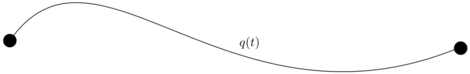
Introduction to Lattice QCD

J. N. Guenther

October 4th 2021 to October 8th 2021

The path integral quantization: from M to QM

Mechanics:



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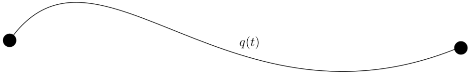
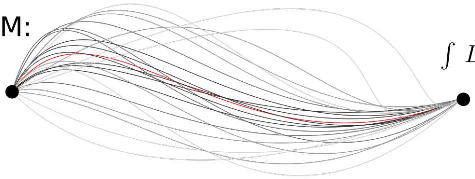


QM:



$$\int Dq(t)e^{\mathrm{i}\int \mathrm{d}t\, L}$$

The path integral quantization: from M to QM

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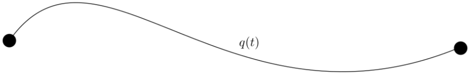

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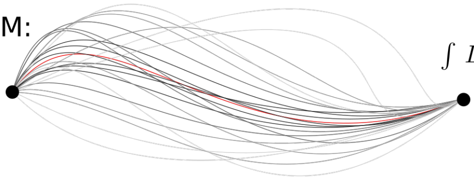
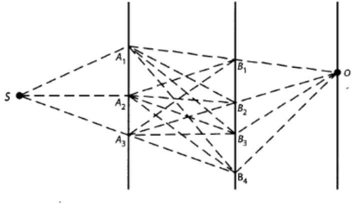


$$\int Dq(t) e^{\mathrm{i} \int \mathrm{d}t\, L}$$

Anecdote of Feynman:



[A. Zee]

The Pathintegral of QM

QM Amplitude:

$$\langle q_F | e^{-\mathrm{i}HT} | q_F \rangle \stackrel{T=N\cdot\delta t}{=} \langle q_F | e^{-\mathrm{i}H\delta t} \underbrace{1}_{\int \mathrm{d}q |q\rangle\langle q|} e^{-\mathrm{i}H\delta t} \underbrace{1}_{\int \mathrm{d}q |q\rangle\langle q|} \dots \underbrace{1}_{\int \mathrm{d}q |q\rangle\langle q|} e^{-\mathrm{i}H\delta t} | q_F \rangle$$

$$= \left(\prod_{j=1}^{N-1} \int \mathrm{d}q_j \right) \langle q_F | e^{-\mathrm{i}H\delta t} | q_{N-1} \rangle \langle q_{N-1} | e^{-\mathrm{i}H\delta t} | q_{N-2} \rangle \dots \langle q_2 | e^{-\mathrm{i}H\delta t} | q_1 \rangle \langle 1 | e^{-\mathrm{i}H\delta t} | q_I \rangle$$

For one Amplitude and $H = \frac{\hat{p}^2}{2m}$

$$\langle q_{j+1} | e^{-\mathrm{i}\frac{\hat{p}^2}{2m}\delta t} | q_j \rangle \stackrel{\int \frac{\mathrm{d}p}{2\pi} |p\rangle\langle p| = 1}{=} \int \frac{\mathrm{d}p}{2\pi} \langle q_{j+1} | e^{-\mathrm{i}\frac{\hat{p}^2}{2m}\delta t} | p \rangle \langle p | q_j \rangle$$

$$= \int \frac{\mathrm{d}p}{2\pi} e^{-\mathrm{i}\frac{p^2}{2m}\delta t} \langle q_{j+1} | p \rangle \langle p | q_j \rangle = \frac{\mathrm{d}p}{2\pi} e^{-\mathrm{i}\frac{p^2}{2m}\delta t} e^{\mathrm{i}p(q_{j+1}-q_j)}$$

$$\stackrel{\text{Gaußintegral}}{=} \left(\frac{\mathrm{i}m}{2\pi\delta t} \right)^{\frac{1}{2}} e^{i\frac{(q_{j+1}-q_j)^2 m}{2\delta t}}$$

The Pathintegral of QM II

Combining the Amplitudes:

$$\langle q_F|e^{-\mathrm{i}HT}|q_F\rangle = \left(-\frac{\mathrm{i}m}{2\pi\delta t}\right)^{\frac{N}{2}}\left(\prod_{j=0}^{N-1}\int \mathrm{d}q_j\right) e^{\mathrm{i}\frac{\delta t m}{2}\sum_{j=1}^{N-1}\left(\frac{q_{j+1}-q_j}{\delta t}\right)^2}$$

Now one could start a Lattice QM simulation or take the continuum limit:

$$\delta t \longrightarrow 0$$

$$\frac{q_{j+1}-q_j}{\delta t} \longrightarrow \dot{q}$$

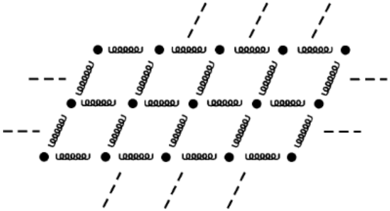
$$\delta t\sum_{j=0}^{N-1} \longrightarrow \int_0^T \mathrm{d}t$$

Definition:

$$\int \mathcal{D}q(t) = \lim_{N\to\infty}\left(\frac{-\mathrm{i}m}{2\pi\delta t}\right)^{\frac{N}{2}}\prod_{j=0}^{N-1}\int \mathrm{d}q_j$$

$$\langle q_F|e^{-\mathrm{i}HT}|q_F\rangle = \int \mathcal{D}q(t)e^{\mathrm{i}\int_0^T \mathrm{d}t\frac{1}{2}m\dot{q}^2} = \int \mathcal{D}q(t)e^{\mathrm{i}\int_0^T \mathrm{d}tL} = \int \mathcal{D}q(t)e^{\mathrm{i}S}$$

From QM to QFT



Going to the continuum:

$$q \longrightarrow \varphi$$
$$a \longrightarrow \vec{x}$$
$$q_a \longrightarrow \varphi(t, \vec{x}) = \varphi(x)$$
$$\sum_a \longrightarrow \int \mathrm{d}^4 x$$

Going to many particles that interact with some potential:

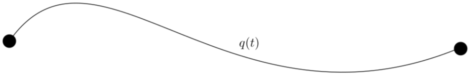
$$S(q) = \int_0^T \mathrm{d}t \left(\sum_a \frac{1}{2} m \dot{q}_a^2 - V(q_1, q_2, \dots) \right)$$

Path integral of $d = (D+1)$ dimensional scalar field theory:

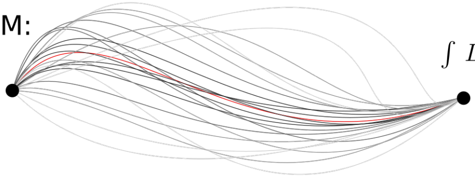
$$Z = \int D\varphi e^{\mathrm{i} \int \mathrm{d}^d x \left(\frac{1}{2} \partial_\mu \varphi \partial^\mu \varphi - V(\varphi) \right)}$$
$$= \int D\varphi e^{\mathrm{i} \int \mathrm{d}^d x \mathcal{L}}$$
$$= \int D\varphi e^{\mathrm{i}S}$$

The path integral quantization: from M to QM to QFT

Mechanics:



QM:



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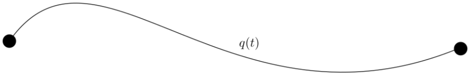
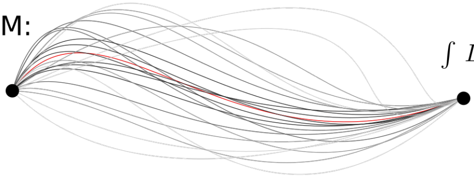
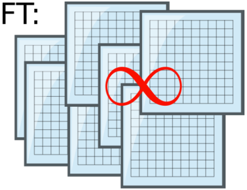


QM:

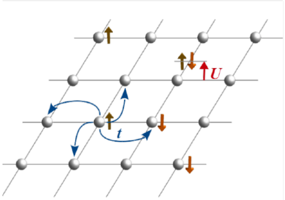


$$\int Dq(t)e^{\mathrm{i}\int \mathrm{d}t\, L}$$

QFT:

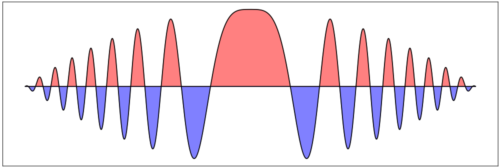


$$\int \mathcal{D}\phi(x)e^{\mathrm{i}\int \mathrm{d}^4x\mathcal{L}}$$



Wick rotation

$e^{\mathrm{i}S}$ is an oscillating function
($e^{\mathrm{i}x} = \cos(x) + \mathrm{i}\sin(x)$)
This has a sign problem!



Solution:
Go from Minkowski space to Euclidean space. This a called a *Wick rotation*.

$$t \longrightarrow \mathrm{i}\tau$$

$$\int D\varphi e^{\mathrm{i}S} \longrightarrow \int D\varphi e^{-S}$$

Price to pay: Some quantities (like real time) become very hard to access.

The QCD Lagrangian

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a_{\mu\nu} F^{a,\mu\nu} + \overline{\psi} \left(\mathrm{i}\gamma_\mu D^\mu - m \right) \psi$$

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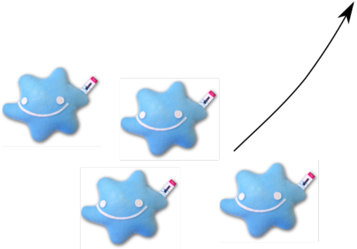

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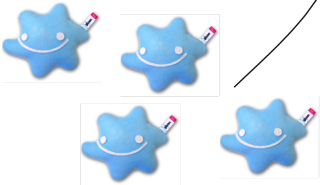

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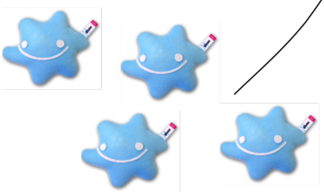


Observables in Lattice QCD

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}[U]\mathcal{D}\bar{\psi}\mathcal{D}\psi \mathcal{O} e^{-S_F - S_G}}{\int \mathcal{D}[U]\mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-S_F - S_G}} = \frac{1}{Z}\int \mathcal{D}[U]\mathcal{D}\bar{\psi}\mathcal{D}\psi \mathcal{O} e^{-S_F[\psi,U] - S_G[U]}$$

Fermions are represented by Grassmann variables: $\psi\overline{\psi} = -\overline{\psi}\psi$

$$\int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-S_F} = \det M[\psi, U]$$

M is the fermion matrix (sorry, no time for the derivation). This leaves us with:

$$\langle \mathcal{O} \rangle = \frac{1}{Z}\int \mathcal{D}[U]\mathcal{O} \det[M] e^{-S_G}$$

The calculation of the fermion determinent M has to be redone everytime the gauge fields change. This is computationally very expensive. If one ingnores the dependence of M on the gauge fields one end up with so called *Quenched QCD*.

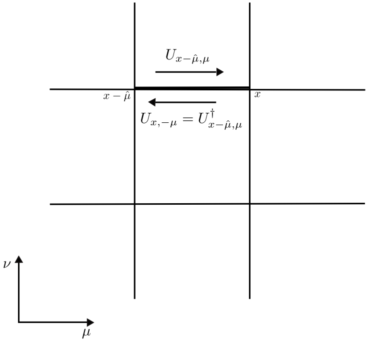
Link variables

In the continuum:

$$\mathcal{L} = -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu}$$

with

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu - \mathrm{i}g[A_\mu, A_\nu]$$

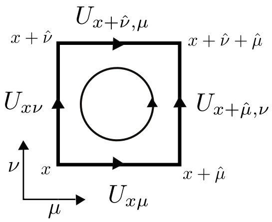


On the lattice instead of the fields A one uses the link variables U. They relate to the continuum A:

$$U_{x\mu} = e^{\mathrm{i}gA_{x\mu}}, \quad U_{x\mu} \in SU(3), \quad (\det U = 1, \; U^{-1} = U^\dagger)$$

Lattice gauge action (unimproved Wilson)

The field strength tensor describes the infinitesimal change of the fields per area, if they are transported in an infinitesimal circle. Due to the discrete nature of the lattice there cannot be an object like an infinitesimal circle. Instead one uses a plaquette, which is the smallest square on the lattice.



Plaquette:

$$U_{x,\mu\nu} = U_{x\mu} U_{x+\hat{\mu},\nu} U^{\dagger}_{x+\hat{\nu},\mu} U^{\dagger}_{x\nu}$$

The gauge action:

$$S[U] = \frac{\beta}{3} \sum_{x} \sum_{\mu<\nu} \Re \operatorname{tr}(1 - U_{x,\mu\nu})$$

From lattice and continuum

Starting from the plaquette:

$$U_{x,\mu\nu} = U_{x\mu} U_{x+\hat{\mu},\nu} U^{\dagger}_{x+\hat{\nu},\mu} U^{\dagger}_{x\nu}.$$

To relate this with the continuum action one can Taylor expand this expression to recover the field strength tensor in equation. Since the gauge fields do not commute with each other on has to make use of the Baker-Cambell-Hausdorff-formula

$$e^{A} e^{B} = e^{A+b+\frac{1}{2}[A,B]+\cdots}$$

during this expansion.
Replacing the link variables in the plaquette with the the continuum fields yields:

$$\begin{aligned}
U_{x,\mu\nu} &= e^{\mathrm{i}gaA_{x\mu}} e^{\mathrm{i}gaA_{x+\hat{\mu},\nu}} e^{-\mathrm{i}gaA_{x+\hat{\nu},\mu}} e^{-\mathrm{i}gaA_{x\nu}} \\
&\overset{\text{BCH}}{=} e^{\mathrm{i}gaA_{x\mu}+\mathrm{i}gaA_{x+\hat{\mu},\nu}-\frac{a^2g^2}{2}[A_{x\mu},A_{x+\hat{\mu},\nu}]+\mathcal{O}(a^3)} e^{-\mathrm{i}gaA_{x+\hat{\nu},\mu}-\mathrm{i}gaA_{x\nu}-\frac{a^2g^2}{2}[A_{x+\hat{\nu},\mu},A_{x\nu}]+\mathcal{O}(a^3)} \\
&\overset{\text{BCH}}{=} \exp\Big(\mathrm{i}gaA_{x\mu} + \mathrm{i}gaA_{x+\hat{\mu},\nu} - \mathrm{i}gaA_{x+\hat{\nu},\mu} - \mathrm{i}gaA_{x\nu} + \frac{a^2g^2}{2}(-[A_{x+\hat{\nu},\mu}, A_{x\nu}] - [A_{x\mu}, A_{x+\hat{\mu},\nu}] \\
&\quad +[A_{x\mu}, A_{x+\hat{\nu},\mu}] + [A_{x\mu}, A_{x\nu}] + [A_{x+\hat{\mu},\nu}, A_{x+\hat{\nu},\mu}] + [A_{x+\hat{\mu},\nu}, A_{x\nu}]) + \mathcal{O}(a^3)\Big)
\end{aligned}$$

From lattice and continuum II

The A fields themselves can now be expanded in a as

$$A_{x+\hat{\mu},\nu} = A_{x\nu} + a\partial_\mu A_{x\nu} + \mathcal{O}(a^2).$$

This results in the expression

$$\begin{aligned} U_{x,\mu\nu} &= e^{\mathrm{i}a^2 g(\partial_\mu A_{x\nu} - \partial_\nu A_{x\mu} + ig[A_{x\mu}, A_{x\nu}]) + \mathcal{O}(a^3)} \\ &= e^{\mathrm{i}a^2 g F_{\mu\nu}} \end{aligned}$$

for the plaquette. Another expansion in a^2 yields

$$U_{x,\mu\nu} = 1 + \mathrm{i}a^2 g F_{\mu\nu} - \frac{a^4 g^2}{2} (F_{\mu\nu})^2 + \mathcal{O}(a^6)$$

Taking the real part removes the a^2 term.
Looking at higher order terms can allow for other construction where some higher order terms are cancelled. This leads to improved gauge actions.

QCD Thermodynamics

Aim: Defining a temperature T.
The partition sum of a QM systhem compared to the path integral:

$$Z(T) = \mathrm{tr}\left(e^{-\frac{\hat{H}}{k_B T}}\right) = \mathrm{tr}\left(e^{-\beta\hat{H}}\right) \quad Z = \int \mathcal{D}[U]\mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-S}$$

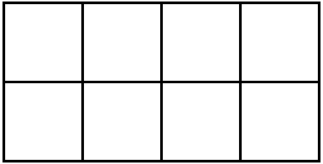
with $\beta = \frac{1}{T}$ and $k_B = 1$. The trace demands periodicity (up to a phase factor) in the time direction. The bosonic fields are periodic in time while the fermionic fields are antiperiodic. This allows to identify the temporal extent of the lattice aN_t with the inverse temperature

$$aN_t = \frac{1}{T} = \beta.$$

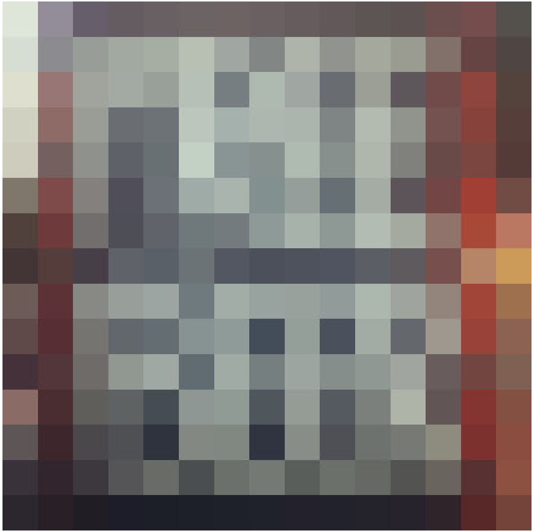
If one takes the limit $\beta \longrightarrow \infty$ at constant N_t the temperature vanishes, while if $\beta \longrightarrow 0$ the temperature rises to infinity. To keep the temperature constant while taking the continuum limit aN_t has to be constant while a goes to zero. This is achieved by keeping the ratio $\frac{N_s}{N_t}$ constant while increasing N_t and N_s to approach the continuum.

The continuum limit

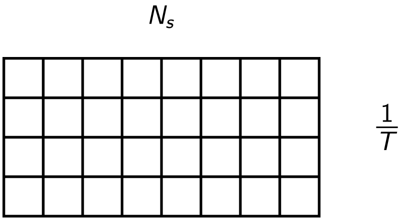
N_s



$\frac{1}{T}$



The continuum limit



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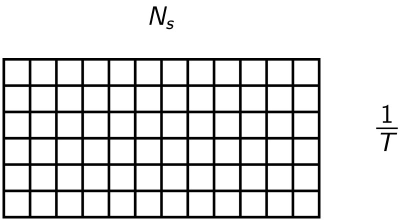
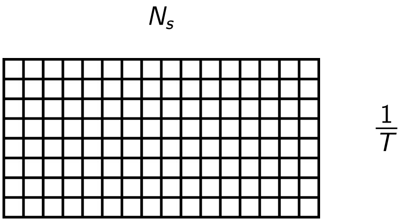


The continuum limit



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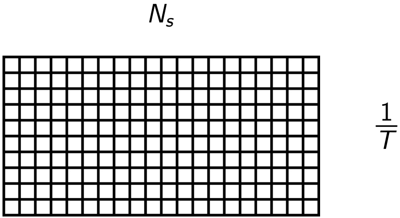

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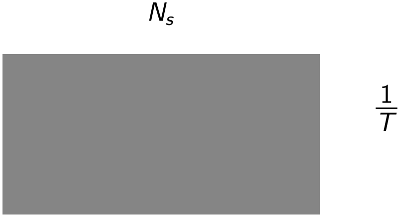
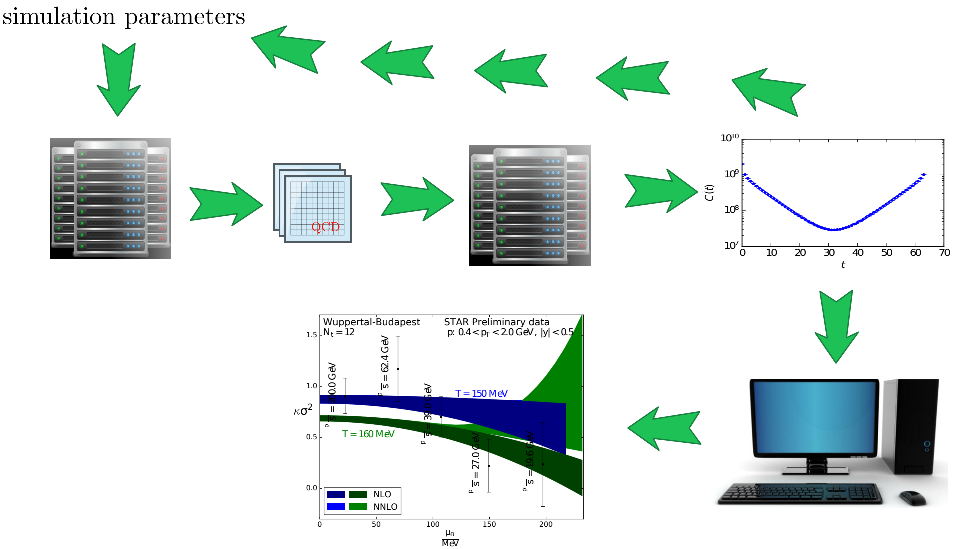


The work flow



$SU(2)$ matrices

The gauge fields U are $SU(2)$ matrices. This means:

$$U^{-1} = U^{\dagger}$$
$$\det U = 1$$

The U can be written in the form

$$X = A_4\sigma_4 + i\sum_{k=1}^{3} A_k\sigma_k$$

where σ_k are the Pauli matrices and σ_4 is the unity matrix.
Alternative:

$$U = \exp\left(\mathrm{i}\sum_{i=1}^{3} a_i\sigma_i\right)$$

```
function get_matrix(A::Array{Float64,1})
   C = zeros(ComplexF64,2,2)
   C[1,1] =  A[4] + im*A[3]
   C[1,2] =  A[2] + im*A[1]
   C[2,1] = -A[2] + im*A[1]
   C[2,2] =  A[4] - im*A[3]
   return C
end
```

$$C = \begin{pmatrix} A_4 + \mathrm{i}A_3 & A_2 + \mathrm{i}A_1 \\ -A_2 + \mathrm{i}A_1 & A_4 - \mathrm{i}A_3 \end{pmatrix}$$

Lattice and neighbor table

- 6 dimensional array
- first three components for N_s^3
- 4th component: N_t
- 5th component: direction of the gauge field
- 6th component: matrix
- initialized by unit matrix

```
function create_lattice(params::SimulationParameters)
    lattice = zeros(Float64, params.Ns, params.Ns,
    params.Ns, params.Nt,4, 4)
    lattice[:,:,:,:,:,4] .= 1.0
    return lattice
end
```

- function that tells you the next or previous lattice side
- keep periodic boundaries in tact
- often stored as a table

```
function pos(x::Int,y::Int,z::Int,t::Int,
  params::SimulationParameters)
    return [mod1(x,params.Ns), mod1(y,params.Ns),
    mod1(z,params.Ns), mod1(t,params.Nt)]
end
```

Update algorithm

Aim: Generating new configurations of U_n.
Conditions for correct configurations:

- For the transition probability $T(U'|U)$ from U to U' it has to be
$$T(U'|U) \geq 0 \quad \forall U$$
- The sum over all transition probabilities is one:
$$\sum_{U'} T(U'|U) = 1 \quad \forall U.$$
- For the probability $P(U')$ to find the systhem in the state U' it has to hold (stability condition)
$$P(U') = \sum_{U} T(U'|U)P(U).$$
- For all U and U' there is a k, so that
$$T^k(U'|U) > 0$$
(ergodicity)

Many algorithms fullfill the *Detailed-Balance-Condition* instead:

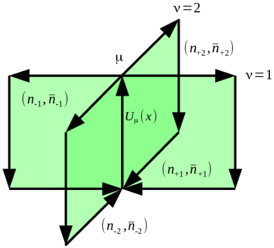
$$T(U'|U)P(U) = T(U|U')P(U')$$

Staple

$$A = \sum_{\nu \neq \mu} \left(U_{x+\hat{\mu},\nu} U_{x+\hat{\mu}+\hat{\nu},-\mu} U_{x+\hat{\nu},-\nu} + U_{x+\hat{\mu},-\nu} U_{x+\hat{\mu}-\hat{\nu},-\mu} U_{x-\hat{\nu},\nu} \right).$$

If one link variable is changed the action changes by:

$$\Delta S = -\frac{\beta}{2} \operatorname{tr}((U'_{x\mu} - U_{x\mu})A).$$



[Gagliardi:2017uag]

```
function single_statple(x::Array{Int,1}, dir::Int,
    lattice::Array{Float64,6}, p::SimulationParameters)
    A = zeros(Float64,4)
    for i in 1:4
        if i != dir
            U1 = get_U(pos(x+ev(dir),p), i,lattice)
            U2 = get_U(pos(x+ev(i),p), dir,lattice)
            U3 = get_U(x,i,lattice)
            A += mult(U1, dagger(U2), dagger(U3))
            U1 = get_U(pos(x+ev(dir)-ev(i),p), i,lattice)
            U2 = get_U(pos(x-ev(i),p), dir,lattice)
            U3 = get_U(pos(x-ev(i),p),i,lattice)
            A += mult(dagger(U1), dagger(U2), U3)
        end
    end
    return A
end
```

Metropolis algorithm

1. starting with a random configuration
2. one U matrix is changed
3. the change in the action ΔS is calculated
4. 1. $\Delta S < 0$ the new configuration is accepted
   2. a random number $r \in [0.1)$ is computed
      - if $r <= e^{-\Delta S}$ the configuration is accepted
      - if $r > e^{-\Delta S}$ the configuration is rejected
5. go back to step 2

```
function single_metropolis!(x::Array{Int,1}, dir::Int,
  lattice::Array{Float64,6}, p::SimulationParameters)
    for k in 1:8
        U = get_U(x, dir, lattice)
        X = zeros(Float64,4)
        r = rand(Float64,4) .- 0.5
        a = sqrt(sum(r[1:3].^2))
        epsilon = 0.1
        X[4] = copysign(sqrt(1-epsilon^2), r[4])
        X[1:3] = epsilon .* r[1:3] ./ a
        U_new = mult(X,U)
        A = single_statple(x,dir,lattice,p)
        delta_S = - p.beta / 2.0 * trace(mult(U_new .- U, A))
        test = rand()
        if test <= exp(-delta_S)

            set_U!(x,dir,lattice,U_new)
        end
    end
end
```

Heatbath algorithm

Create $X \in SU(2)$ as: $X = a_0\sigma_0 + i\sum_{l=1}^{3} a_l\sigma_l$
Where the a_l are random numbers drawn from a spherical distribution with radius $\sqrt{1-a_0^2}$.
a_0 is created from a distribution proprtional to $\sqrt{1-a_0^2}e^{ka_0}$:

1. Draw 4 random numbers r_1 to r_4 from a unity distribution of the interval $[0,1]$.
2. Calculate $x = -\frac{\ln(r_1)}{k}$ und $x' = -\frac{\ln(r_2)}{k}$
3. Calculate $c = \cos^2(2\pi r_3)$.
4. Calculate $a = xc$ and $\delta = x' + a$.

If $r_3^2 > 1 - \frac{\delta}{2}$ go back to step 1. Else you get: $a_0 = 1 - \delta$ and $U_{new} = XU^\dagger$

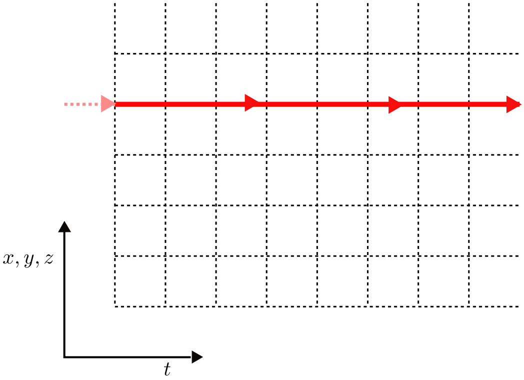
Advantage:

- Lattice is changed every time
- Smaller auto-correlation

```
function single_kennedy_pendleton!(x::Array{Int,1}, dir::Int,
 lattice::Array{Float64,6}, p::SimulationParameters)
    staple = single_statple(x,dir,lattice,p)
    k = sqrt(det(staple))
    U_bar = staple ./ k
    a = sphaeric_distribution()
    U = zeros(Float64,4)
    a_0 = a_0_kennedy_penleton(k,p)
    U[4] = a_0
    r = sqrt(1 - a_0^2)
    U[1:3] = r .* a
    set_U!(x,dir,lattice, mult(U, dagger(U_bar)))

end
```

Polyakov Loop



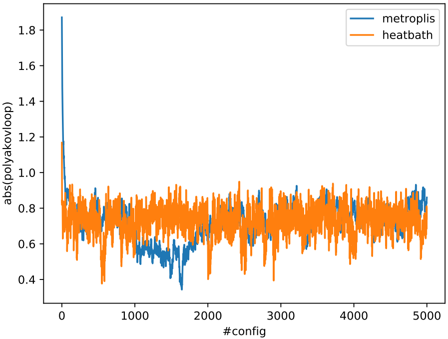
$$P(x) = \mathrm{tr}\left(\prod_{k=0}^{N_t-1} U_{x+k\hat{t},t}\right)$$

```
function single_ploop!(x::Array{Int,1}, lattice::Array{Float64,6},
        p::SimulationParameters)
    W = zeros(Float64,4)
    W[4] = 1.0
    for x[4] in 1:p.Nt
        W = mult(W,get_U(x,4,lattice))
    end
    return trace(W)
end
```

Timeseries

Things to note:

- Thermalization time
- Both algorithms give the same number
- longer auto-correlation time in Metropolis
- more jumps in Heatbath



Jack-Knife

We need a way to calculate the statistical error through out our analysis that also allows to account for correlations. Solution: Jack-Knife (or Boostrap) method

- Divide the data in N blocks. Each block should be larger than two autocorrelation times.
- Calculate the mean of the data where the kth block is missing (you end up with N mean values O_k. The error is:

$$\sigma_{\langle\mathcal{O}\rangle} = \sqrt{\frac{\left(\sum_{k=1}^{N}\mathcal{O}_k^2 - \frac{1}{N}\left(\sum_{k=1}^{N}\mathcal{O}_k\right)^2\right)(N-1)}{N}}$$

```
function createJK(C::Array{Float64,1}, NJK::Int)
    blockl = mod(length(C), NJK)
    result = ones(NJK+2)*sum(C[1:blockl*NJK])
    for i in 1:blockl*NJK
        current_block = mod((i-1), blockl+1)
        result[current_block+1] -= C[i]
    end
    result[2:NJK+1] /= blockl*(NJK-1)
    result[1] /= blockl*NJK
    error = sqrt((sum(result[2:NJK+1].^2)
        -sum(result[2:NJK+1])^2/NJK)*(NJK-1)/NJK)
    result[NJK+2] = error
    return result
end
```

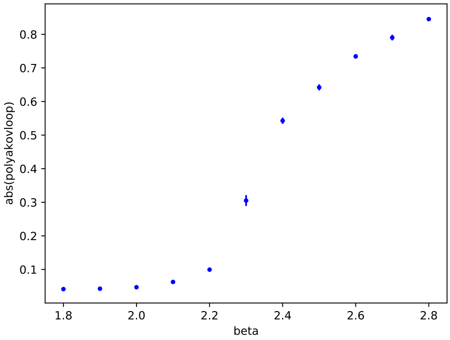
Beta scan

```
function betaScan(Ns::Int, Nt::Int, betas::Array{Float64,1}, N:
   pl = zeros(Float64,length(betas),4)

   open(@sprintf("%ix%i_ploop.dat", Ns,Nt),"w") do file

       for (i,beta) in enumerate(betas)
           println("beta = ", beta)
           pl_traj = zeros(Float64,N)
           params = SimulationParameters(Ns,Nt,beta)
           lattice = create_lattice(params)
           for k in 1:N
               kennedy_pendleton!(lattice,params)
               pl_traj[k] = ploop(lattice,params)
           end
           result = createJK(pl_traj[100:end],50)
           pl[i,1] = result[1]
           pl[i,2] = result[end]
           result2 = createJK(abs.(pl_traj[100:end]),50)
           pl[i,3] = result2[1]
           pl[i,4] = result2[end]

           println(file,@sprintf("%.2f\t%.5e\t%.5e\t%.5e\t%.5e"
       end
   end
   return pl
end
```



(phase) transitions

Finding a first order phase transition:

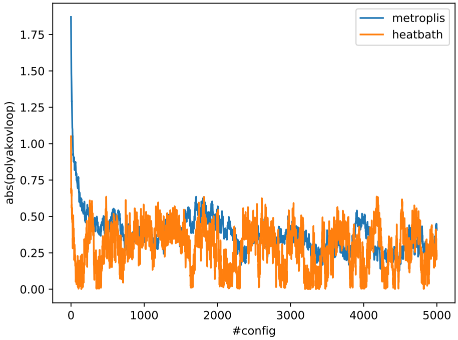
- two distinct phases are visible
- jump in order parameter becomes steeper with larger volumes
- hysteresis curve
- volume scaling of susceptibility

Finding a second order phase transition:

- critical volume scaling

Finding an analytic transition:

- slow change in order parameter
- no change with volume



Correlators and masses I

The Euclidean correlator $\langle \mathcal{O}_2(t)\mathcal{O}_1(0)\rangle_T - \langle \mathcal{O}_2\rangle\langle \mathcal{O}_1\rangle$ can be calculated as:

$$\langle \mathcal{O}_2(t)\mathcal{O}_1(0)\rangle_T = \frac{1}{Z_T}\,\mathrm{tr}\left[e^{-(T-t)\hat{H}}\mathcal{O}_2 e^{-t\hat{H}}\mathcal{O}_1\right] - \langle 0|\mathcal{O}_1|0\rangle\langle 0|\mathcal{O}_1|0\rangle$$

with

$$Z_T = \mathrm{tr}\left[e^{-T\hat{H}}\right] = \sum_n \langle n|e^{-T\hat{H}}|n\rangle = \sum_n e^{-TE_n}$$

with a complete basis $|n\rangle$ where E_n are corresponding eigenvalues/energy levels.

$$\begin{aligned}
\langle \mathcal{O}_2(t)\mathcal{O}_1(0)\rangle_T &= \frac{1}{Z_T}\,\mathrm{tr}\left[e^{-(T-t)\hat{H}}\mathcal{O}_2 e^{-t\hat{H}}\mathcal{O}_1\right] \\
&= \frac{1}{Z_T}\sum_m \langle m|e^{-(T-t)\hat{H}}\mathcal{O}_2 e^{-t\hat{H}}\mathcal{O}_1|m\rangle. \\
&= \frac{1}{Z_T}\sum_{m,n} \langle m|e^{-(T-t)\hat{H}}\mathcal{O}_2|n\rangle\langle n|e^{-t\hat{H}}\mathcal{O}_1|m\rangle \\
&= \frac{1}{Z_T}\sum_{m,n} e^{-(T-t)E_m}\langle m|\mathcal{O}_2|n\rangle e^{-tE_n}\langle n|\mathcal{O}_1|m\rangle.
\end{aligned}$$

Correlators and masses II

Plugging in Z_T:

$$\begin{aligned}\langle \mathcal{O}_2(t)\mathcal{O}_1(0)\rangle_T &= \frac{\sum_{m,n} e^{-(T-t)E_m} e^{-tE_n} \langle m|\mathcal{O}_2|n\rangle\langle n|\mathcal{O}_1|m\rangle}{\sum_n e^{-TE_n}} \\ &= \frac{e^{-tE_0} e^{-(T-t)E_0} \sum_{m,n} e^{-(T-t)(E_m-E_0)} e^{-t(E_n-E_0)} \langle m|\mathcal{O}_2|n\rangle\langle n|\mathcal{O}_1|m\rangle}{e^{-TE_0}\sum_n e^{-T(E_n-E_0)}} \\ &= \frac{\sum_{m,n} e^{-(T-t)(E_m-E_0)} e^{-t(E_n-E_0)} \langle m|\mathcal{O}_2|n\rangle\langle n|\mathcal{O}_1|m\rangle}{\sum_n e^{-T(E_n-E_0)}},\end{aligned}$$

Taking the limit $T \to \infty$ leaves only one term of the sum over m, where $E_m = E_0$. In the denominator only the first term is left. It becomes 1.

$$\langle \mathcal{O}_2(t)\mathcal{O}_1(0)\rangle = \sum_n \langle 0|\mathcal{O}_2|n\rangle\langle n|\mathcal{O}_1|0\rangle e^{-t(E_n-E_0)}.$$

Putting $E_n - E_0 = \Delta E_n$:

$$\langle \mathcal{O}_2(t)\mathcal{O}_1(0)\rangle = \sum_n \langle 0|\mathcal{O}_2|n\rangle\langle n|\mathcal{O}_1|0\rangle e^{-t\Delta E_n}$$

Correlators and masses III

$$\langle \mathcal{O}_2(t)\mathcal{O}_1(0)\rangle = \sum_n \langle 0|\mathcal{O}_2|n\rangle\langle n|\mathcal{O}_1|0\rangle e^{-t\Delta E_n}$$

For large t large ΔE_n are suppresed. The ground state E dominates. The expression is proportional to e^{-tE} with a constant C:

$$C = \langle 0|\mathcal{O}_2|0\rangle\langle 0|\mathcal{O}_1|0\rangle.$$

If one choses $\mathcal{O}_1$ and $\mathcal{O}_2$ as creation and anhiliation operators of a particle one can determen its mass by defining

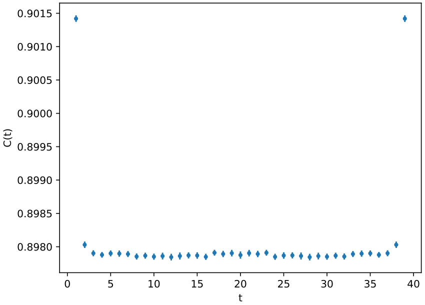
$$\Gamma_{\mathcal{O}}(t) = \sum_{t_0=0}^{N_t-1} \langle \mathcal{O}(t_0)\mathcal{O}(t_0+t)\rangle - \langle \mathcal{O}\rangle^2$$

for periodic boundary conditions this will have the form

$$\Gamma(t) = A\cosh\left(M\left(\frac{N_t}{2}-t\right)\right) + C$$

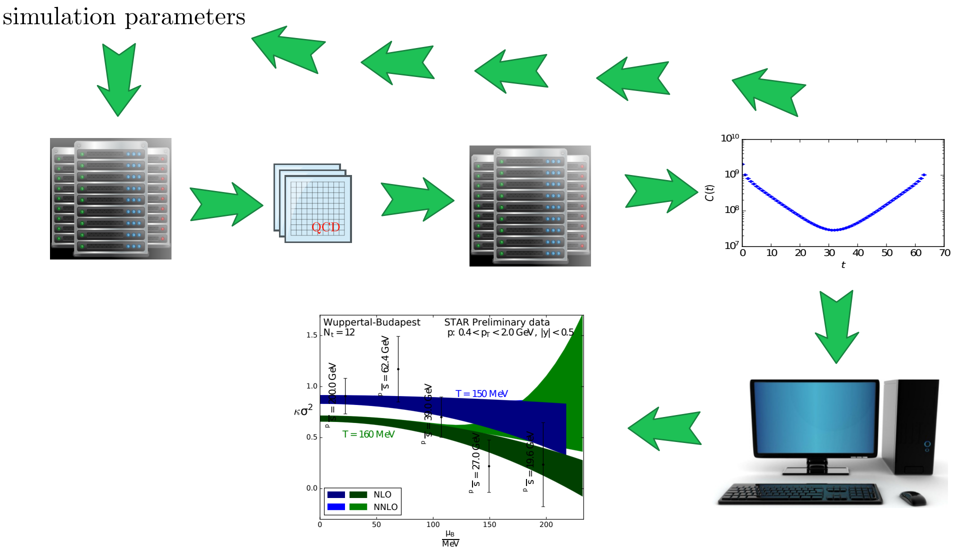
Correlators and masses - numerics

- There are no real particles in $SU(2)$ gauge
- Looking at the correlator of the plaquette
- In QCD typical: Ω mass, or decay constants f_π, f_K
- Deciding when the excited states are gone
- Fitting the rest of the correlator (strong correlaton!)



- Here: only 1 parameter β. No tuning necessary, just determining the temperature/lattice spacing
- in QCD: each quark brings an adittional parameter m_q they have to be tuned to match physical parameters m_π, m_K
- The choice of parameters is called *Line of constant physics* (LCP)
- The tuning has to be repeated for each lattice size

The work flow



Fermions on the lattice

- free fermionic action in the continuum (one flavor):

$$S_F(\psi,\overline{\psi}) = \int \mathrm{d}^4x\overline{\psi}(x)(\gamma_\mu\partial_\mu + m)\psi(x)$$

- Naive discetiziation:

$$S_F(\psi,\overline{\psi}) = \sum_{n\in\Lambda}\overline{\psi}(n)\left(\sum_{\mu=1}^{4}\gamma_\mu\frac{\psi(n+\mu)-\psi(n-\mu)}{2a} + m\psi(n)\right)$$

Gauge invariance

- QCD is a gauge invariant theory $\longrightarrow$ S_F is supposed to be gauge invariant
- gauge transformation $\Omega \in SU(3)(\Omega^{-1} = \Omega^\dagger, \det \Omega = 1)$:

$$\psi(n) \longrightarrow \psi'(n) = \Omega(n)\psi(n)$$
$$\overline{\psi}(n) \longrightarrow \overline{\psi}'(n) = \overline{\psi}(n)\Omega^\dagger(n)$$

- gauge invariance $S_F = S'_F$
- mass term is gauge invariant

$$\overline{\psi}(n)m\psi(n) \longrightarrow \overline{\psi}(n)\Omega^\dagger(n)m\Omega(n)\psi(n) = \overline{\psi}(n)m\psi(n)$$

Restore gauge invariance

- $\overline{\psi}(n)\psi(n \pm \mu)$ is not gauge invariant:

$$\begin{aligned}\overline{\psi}(n)\psi(n \pm \mu) \longrightarrow \overline{\psi}'(n)\psi'(n \pm \mu) \\ = \overline{\psi}(n)\Omega^\dagger(n)\Omega(n+\mu)\psi(n+\mu)\end{aligned}$$

- Solution: $\psi(n \pm \mu) \longrightarrow U_{\pm\mu}(n)\psi(n \pm \mu)$

$$S_F(\psi, \overline{\psi}) = \sum_{n \in \Lambda} \overline{\psi}(n) \left(\sum_{\mu=1}^{4} \gamma_\mu \frac{U_\mu(n)\psi(n+\mu) - U_{-\mu}(n)\psi(n-\mu)}{2a} + m\psi(n) \right)$$

Fermion doublers

- Naive fermionic action:

$$S_F(\psi, \overline{\psi}) = \sum_{n\in\Lambda} \overline{\psi}(n) \left(\sum_{\mu=1}^{4} \frac{U_\mu(n)\psi(n+\mu) - U_{-\mu}(n)\psi(n-\mu)}{2a} + m\psi(n) \right)$$

- if a massless, free fermion propagator is calculated from this action on gets a term

$$\propto \frac{1}{\sum_\mu \sin^2(p_\mu a)}$$

- Continuum propagator

$$\propto \frac{1}{p^2}$$

- Continuum: one pole at $p = 0$ corresponding to one fermion
- Lattice: pole whenever $p_\mu \in \{0; \frac{\pi}{a}\}$
- 16 fermions on the lattice (15 are called doublers)

Wilson quarks

- aim: elimination of doublers
- doublers are made heavy in the continuum limit
- adding a new term to the Dirac operator that vanishes in the continuum limit
- adds an additional mass term to the Naive fermionic action:

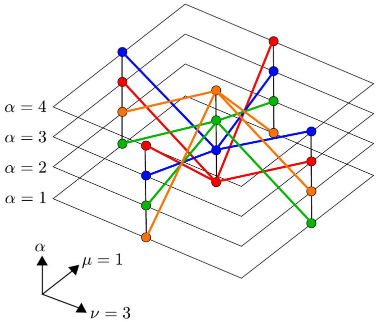
$$m \longrightarrow m + \frac{2l}{a}$$

  l is how often $\frac{\pi}{a}$ appears in p_μ
- Only the one fermion $p_\mu = (0,0,0,0)$ remains
- this extra term breaks chiral symmetry

p_μ	mass $m + \frac{2l}{a}$
$(0,0,0,0)$	m
$(\frac{\pi}{a},0,0,0)$	$m + \frac{2}{a}$
$(\frac{\pi}{a},\frac{\pi}{a},0,0)$	$m + \frac{4}{a}$
$(\frac{\pi}{a},\frac{\pi}{a},\frac{\pi}{a},0)$	$m + \frac{6}{a}$
$(\frac{\pi}{a},\frac{\pi}{a},\frac{\pi}{a},\frac{\pi}{a})$	$m + \frac{8}{a}$

Staggered Fermions

- Also named Kogut-Susskind-Fermions
- Constructing an action diagonal in Spinor space
- These leads to four groups, that are exact copies of each other
- Three groups can be dropped (spinors only have self and nearest neighbour coupling)
- In the process of rearranging the γ matrices get replaced by the staggered sign functions η



The staggered action in terms of quark fields:

$$S_F[q,\bar{q}] = (2a)^4 \sum_n \left(m\bar{q}(n)q(n)\right) + \sum_\mu \mathrm{tr}\left(\bar{q}(n)\gamma_\mu \nabla_\mu q(n)\right) - \underbrace{a \sum_\mu \mathrm{tr}\left(\bar{q}(n)\gamma_5 \triangle_\mu q(n)\gamma_\mu\gamma_5\right)}_{\text{taste breaking term}}$$

Going to one taste by taking the 4th root of the action. This is called rooting and is not local.

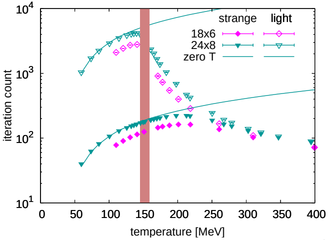
Overlap quarks

- theoretically most elegant (implement exact chiral symmetry)
- Dirac operator fulfills lattice Ginspark-Wilson relation: $D\gamma_5 + \gamma_5 D = aD\gamma_5 D$
- $D_{\text{overlap}} = \frac{1}{a}\left(1 + \gamma_5 \text{sgn} H\right)$
- (H is an appropriate kernel)
- The sng() function requires taking the square root of a large matrix
- this is expensive

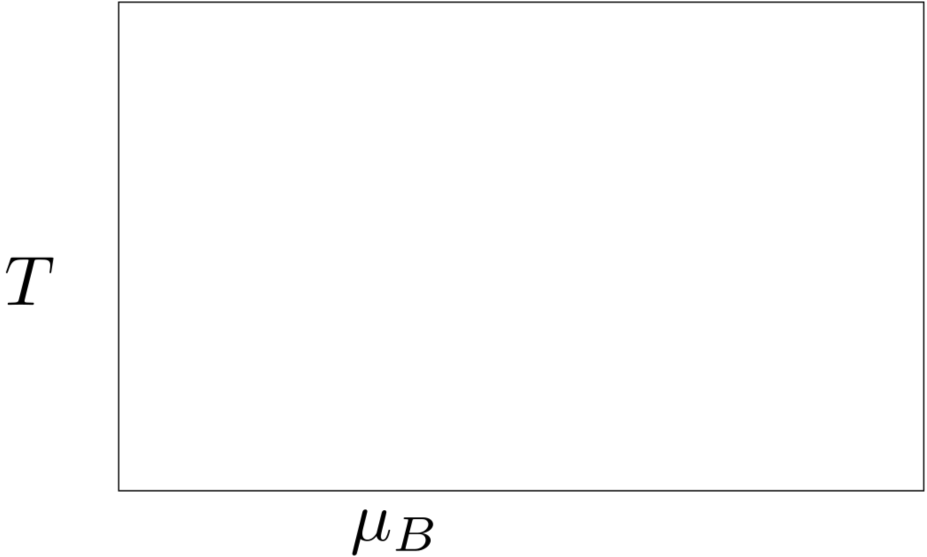
Why aren't we finished yet?

- Simulations take a lot of computer time
- Not everything can be calculated directly. For example:
  - Only thermal equilibrium
  - Only simulations at $\mu_B = 0 \Rightarrow \langle n_B \rangle = 0$
    heavy ion collision experiments

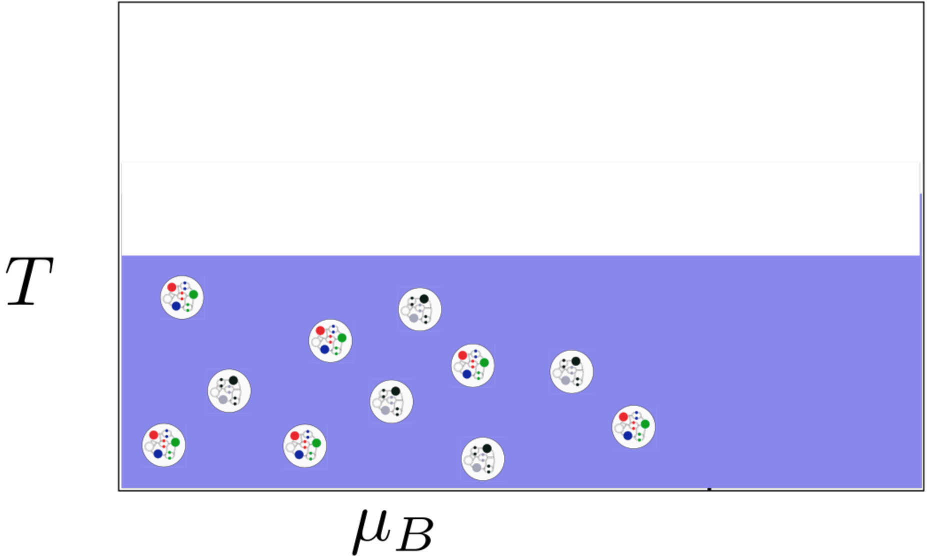
1000 configurations on a $64^3 \times 16$ lattice cost about 1 million core hours



The (T, μ_B)-phase diagram of QCD



The (T, μ_B)-phase diagram of QCD



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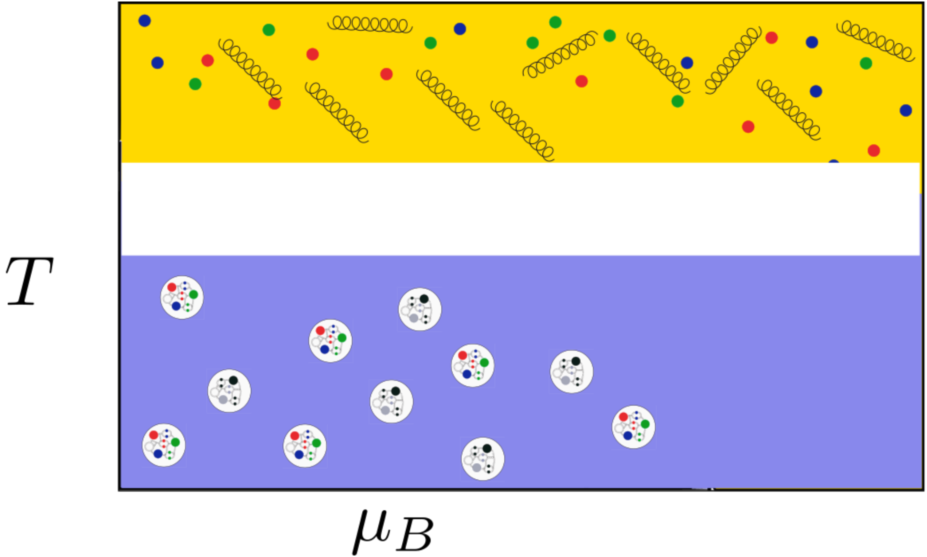

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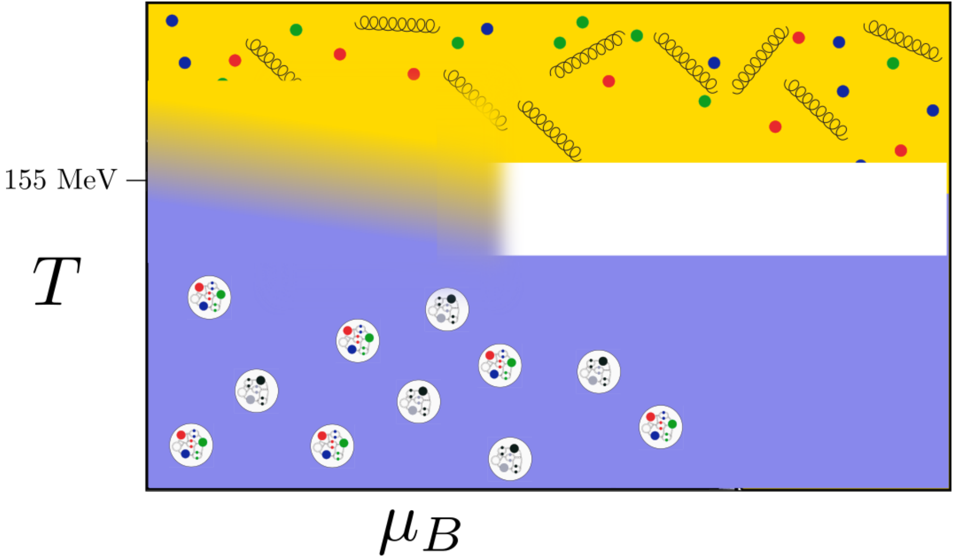

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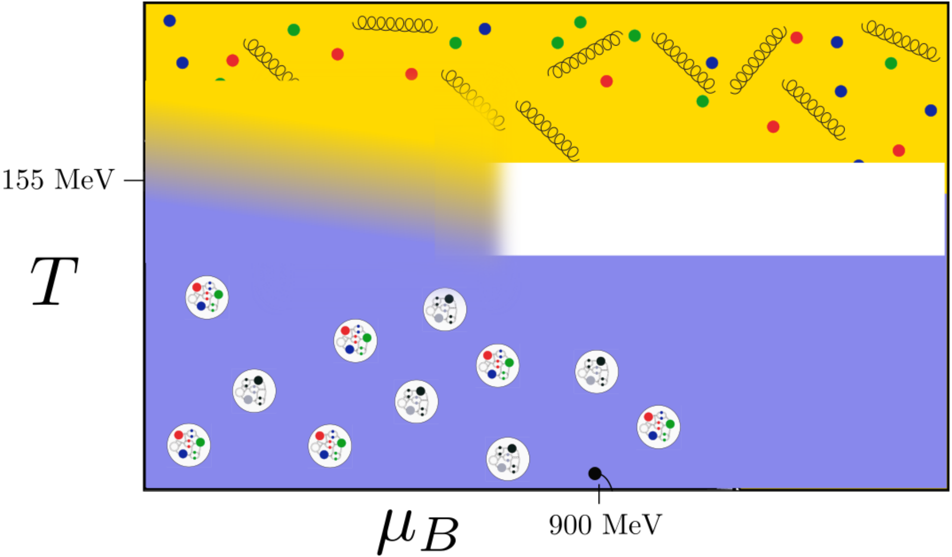

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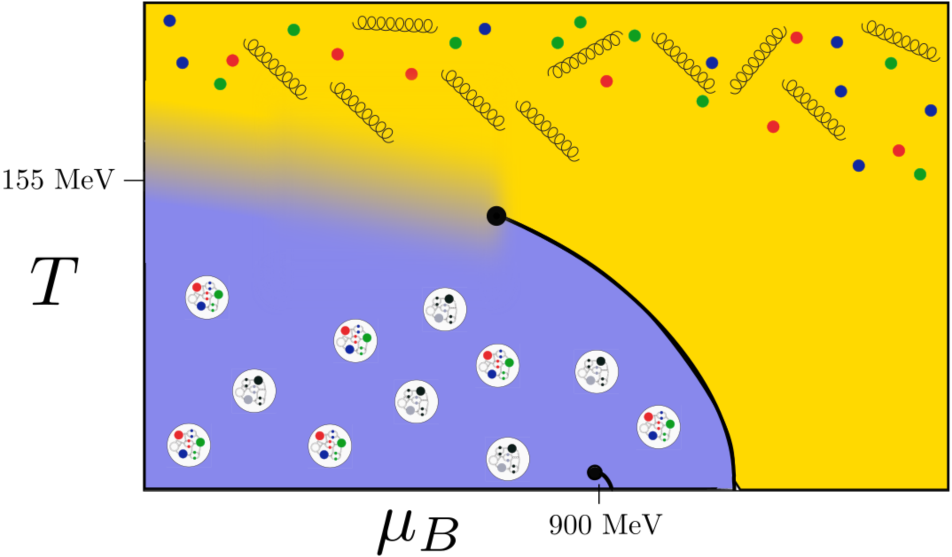

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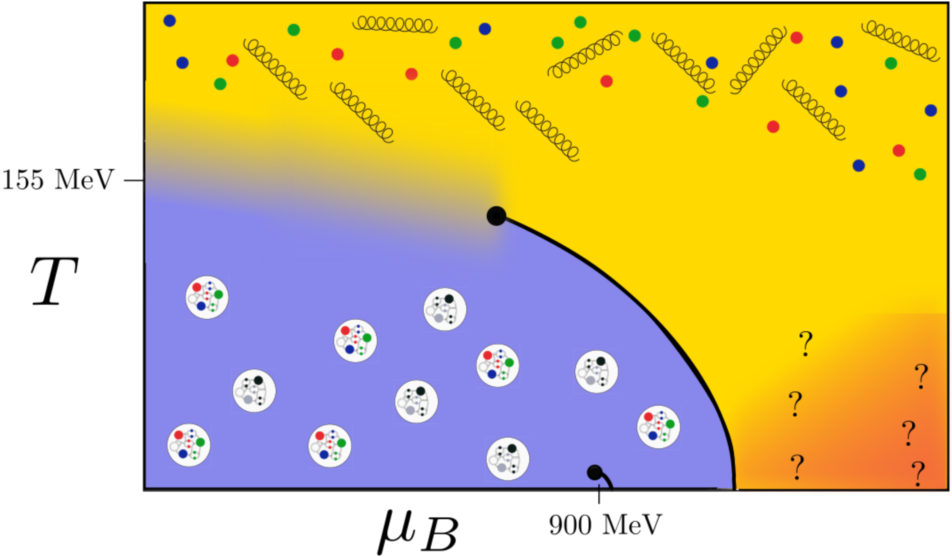

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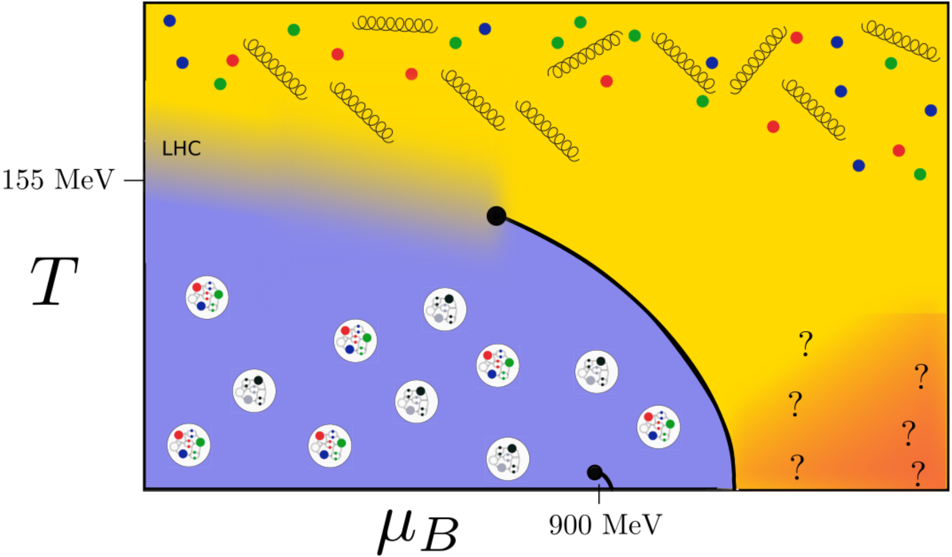
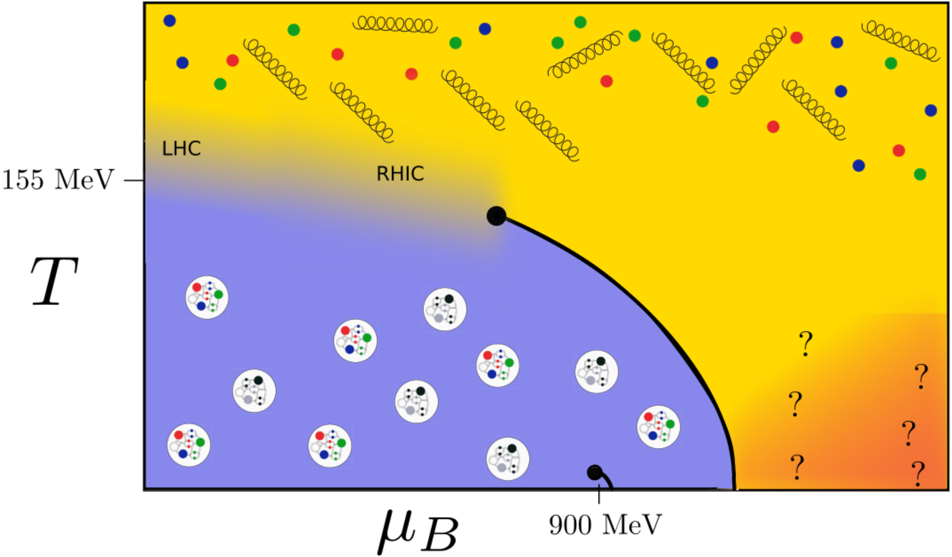
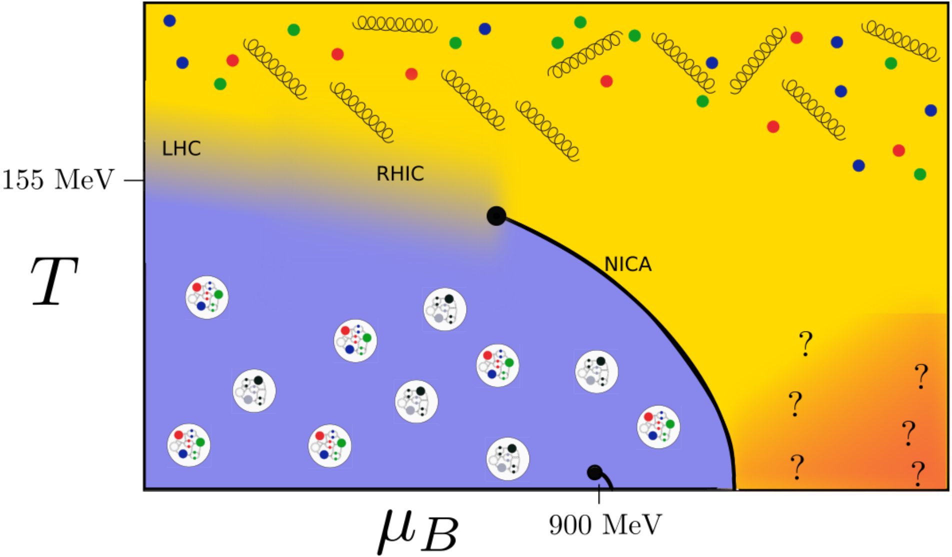


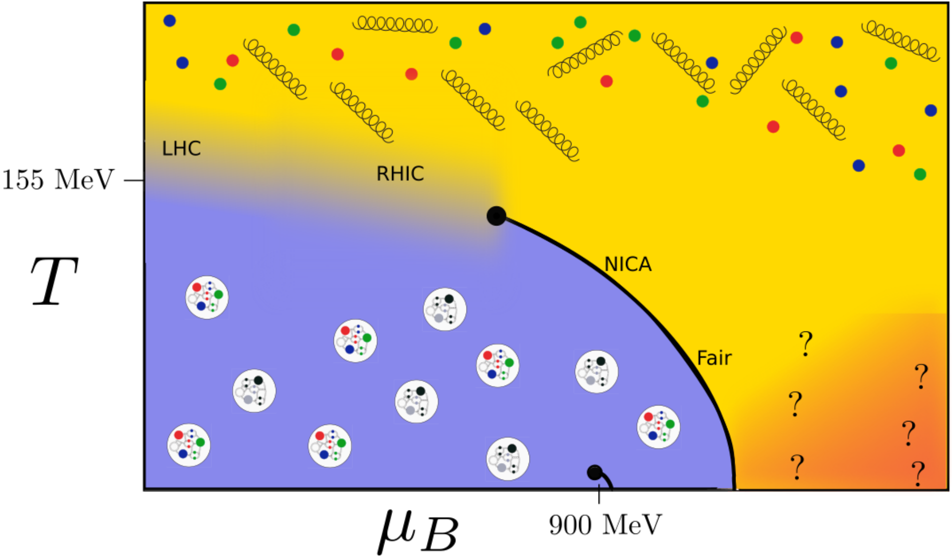
The (T, μ_B)-phase diagram of QCD



The (T, μ_B)-phase diagram of QCD



The (T, μ_B)-phase diagram of QCD



The sign problem

The QCD partition function:

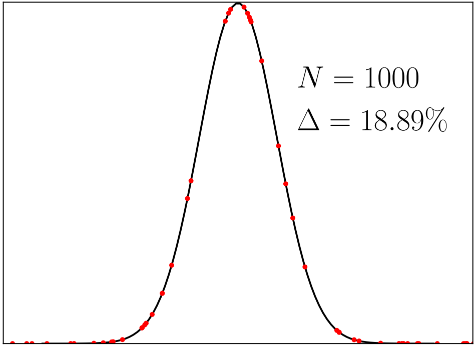
$$Z(V,T,\mu) = \int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar{\psi}\ e^{-S_F(U,\psi,\bar{\psi})-\beta S_G(U)}$$
$$= \int \mathcal{D}U \ \det M(U) e^{-\beta S_G(U)}$$

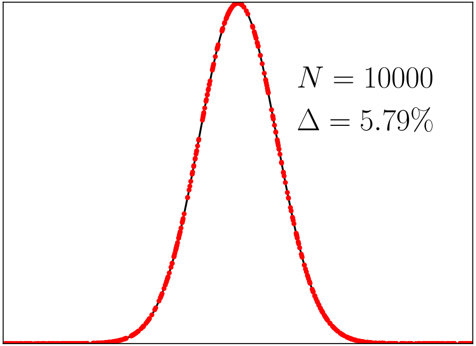
- For Monte Carlo simulations $\det M(U) e^{-\beta S_G(U)}$ is interpreted as Boltzmann weight
- If there is particle-antiparticle-symmetry $\det M(U)$ is real
- If $\mu^2 > 0$ $\det M(U)$ is complex

The sign problem

$$\int_{-\infty}^{\infty}(100-x^2)\frac{e^{-\frac{1}{2}x^2}}{\sqrt{2\pi}} \approx \int_{-100}^{100}(100-x^2)\frac{e^{-\frac{1}{2}x^2}}{\sqrt{2\pi}} = \sum_{i=1}^{N}(100-x_i^2)\frac{e^{-\frac{1}{2}x_i^2}}{\sqrt{2\pi}}\cdot\frac{200}{N}$$

The x_i are drawn from a uniform distribution in the interval $[-100, 100]$

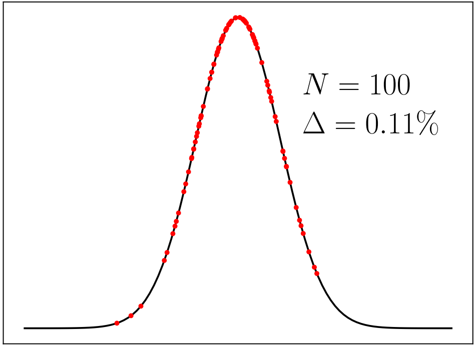


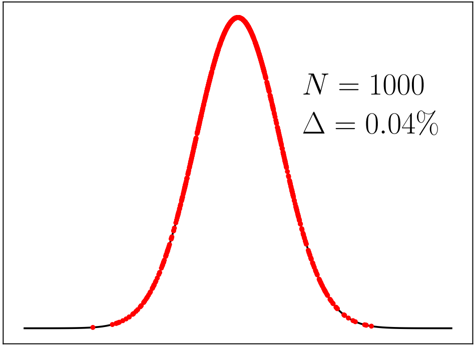


Importance sampling

$$\int_{-\infty}^{\infty}(100 - x^2)\frac{e^{-\frac{1}{2}x^2}}{\sqrt{2\pi}} = \sum_{i=1}^{N}(100 - x_i^2)\cdot\frac{1}{N}$$

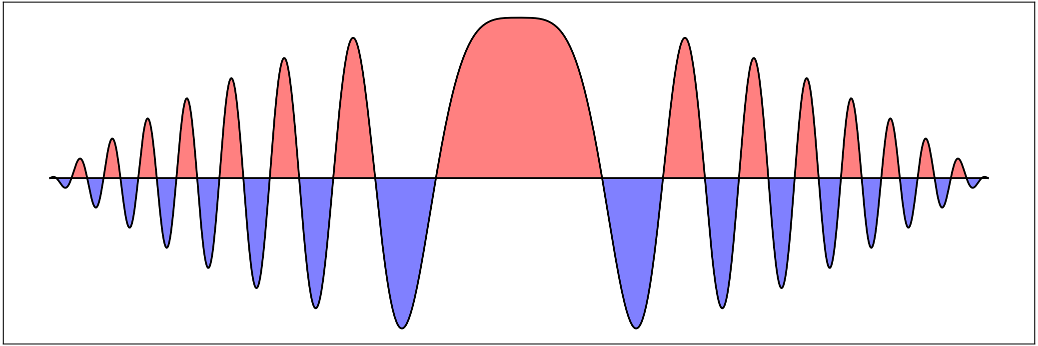
The x_i are drawn from a normal distribution





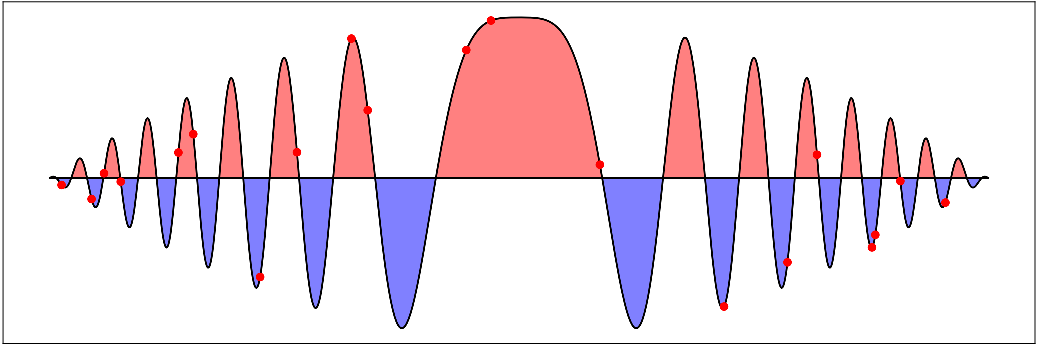
The sign problem

$$\int_{-\infty}^{\infty} (100 - x^2) \frac{e^{-\frac{i}{2}x^2}}{\sqrt{2\pi}}$$



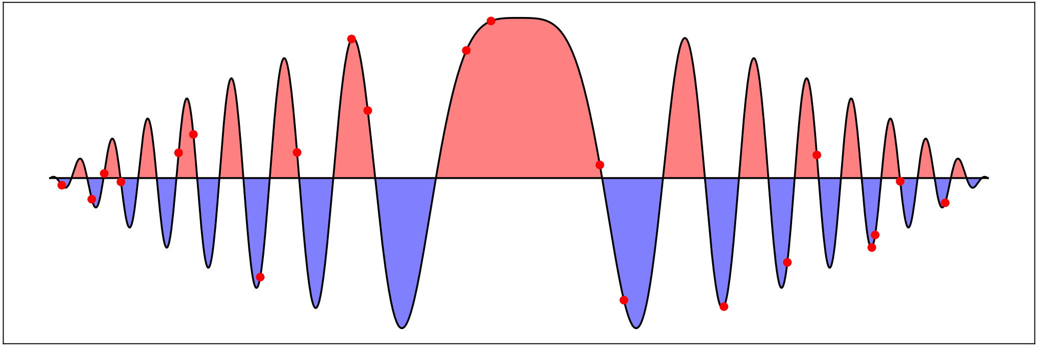
The sign problem

$$\int_{-\infty}^{\infty} (100 - x^2) \frac{e^{-\frac{i}{2}x^2}}{\sqrt{2\pi}}$$



The sign problem

$$\int_{-\infty}^{\infty} (100 - x^2) \frac{e^{-\frac{i}{2}x^2}}{\sqrt{2\pi}}$$



Dealing with the sign problem

- (Sign) Reweighting techniques
- Canonical ensemble
- Lefshetz Thimble
- Density of state methods
- Dual variables
- Complex Langevin
- ...

Dealing with the sign problem

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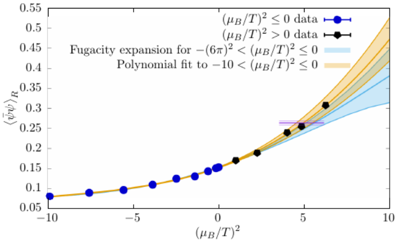

[Borsanyi:2021hbk]

Dealing with the sign problem

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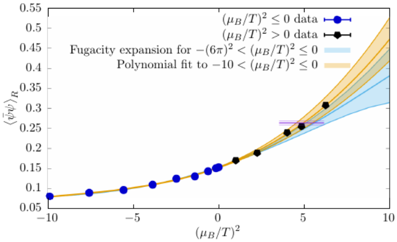
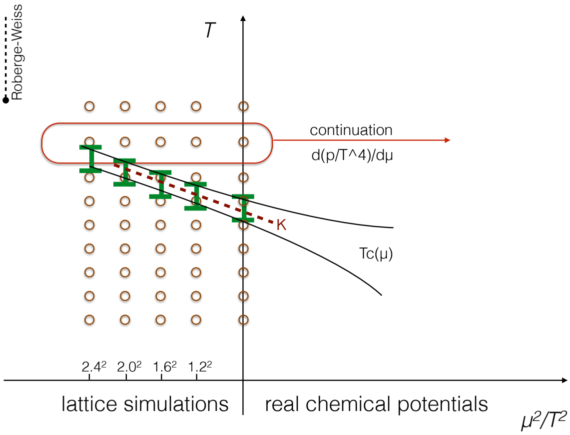


[Borsanyi:2021hbk]

- (Taylor) expansion
- Imaginary μ

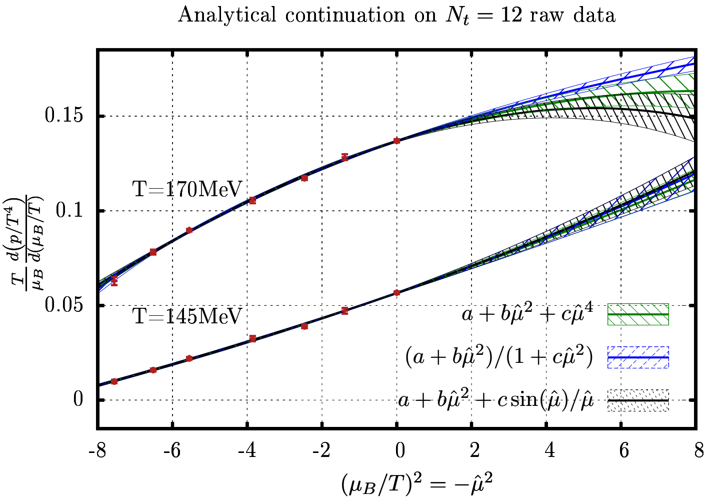
Analytic continuation from imaginary chemical potential



Common technique:

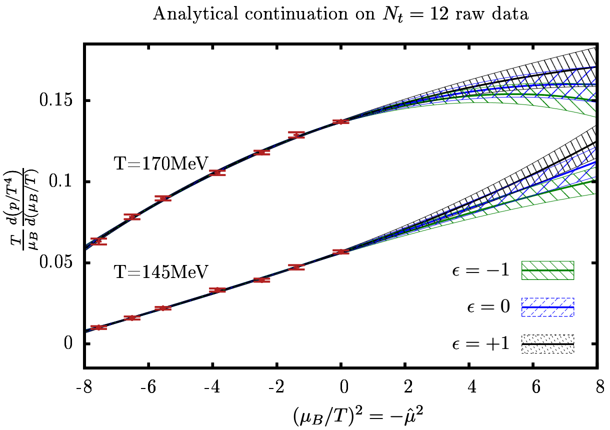
- [deForcrand:2002hgr]
- [Bonati:2015bha]
- [Cea:2015cya]
- [DElia:2016jqh]
- [Bonati:2018nut]
- [Borsanyi:2018grb]
- [Borsanyi:2020fev]
- [Bellwied:2021nrt]
- ...

Different functions

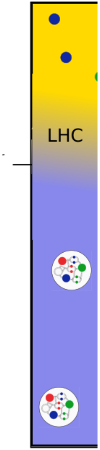


Different functions

Condition: $\chi_8 \lesssim \chi_4 \longrightarrow f(\hat{\mu}_B) = a + b\hat{\mu}_B^2 + c\hat{\mu}_B^4 + \frac{b\epsilon}{840}\hat{\mu}_B^6$



Expansion from $\mu = 0$



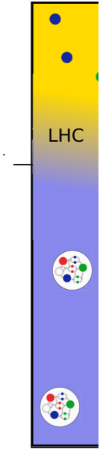
Taylor expansion

$$\frac{p}{T^4} = \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{1}{j!k!} \chi_{jk}^{BS} \hat{\mu}_B^j \hat{\mu}_S^k$$

with $\hat{\mu} = \frac{\mu}{T}$

- rapid convergence in Stephan-Boltzmann ($T = \infty$) limit
- expansion coefficients are lattice observables

Expansion from $\mu = 0$



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Fugacity expansion/sector method

$$\frac{p}{T^4} = \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} P_{jk}^{BS} \cosh(j\hat{\mu}_B - k\hat{\mu}_S)$$

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- information about particle content

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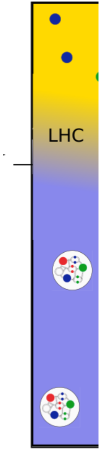

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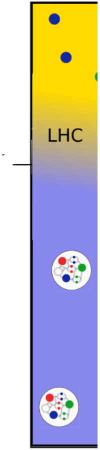
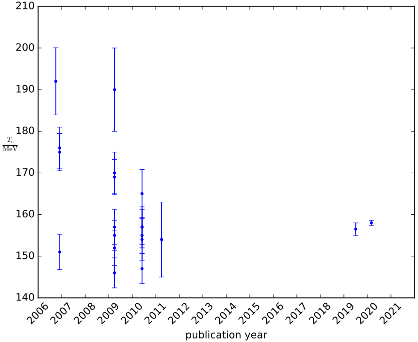
- information about particle content

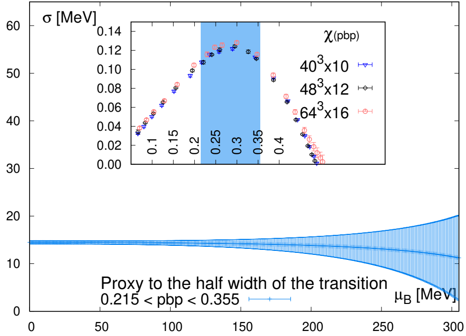
- often the expansion is done for a specific choice of μ_S

The transition temperature





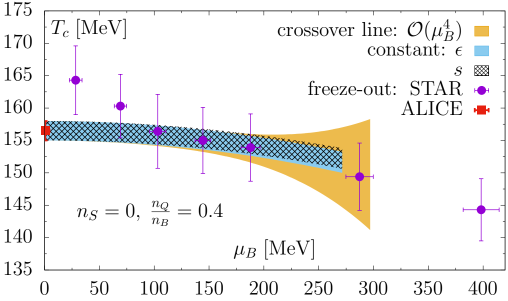
[Cheng:2006qk], [Aoki:2006br], [Aoki:2009sc], [Bazavov:2009zn], [Borsanyi:2010bp], [Bazavov:2011nk], [Bazavov:2018mes], [Borsanyi:2020fev]



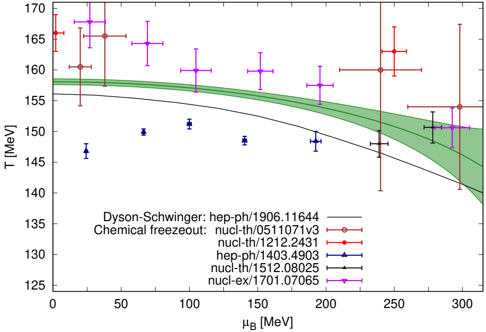
[Borsanyi:2020fev]

Extrapolation of the transition temperature

[Bazavov:2018mes]
Results from the Taylor expansion method
HISQ quarks
Continuum limit from $N_t = 6, 8, 12$



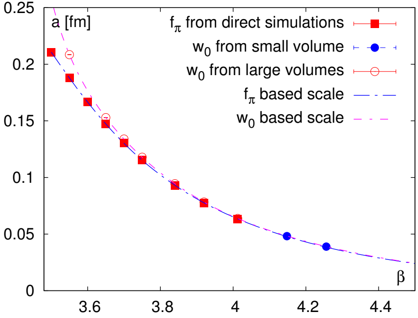
[Borsanyi:2020fev]
Results from the imaginary potential method
staggered quarks
Continuum limit from $N_t = 10, 12, 16$



chemical freezeout: abundancies of hadrons are fixed (frozen-in)

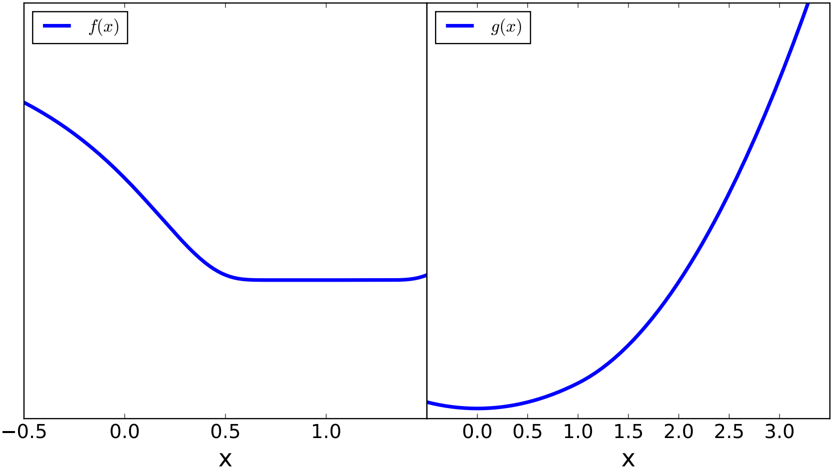
kinetic freezeout: momentum distributions are fixed

Actual-Analysis



- Action: tree-level Symanzik improved gauge action, with four times stout smeared staggered fermions
- 2+1+1 flavour, on LCP with pion and kaon mass
- Simulation at $\langle n_S \rangle = 0$ and $\langle n_Q \rangle = 0.4 \langle n_B \rangle$
- Continuum extrapolation from lattice sizes: $40^3 \times 10$, $48^3 \times 12$ and $64^3 \times 16$
- $\frac{\mu_B}{T} = \mathrm{i}\frac{j\pi}{8}$ with $j = 0, 3, 4, 5, 6, 6.5$ and 7
- Two methods of scale setting: f_π and w_0, $Lm_\pi > 4$

Does that mean there is no critical endpoint?



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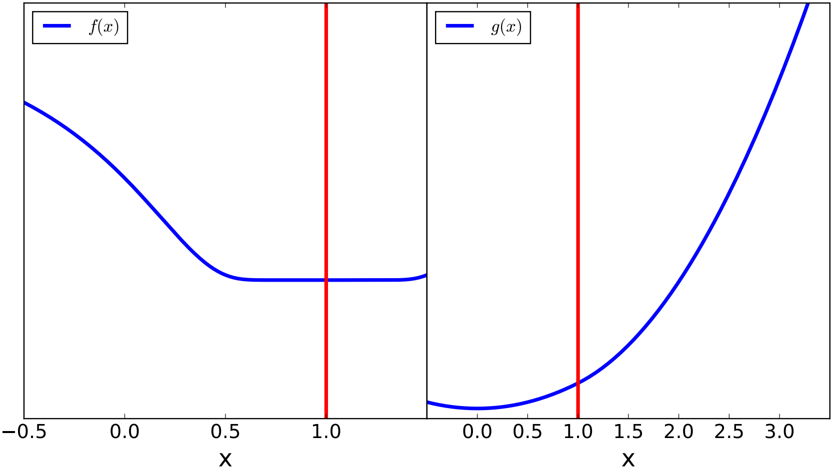

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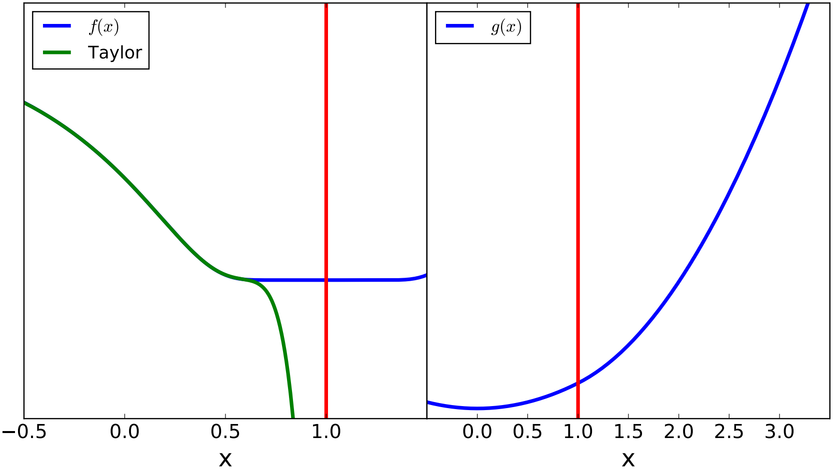

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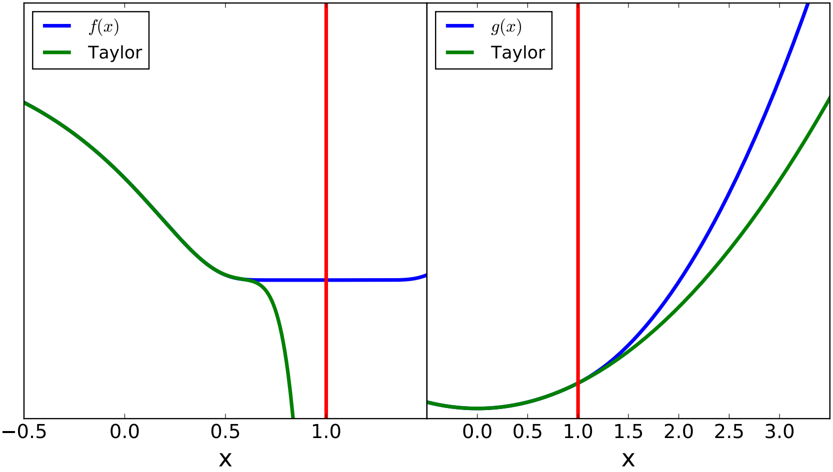
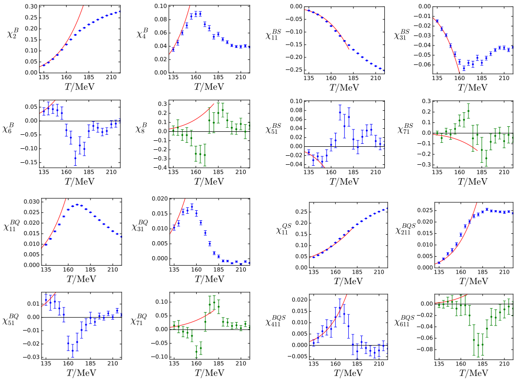


Fluctuations on the lattice

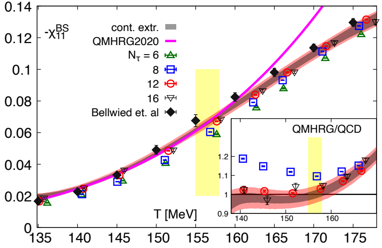
$$\chi^{B,Q,S}_{i,j,k} = \frac{\partial^{i+j+k}(p/T^4)}{(\partial\hat{\mu}_B)^i(\partial\hat{\mu}_Q)^j(\partial\hat{\mu}_S)^k}\,,\quad \hat{\mu}_i = \frac{\mu}{T}$$

- can be calculated on the lattice
- can be compared to various models
- can be compared to experiment
- can be used as building blocks for various observables



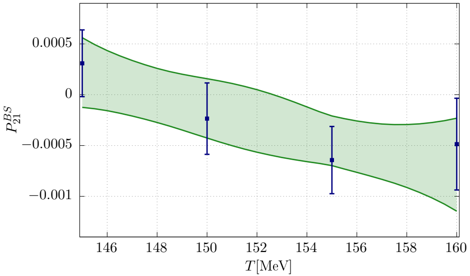
[Borsanyi:2018grb]

Low order fluctuations with high precision



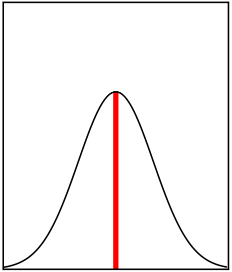
- [Bollweg:2021vqf]
- HISQ
- New continuum extrapolated results ($N_t = 6, 8, 12, 16$) allow for detailed comparisons with various models
- Quark model states are needed for HRG

- [Bellwied:2021nrt]
- continuum estimate from $N_t = 8, 10, 12$
- stout smeared staggered
- contributions vom $N - \Lambda$, $N - \Sigma$ scattering
- negative contribution in the Fugacity expansion indicate repulsive interaction that cannot be described with more resonances

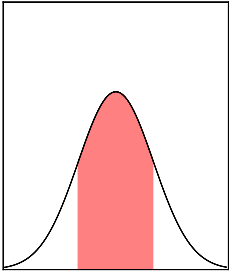


Observables

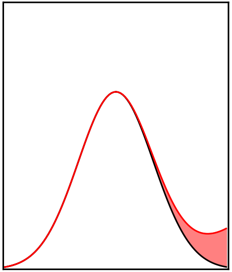
Cumulants of the net baryon number distributions:



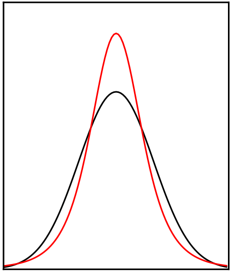
mean
$M_B = \chi_1^B$



variance
$\sigma_B^2 = \chi_2^B$



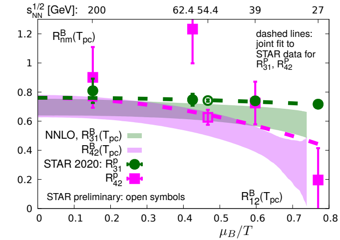
skewness
$S_B = \frac{\chi_3^B}{\left(\chi_2^B\right)^{3/2}}$
asymmetry of the distribution



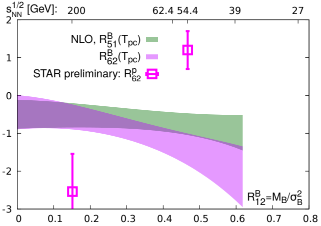
kurtosis
$\kappa_B = \frac{\chi_4^B}{\left(\chi_2^B\right)^2}$
"tailedness" of the distribution

Comparison with heavy ion collision experiments

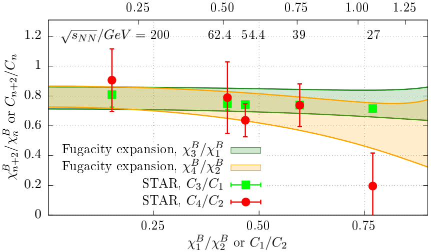
Continuum estimate from $N_t = 8, 12$



$N_t = 8$



- [Bazavov:2020bjn]
- Taylor method
- HISQ



- [Bellwied:2021nrt]
- continuum estimate from $N_t = 8, 10, 12$
- stout smeared staggered

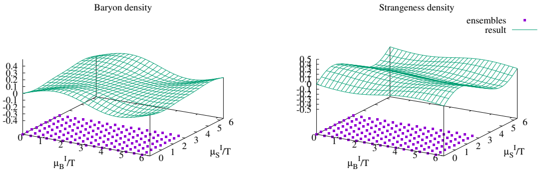
- 2d-extrapolation in μ_B and μ_S
- Fugacity expansion and imaginary chemical potential

Extrapolations are done along the transition line.

2d-Extrapolation: [Bellwied:2021nrt]

144 ensembles for each temperature and lattice

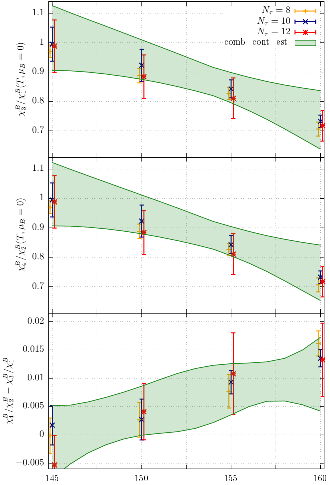
Example at $T = 155$ MeV:



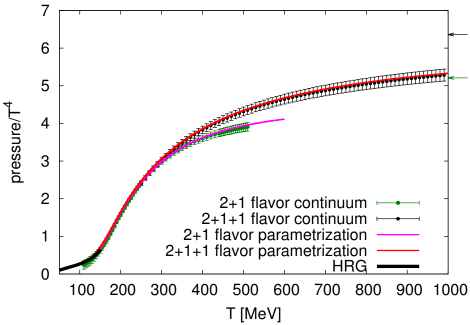
$$P(T, \hat{\mu}_B^I, \hat{\mu}_S^I) = \sum_{j,k} P_{jk}^{BS}(T) \cos(j\hat{\mu}_B^I - k\hat{\mu}_S^I) \ .$$

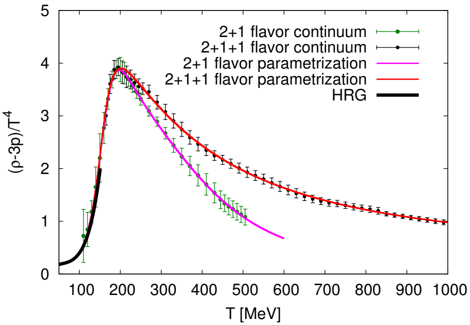
$$-S = -1, 0, 1, 2, 3; \quad B = 0, 1, 2, 3$$

A surface is fitted on the baryon and strangeness densities, as well as on their susceptibilities.



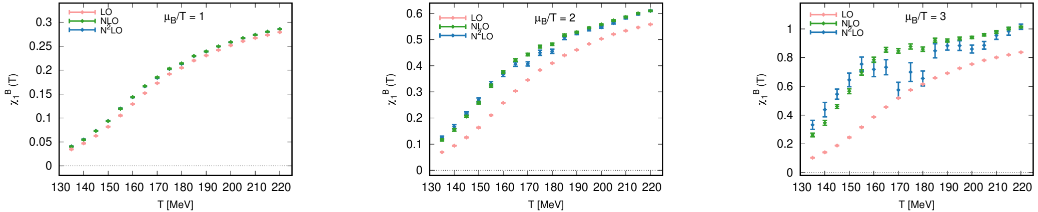
$\mu_B = 0$ and high T: Influence of the charm quark





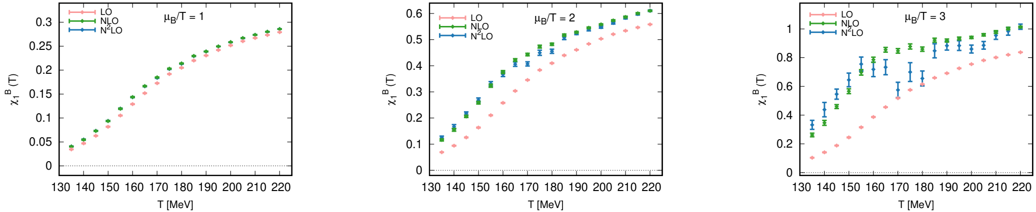
[Borsanyi:2016ksw]

Trouble with the equation of state

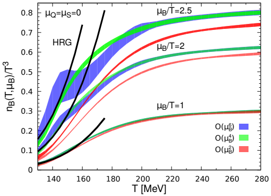


[Borsanyi:2021sxv], [Borsanyi:2018grb], $N_t = 12$

Trouble with the equation of state

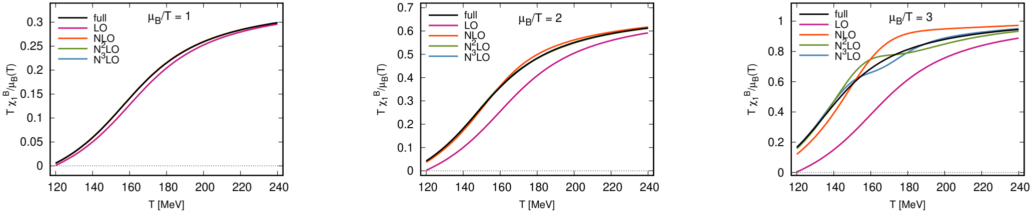


[Borsanyi:2021sxv], [Borsanyi:2018grb], $N_t = 12$

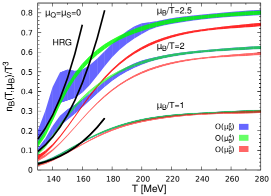


[Bazavov:2017dus]
Taylor method
$N_t = 6, 8, 12, (16)$ (2nd Order)
$N_t = 6, 8$ (4th and 6th Order)

Trouble with the equation of state



[Borsanyi:2021sxv]



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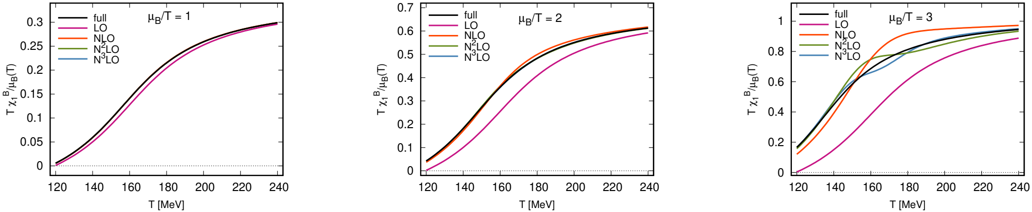

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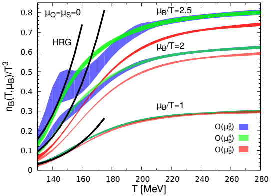
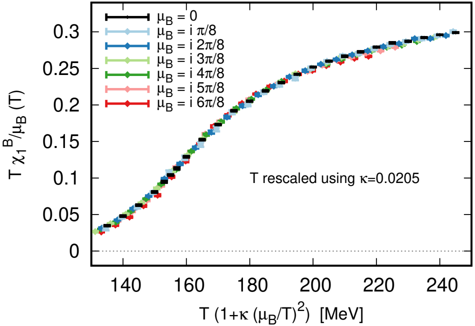


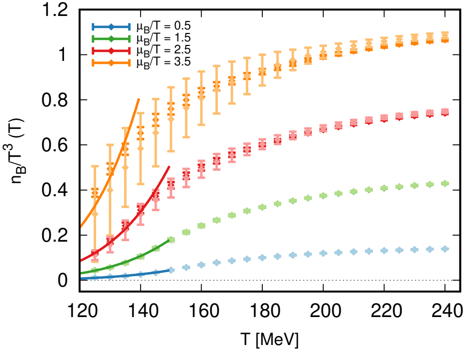
[Bazavov:2017dus]
Taylor method
$N_t = 6, 8, 12, (16)$ (2nd Order)
$N_t = 6, 8$ (4th and 6th Order)

- extrapolation at fixed T cross the transition line
- bad convergence with low order Taylor coefficients

Equation of state

Find a different extrapolation scheme for extrapolating to higher μ_B.

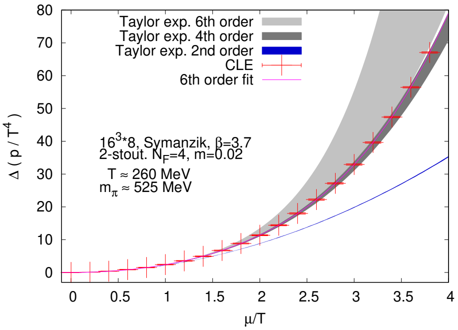




- [Borsanyi:2021sxv]
- $N_t = 10, 12, 16$

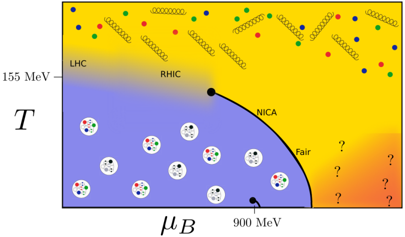
Progress on Complex Langevin

Evolution in a fictitious Langevin time generates configurations with a complex measure.

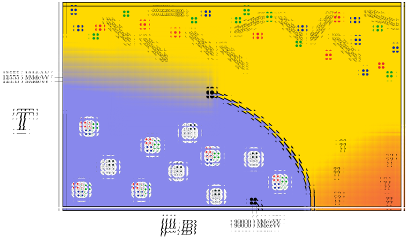


- [Sexty:2019vqx]
- Results with improved actions
- Comparison with extrapolation methods
- Progress on convergence control during Lattice2021

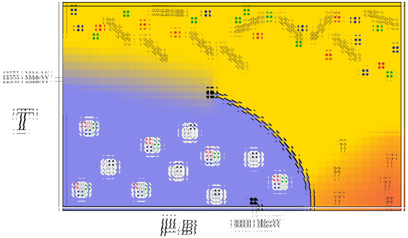
Outlook on higher μ_B with Complex Langevin I

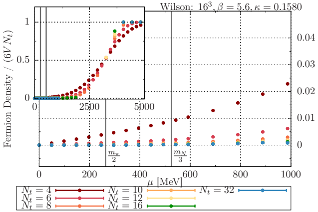


Outlook on higher μ_B with Complex Langevin I



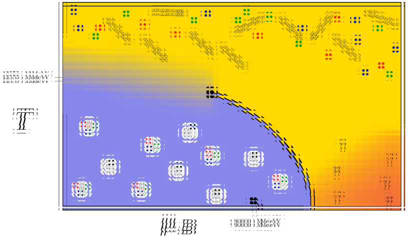
Outlook on higher μ_B with Complex Langevin I

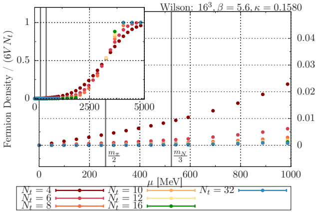


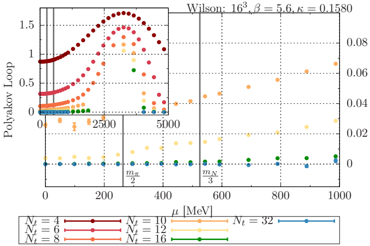


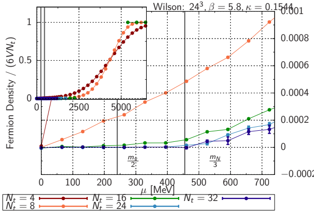
- [Benjamin Jaeger at Lattice2021]
- $N_f = 2$, $m_\pi = 550$ MeV, Wilson fermions

Outlook on higher μ_B with Complex Langevin I





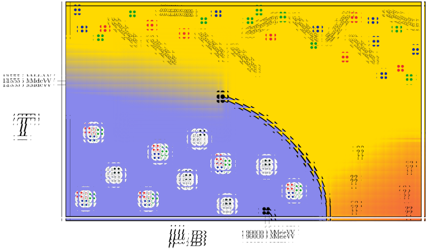


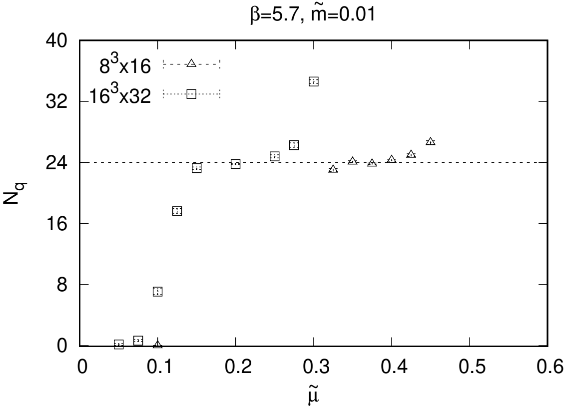


- [Benjamin Jaeger at Lattice2021]
- $N_f = 2$, $m_\pi = 550$ MeV, Wilson fermions

- unrenormalized Polyakov Loop
- saturation at higher μ_B
- extrapolation in Langevin time still missing

Outlook on higher μ_B with Complex Langevin II





- [Ito:2020mys]
- $N_f = 4$, $\tilde{\mu} = \mu a$, $a^{-1} \approx 4.7$ GeV
- plateau might be connected to a Fermi surface and color superconductivity
- this is done in a small box