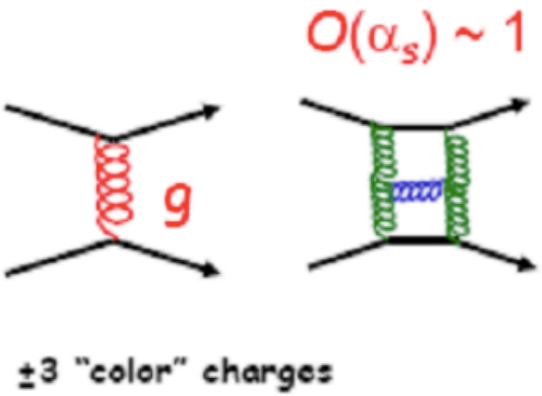
→ we can apply perturbation theory reaching whatever accuracy we like

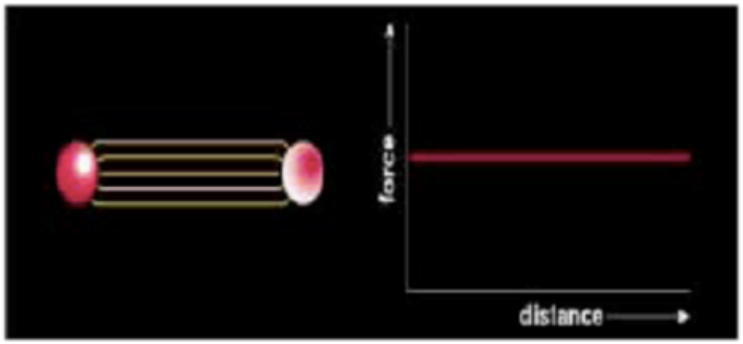




QCD: Interaction due to exchange of gluons. In the energy range of ~ 1GeV the coupling constant is ~1

→ We can no longer use perturbation theory





LATTICE QCD GENERAL

QCD on the lattice

Why Lattice QCD?

- Discrete space-time lattice acts as a non-perturbative regularization scheme with the lattice spacing a providing an ultraviolet cutoff at $\pi/a \longrightarrow$ no infinities. Furthermore, renormalized physical quantities have a finite well behaved limit as $a \longrightarrow 0$.
- Can be simulated on the computer using methods analogous to those used for Statistical Mechanics systems. These simulations allow us to calculate correlation functions of hadronic operators and matrix elements of any operator between hadronic states in terms of the fundamental quark and gluon degrees of freedom.

Like continuum QCD lattice QCD has as unknown input parameters the coupling constant α_s and the masses of the up, down, strange, charm and bottom quarks (the top quark is too short lived).
$\Longrightarrow$Lattice QCD provides a well-defined approach to calculate observables non-perturbative starting directly from the QCD Langragian.

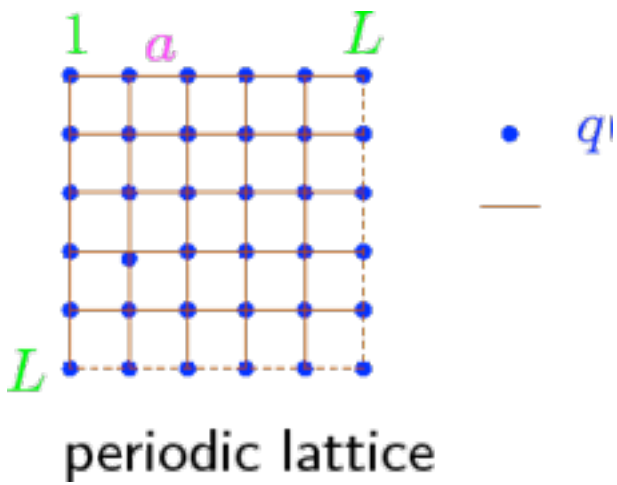
LATTICE QCD GENERAL

In lattice QCD,

fields representing quarks are defined at lattice sites (which leads to fermion doubling)

gluon fields are defined on the links connecting neighboring sites.

This approximation approaches continuum QCD as the spacing between lattice sites is reduced to zero (a = 0)



GENERAL REMARKS

The Nielsen–Ninomiya theorem

Nielsen and Ninomiya proved a theorem stating that a local, real, free fermion lattice action, having chiral and translational invariance, necessarily has fermion doubling. The only way to get rid of the doublers is by violating one of the presuppositions of the theorem —for example:

- Wilson fermions explicitly violate chiral symmetry, giving an infinitely high mass to the doublers which then decouple.
- So-called "perfect lattice fermions" have a nonlocal action.
- Staggered fermions
- Twisted mass fermions
- Ginsparg–Wilson fermions
- Domain wall fermions
- Overlap fermions

Lattice QCD predicts that confined quarks will become released to quark-gluon plasma around energies of 170 MeV. Monte Carlo methods are free from the sign problem when applied to the case of QCD with gauge group SU(2) (QC_2D).

Lattice QCD has already made successful contact with many experiments. For example the mass of the proton has been determined theoretically with an error of less than 2 percent.

GENERAL REMARKS

Chiral symmetry at non-zero lattice spacing is realized if the Ginsparg-Wilson relation is satisfied

$$D\gamma_5 + \gamma_5 D = aD\gamma_5 D.$$

This amounts to adding a contact term that vanishes in the continuum limit.
Using D we can define a chiral rotation which reduces to the continuum one as $a \to 0$

$$\psi' = e^{i\theta\gamma_5\left(1-\frac{a}{2}D\right)}\psi, \quad \bar{\psi}' = \bar{\psi}' e^{i\theta\left(1-\frac{a}{2}D\gamma_5\right)}$$

leaving $L(\bar{\psi}, \psi) = \bar{\psi} D \psi$ invariant.
Explicit construction of D is provided by:

- Overlap operator:

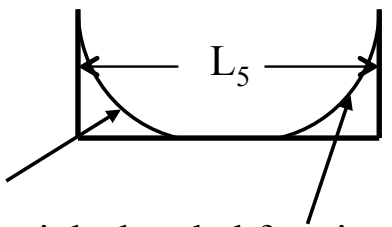
$$D_{ov} = \frac{1}{a}\left[1 - \frac{A}{\sqrt{A^\dagger A}}\right], \quad A = 1 - aD_W$$

  where D_W is the massless Wilson-Dirac operator.
  The main drawback is that its expensive.

- Domain wall operator is defined on a 5-D lattice:

$$D_{DW}(n_1, s_1; n_2, s_2) = \delta_{s_1,s_2} D_W(n_1; n_2) + \delta_{n1,n_2} D_{DW5}(s_1; s_2)$$

  where s_1, s_2 denote the fifth direction. D_W is the 4-D Wilson Dirac operator.
  The link variables are define in 4-D as before and the operator D_{DW5} act in the 5th direction.
  Left and right handed fermions live on the opposite boundaries of the fifth dimension



NUMERICAL PATH INTEGRAL

$$\langle x_{\rm f}|\, {\rm e}^{-\tilde{H}(t_{\rm f}-t_{\rm i})}\, |x_{\rm i}\rangle = \int \mathcal{D}x(t)\, {\rm e}^{-S[x]}. \qquad (1)$$

Here the $\int \mathcal{D}x(t)$ designates a sum over all possible particle paths

$$\{x(t) \quad \text{for} \quad t = t_{\rm i} \to t_{\rm f}\} \qquad (2)$$

with

$$x(t_{\rm i}) = x_{\rm i} \qquad x(t_{\rm f}) = x_{\rm f}. \qquad (3)$$

The hamiltonian is $\tilde{H}$, and $S[x]$ is the classical action,

$$S[x] \equiv \int_{t_{\rm i}}^{t_{\rm f}} dt\, L(x,\dot{x}) \equiv \int_{t_{\rm i}}^{t_{\rm f}} dt\, \left[\frac{m\,\dot{x}(t)^2}{2} + V(x(t))\right], \qquad (4)$$

For details click here

NUMERICAL PATH INTEGRAL

Knowledge of the propagator, Eq. (1), as a function of $x_\mathrm{i}, t_\mathrm{i}, x_\mathrm{f}, t_\mathrm{f}$ gives us complete information about the quantum theory. For example, we can easily determine the groundstate energy and wavefunction. Setting

$$x_\mathrm{i} = x_\mathrm{f} \equiv x \qquad t_\mathrm{f} - t_\mathrm{i} \equiv T, \tag{5}$$

the propagator can be rewritten

$$\langle x|\, \mathrm{e}^{-\tilde{H}T}\, |x\rangle = \sum_n \langle x|\, E_n\rangle\, \mathrm{e}^{-E_n T}\, \langle E_n|\, x\rangle \tag{6}$$

where $|E_n\rangle$ is the energy eigenstate with eigenvalue E_n. The sum is dominated by the lowest-energy states when T is large, because of the exponentials, and in the limit of very large T only the groundstate, $|E_0\rangle$, contributes:

$$\langle x|\, \mathrm{e}^{-\tilde{H}T}\, |x\rangle \overset{T\to\infty}{\longrightarrow} \mathrm{e}^{-E_0 T}\, |\langle x|\, E_0\rangle|^2 . \tag{7}$$

We extract the groundstate energy E_0 by integrating over x,

$$\int dx\, \langle x|\, \mathrm{e}^{-\tilde{H}T}\, |x\rangle \overset{T\to\infty}{\longrightarrow} \mathrm{e}^{-E_0 T}, \tag{8}$$

and then, going back to the previous equation, we determine the groundstate wavefunction $\psi_{E_0}(x) \equiv \langle x|\, E_0\rangle$.

IN THE LATTICE

$$t_j = t_\mathrm{i} + j\,a \qquad \text{for } j = 0, 1 \ldots N \tag{9}$$

where a is the grid spacing,

$$a \equiv \frac{t_\mathrm{f} - t_\mathrm{i}}{N}. \tag{10}$$

Then a path is described by a vector of numbers,

$$x = \{x(t_0), x(t_1) \ldots x(t_N)\}. \tag{11}$$

It is common practice to refer to such a path as a "configuration". The integral over all paths in this approximation becomes an ordinary integral over all possible values for each of the $x(t_j)$'s: that is,

$$\int \mathcal{D}x(t) \to A \int_{-\infty}^{\infty} dx_1\, dx_2 \ldots dx_{N-1} \tag{12}$$

IN THE LATTICE

The second issue we must address concerns the evaluation of the action given only a discretized path $\{x_j\}$. Focusing just on the contribution from $t_j \le t \le t_{j+1}$, the obvious approximation is

$$\int_{t_j}^{t_{j+1}} dt\, L \;\approx\; a\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{a}\right)^2 + \frac{1}{2}\left(V(x_{j+1})+V(x_j)\right)\right] \tag{15}$$

With this approximation, our numerical representation of the path integral is complete, and we have an approximate expression for the quantum mechanical propagator: for example,

$$\langle x|\, \mathrm{e}^{-\tilde{H}T}\, |x\rangle \approx A \int_{-\infty}^{\infty} dx_1 \ldots dx_{N-1}\, \mathrm{e}^{-S_{\mathrm{lat}}[x]} \tag{16}$$

where

$$S_{\mathrm{lat}}[x] \equiv \sum_{j=0}^{N-1}\left[\frac{m}{2a}(x_{j+1}-x_j)^2 + aV(x_j)\right], \tag{17}$$

$x_0 = x_N = x$, and $a = T/N$. We have reduced quantum mechanics to a problem in numerical integration.

IN THE LATTICE

$$\langle\langle x(t_2)x(t_1)\rangle\rangle \equiv \frac{\int \mathcal{D}x(t)\, x(t_2)x(t_1)\, \mathrm{e}^{-S[x]}}{\int \mathcal{D}x(t)\, \mathrm{e}^{-S[x]}} \tag{21}$$

$$\int dx\, \langle x|\, \mathrm{e}^{-\tilde{H}(t_\mathrm{f}-t_2)}\, \tilde{x}\, \mathrm{e}^{-\tilde{H}(t_2-t_1)}\, \tilde{x}\, \mathrm{e}^{-\tilde{H}(t_1-t_\mathrm{i})}\, |x\rangle\,. \tag{22}$$

Setting $T = t_\mathrm{f} - t_\mathrm{i}$ and $t = t_2 - t_1$ we can rewrite the full expression as

$$\langle\langle x(t_2)x(t_1)\rangle\rangle = \frac{\sum \mathrm{e}^{-E_n T}\, \langle E_n|\, \tilde{x}\, \mathrm{e}^{-(\tilde{H}-E_n)t}\, \tilde{x}\, |E_n\rangle}{\sum \mathrm{e}^{-E_n T}}. \tag{23}$$

If $T \gg t$ and large, then the groundstate $|E_0\rangle$ dominates the sums and

$$G(t) \equiv \langle\langle x(t_2)x(t_1)\rangle\rangle \to \langle E_0|\, \tilde{x}\, \mathrm{e}^{-(\tilde{H}-E_0)t}\, \tilde{x}\, |E_0\rangle\,. \tag{24}$$

In our harmonic oscillator example, the state propagating between the two $\tilde{x}$'s cannot be $|E_0\rangle$ since $\tilde{x}$ switches the parity of the state. Thus if we now make t large (but still $\ll T$)

$$G(t) \overset{t\ \text{large}}{\longrightarrow} |\langle E_0|\, \tilde{x}\, |E_1\rangle|^2\, \mathrm{e}^{-(E_1-E_0)t} \tag{25}$$

IN THE LATTICE

$$\log(G(t)/G(t+a)) \to (E_1 - E_0)a, \tag{26}$$

In principle, path integral averages $\langle\langle \Gamma[x] \rangle\rangle$ of arbitrary functionals $\Gamma[x]$ can be used to compute any physical property of the excited states in the quantum theory. Also we note in passing that

$$\langle\langle \Gamma[x] \rangle\rangle = \frac{\sum \mathrm{e}^{-E_n T} \langle E_n | \Gamma[\tilde{x}] | E_n \rangle}{\sum \mathrm{e}^{-E_n T}} \tag{27}$$

becomes a (quantum mechanical) thermal average if we replace

$$T \to \beta \equiv 1/k_B T_{\mathrm{temp}}. \tag{28}$$

Thus any computer code designed to compute path integral averages can be used for thermal physics as well. Here we focus on the zero-temperature limit of large T.

MONTECARLO CALCULATIONS

$$\langle\langle \Gamma[x] \rangle\rangle = \frac{\int \mathcal{D}x(t)\, \Gamma[x]\, \mathrm{e}^{-S[x]}}{\int \mathcal{D}x(t)\, \mathrm{e}^{-S[x]}}, \tag{29}$$

is a weighted average over paths with weight $\exp(-S[x])$, we generate a large number, N_{cf}, of random paths or configurations,

$$x^{(\alpha)} \equiv \{x_0^{(\alpha)} x_1^{(\alpha)} \dots x_{N-1}^{(\alpha)}\} \qquad \alpha = 1, 2 \dots N_{\mathrm{cf}}, \tag{30}$$

Text

on our grid in such a way that the probability $P[x^{(\alpha)}]$ for obtaining any particular path $x^{(\alpha)}$ is

$$P[x^{(\alpha)}] \propto \mathrm{e}^{-S[x^{(\alpha)}]}. \tag{31}$$

Then an unweighted average of $\Gamma[x]$ over this set of paths approximates the weighted average over uniformly distributed paths:

$$\langle\langle \Gamma[x] \rangle\rangle \approx \overline{\Gamma} \equiv \frac{1}{N_{\mathrm{cf}}} \sum_{\alpha=1}^{N_{\mathrm{cf}}} \Gamma[x^{(\alpha)}]. \tag{32}$$

MONTECARLO UNCERTAINTIES

$$\sigma^2_{\overline{\Gamma}} \approx \frac{1}{N_{\rm cf}} \left\{ \frac{1}{N_{\rm cf}} \sum_{\alpha=1}^{N_{\rm cf}} \Gamma^2[x^{(\alpha)}] - \overline{\Gamma}^2 \right\}. \tag{33}$$

This becomes

$$\sigma^2_{\overline{\Gamma}} = \frac{\langle\langle \Gamma^2 \rangle\rangle - \langle\langle \Gamma \rangle\rangle^2}{N_{\rm cf}} \tag{34}$$

for large $N_{\rm cf}$. Since the numerator in this expression is independent of $N_{\rm cf}$ (in principle, it can be determined directly from quantum mechanics), the statistical uncertainties vanish as $1/\sqrt{N_{\rm cf}}$ when $N_{\rm cf}$ increases.

METROPOLIS HASTINGS

Metropolis Algorithm

We need an algorithm to to create our set of random paths $x^{(\alpha)}$ with probability $\frac{e^{-S[x]}}{Z}$, where $Z = \int \mathcal{D}[x(t)] e^{-S[x]}$.

$\Longrightarrow$ a simple procedure, though not always the best, is the Metropolis Algorithm:

- Start with an arbitrary path $x^{(0)}$
- Modify by visiting each of the sites on the lattice, and randomizing the x_j's at those sites, one at a time, in a particular fashion as described below $\longrightarrow$ generate a new random path from the old one: $x^{(0)} \longrightarrow x^{(1)}$. This is called "updating" the path.
- Apply to $x^{(1)}$ to generate path $x^{(2)}$, and so on until we have N_{cf} random paths.

The algorithm for randomizing x_j at the j^{th} site is:

- Generate a random number $-\epsilon < \zeta \leq \epsilon$, with uniform probability;
- Let $x_j \longrightarrow x_j + \zeta$ and compute the change ΔS in the action;
- If $\Delta S < 0$ retain the new value for x_j, and proceed to the next site;
- If $\Delta S > 0$ accept change with probability $\exp(-\Delta S)$ i.e. generate a random number η uniformly distributed between 0 and 1; retain the new value for x_j if $\exp(-\Delta S) > \eta$, otherwise restore the old value; proceed to the next site.

Comments:

- Choice of ϵ: should be tuned so that 40%–60% of the x_j's are changed on each pass (or "sweep") through the lattice. Then ϵ is of order the typical quantum fluctuations expected in the theory. Whatever the ϵ, successive paths are going to be quite similar and so contain rather similar information about the theory. Thus when we accumulate random paths $x^{(\alpha)}$ for our Monte Carlo estimates we should keep only every N_{cor}-th path; the intervening sweeps erase correlations, giving us configurations that are statistically independent. The optimal value for N_{cor} depends upon the theory, and can be found by experimentation. It also depends on the lattice spacing a.
- Initial configuration: Guess the first configuration $\longrightarrow$ discard some number of configurations at the beginning, before starting to collect $x^{(\alpha)}$'s. This is called "thermalizing the lattice."

RANDOMIZING ALGORITHM

The algorithm for randomizing x_j at the j^{th} site is:

- generate a random number ζ, with probability uniformly distributed between $-\epsilon$ and ϵ for some constant ϵ;
- replace $x_j \to x_j + \zeta$ and compute the change ΔS in the action caused by this replacement (generally only a few terms in the lattice action involve x_j, since lagrangians are local; only these need be examined);
- if $\Delta S < 0$ (the action is reduced) retain the new value for x_j, and proceed to the next site;
- if $\Delta S > 0$ generate a random number η unformly distributed between 0 and 1; retain the new value for x_j if $\exp(-\Delta S) > \eta$, otherwise restore the old value; proceed to the next site.

STATISTICAL ERRORS

An important part of any Monte Carlo analysis is the estimate of the statistical errors.

- **The "statistical bootstrap," method:**
  The bootstrap procedure provides new, almost *zero-cost* random ensembles of measurements by synthesizing them from the original ensemble of N_{cf} measurements.

  Consider an ensemble $\{G^{(\alpha)}, \alpha = 1 \ldots N_{cf}\}$ of Monte Carlo measurements

  - Construct a "bootstrap copy" of that ensemble by selecting $G^{(\alpha)}$'s at random from the original ensemble, taking N_{cf} in all while allowing duplications and omissions
    $\rightarrow$ resulting ensemble of G's may have two or three copies of some $G^{(\alpha)}$'s, and no copies of others
  - Use new ensemble to obtain a new estimate of some the quantity of interest.
  - Repeat this procedure to generated as many bootstrap copies of the original ensemble as one wishes, and from each we can generate a new estimate.

  The distribution of these estimates approximates the distribution of the quantity that would have been obtained from the original Monte Carlo, and so can be used to estimate the statistical error in our original estimate.
- **The "Jackknife" method:** Similar to boostrap but remove a set of measurements at a time from the sample set. In general easier to use than boostrap.
- **The "binning" method:**
  At the end of a simulation we have set of configurations $x^{(\alpha)}$, and for each a set of measurements like $G^{(\alpha)}$, our propagator. We partially average or bin the measurements: For example, instead of storing each of

  $$G^{(1)} \quad G^{(2)} \quad G^{(3)} \quad G^{(4)} \quad G^{(5)} \ldots$$

  we might instead store

  $$\overline{G}^{(1)} \equiv \frac{G^{(1)} + G^{(2)} + G^{(3)} + G^{(4)}}{4} \qquad \overline{G}^{(2)} \equiv \frac{G^{(5)} + G^{(6)} + G^{(7)} + G^{(8)}}{4} \qquad \ldots$$

  Binning reduces or can even remove the effects of correlations between different configurations.

METROPOLIS HASTINGS

The following snippet is in Python. You should go to www.python.org and install python if you don't have it already installed. Or even better.: You should get pyROOT.

```
def update(x):
    for j in range(0,N):
        old_x = x[j]                          # save original value
        old_Sj = S(j,x)
        x[j] = x[j] + uniform(-eps,eps)       # update x[j]
        dS = S(j,x) - old_Sj                  # change in action
        if dS > 0 and exp(-dS) < uniform(0,1):
            x[j] = old_x                      # restore old value

def S(j,x):          # harm. osc. S
    jp = (j+1) % N   # next site
    jm = (j-1) % N   # previous site
    return a*x[j]**2/2 + x[j]*(x[j]-x[jp]-x[jm])/a
```

Python code for one Metropolis update of path $\{x_j\ , j = 0 \ldots N-1\}$. The path is stored in array x[j]. Function S(j,x) returns the value of the part of the action that depends on x_j . Function uniform(a,b) returns a random number between a and b. A sample S(j,x) is shown, for a harmonic oscillator with $x_N = x_0$.

STATISTICAL ERRORS

```
def bootstrap(G):
    N_cf = len(G)
    G_bootstrap = []                    # new ensemble
    for i in range(0,N_cf):
        alpha = int(uniform(0,N_cf))    # choose random config
        G_bootstrap.append(G[alpha])    # keep G[alpha]
    return G_bootstrap
```

code for producing a bootstrap copy of an ensemble of measurements G. The original ensemble consists of individual measurements G[alpha], one for each configuration. The function bootstrap(G) returns a single bootstrap copy of ensemble G, consisting of N cf measurements. Function uniform(a,b) returns a random number between a and b.

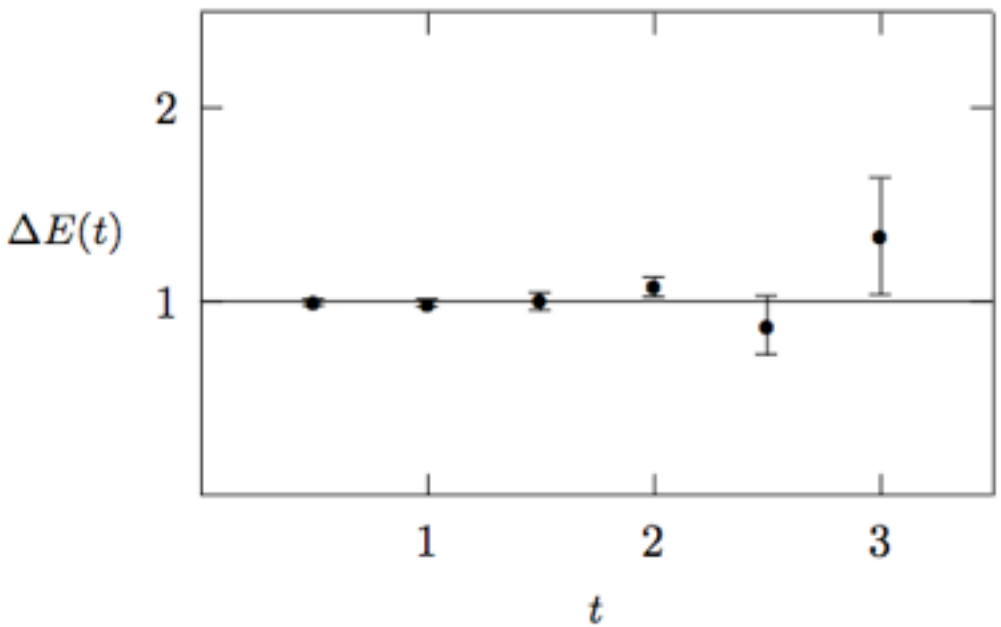
```
def bin(G,binsize):
    G_binned = []                       # binned ensemble
    for i in range(0,len(G),binsize):   # loop on bins
        G_avg = 0
        for j in range(0,binsize):      # loop on bin elements
            G_avg = G_avg + G[i+j]
        G_binned.append(G_avg/binsize)  # keep bin avg
    return G_binned
```

code for producing a binned copy of an ensemble of measure- ments G. The original ensemble consists of individual measurements G[alpha], one for each configuration. The function bin(G,binsize) bins the ensemble into bins of size binsize, averages the G's within each bin, and returns an ensemble consisting of the averages.

CODE TO RUN

Run the code Lattice_Simulation.py
in order to run it

python Lattice_Simulation.py



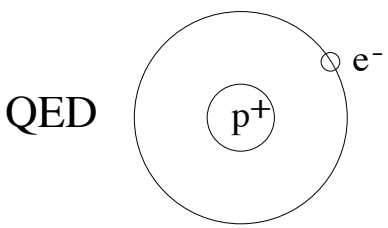
Results are for a one dimensional lattice with N = 20 sites, lattice spacing a = 1/2, and Ncf = 1000 configurations, keeping configurations only every Ncor = 20 sweeps. The Metropolis step size eps was 1.4, resulting in a Metropolis acceptance ratio of 0.5.

SUMMARY

QCD vs QED

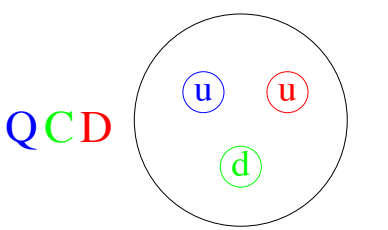
QCD versus QED

- QCD is the theory of strong interactions formulated in terms of quarks and gluons as the basic degrees of freedom of hadronic matter.
- Conventional perturbative approach cannot be applied for hadronic process at scales $\lesssim$ 1 GeV since the strong coupling constant $\alpha_s \sim 1$
  $\Longrightarrow$ we cannot calculate the masses of mesons and baryons from QCD even if we are given α_s and the masses of quarks.
- Bound state in QCD very different from QED e.g. the binding energy of a hydrogen atom is to a good approximation the sum of it constituent masses. Similarly for nuclei the binding energy is $\mathcal{O}(\mathrm{MeV})$. For the proton almost all the mass is attributed to the strong non-linear interactions of the gluons.



$M_e = 0.5$ MeV
$M_p = 938$ MeV
$E_{\text{binding}} = 13.6$ eV

Hydrogen Atom (EM force)



$M_u \sim 3$ MeV
$M_d \sim 6$ MeV
$M_p = 938$ MeV

Proton (Strong force)