Lattice SYM and Monte Carlo methods

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the aim of investigations

- the expectation value of an Operator A is defined nonpertubatively by the functional integral

$$\langle A \rangle = Z^{-1} \int (D\phi)\, e^{-S[\phi]} A\,[\phi]$$

  - normalization constant Z is chosen, such that $< 1 >= 1$
  - $(D\phi)$ is the appropriate functional measure
  - $S\,[\phi]$ is the given action

- In QFT there is one integration per degree of freedom
  - we are dealing with an infinite dimensional functional integral
  - well-defined only in euclidean space-time

the strategy

- lattice regularisation by the functional integral
  - continuum limit (lattice spacing $a \to 0$)
  - thermodynamic limit (physical volume $V \to \infty$)
- problem:
  - hoplessly many integrations
- solution: Monte Carlo integration
  - power sampling is based on the identification of probabilities with measures

how does it work?

- start: generate a sequence of random field configurations $\{\phi_1, \phi_2, \phi_3, ..., \phi_N\}$ chosen from the probability distribution

$$P(\phi_t)D(\phi_t) = \frac{1}{Z}\mathrm{e}^{-S[\phi_t]}$$

- use the Markov process
  - consider stochastic transitions to generate the correct probability distribution Q

$$P : Q_1 \rightarrow Q_2$$

  - the transitions are ergodic
  - distribution converges to a unique fixed point

$$\bar{Q} = \lim_{n\rightarrow\infty} P^n Q_1$$

the Markov Chain

- again:
  - start with an arbitrary state
  - iterate the Markov process until it has thermalised
  - sucessive configurations will be distributed according to $\bar{Q}$
- Markov chain
  - detailed balance

$$P(y \leftarrow x)\bar{Q}(x) = P(x \leftarrow y)\bar{Q}(y)$$

  - Markov step

$$P(x \leftarrow y) = \min\left(1, \frac{\bar{Q}(x)}{\bar{Q}(y)}\right)$$

the thermalisation

- when do we have reached the equilibrium?
- measure the value of A on each configuration and compute the average

$$\bar{A} \equiv \frac{1}{N} \sum_{t=1}^{N} A(\phi_t)$$

- limit of large numbers guarantees

$$\langle A \rangle = \lim_{N \to \infty} \bar{A}$$

- central limit theorem guarantees

$$\langle A \rangle \sim \bar{A} + O\left(\sqrt{\frac{\sigma}{N}}\right)$$

with

$$\sigma \equiv \left\langle (A - \langle A \rangle)^2 \right\rangle$$

the thermalisation

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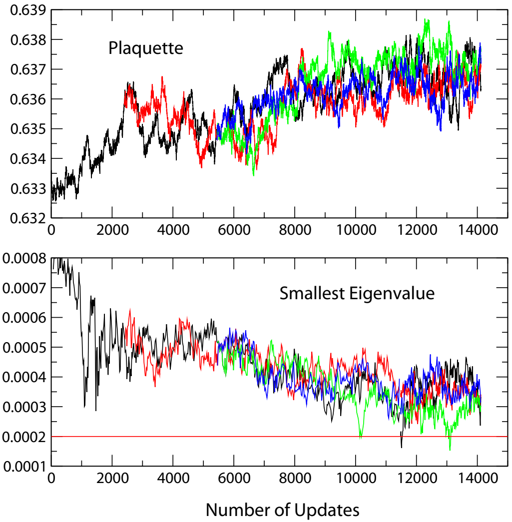


claim on the algorithm

- we want an algorithm which
  - updates the fields globally
    $\longrightarrow$ since single updates are expensive for non-local actions
  - takes large steps through configuration space
    $\longrightarrow$ in order to decorrelate successive configuration
  - does not introduce systematical errors

Hybrid Monte Carlo

- the Hybrid Monte Carlo method is an useful algorithm with these properties
- the central idea is to introduce a fictitious momentum p conjugate to each dynamical degree of freedom q
- next find a Markov Chain with fixed point

$$\propto \mathrm{e}^{-H(p,q)}$$

  with the Hamiltonian

$$H(p,q) = \frac{1}{2}p^2 + S(q)$$

  - the action $S(q)$ of the underlying QFT plays the role of the potential in a fictitious classical mechanics system
  - the hamiltonian gives the evolution in a fifth dimension, fictitious or Monte-Carlo time
- ignoring the momenta p, this generates the desired distribution $S(q)$

the considered action

- the SYM action consists of two parts

$$S_{SYM} = S_g + S_f$$

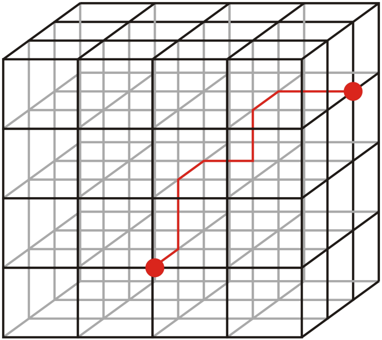
- in detail the continuum action

$$S_{SYM} = \int d^4x \left\{ \frac{1}{4} F^a_{\mu\nu}(x) F^a_{\mu\nu}(x) + \frac{1}{2} \overline{\lambda}^a(x) \gamma_\mu D_\mu \lambda^a(x) \right\}$$

- with Majorana Spinors instead of the quark fields

the lattice

- discretize euclidean space-time
- hypercubic L^4-lattice with lattice spacing a
- derivatives $\rightarrow$ finite differences
- integrals $\rightarrow$ sums
- gauge potentials A_μ in $F_{\mu\nu}$ $\rightarrow$ link matrices U_μ



the lattice action

- discrete gauge part

$$S_g\left[U\right] = \beta \sum_x \sum_{\mu\nu} \left[1 - \frac{1}{N_c} \mathrm{ReTr} U_{\mu\nu}\right]$$

- the fermionic part is more involved. a naive discretization would result in $2^d = 16$ fermions on the lattice (Nielsen Ninomiya theorem)
- giving the doublers the weight $\mathcal{O}(a^{-1})$ leads to the Wilson Fermions

$$\begin{aligned} S_f\left[U, \overline{\lambda}, \lambda\right] &= \frac{1}{2} \sum_x \overline{\lambda}(x)\lambda(x) \\ &+ \frac{\kappa}{2} \sum_x \sum_\mu \left[\overline{\lambda}(x+\hat{\mu}) V_\mu(x)(r+\gamma_\mu)\lambda(x)\right. \\ &\left.+ \overline{\lambda}(x) V_\mu^T(x)\left(r-\gamma_\mu\right)\lambda(x+\hat{\mu})\right] \end{aligned}$$

the involved magnitudes

- the bare coupling

$$\beta = \frac{2N_c}{g}$$

- the hopping parameter

$$\kappa = (2m_0 + 8r)^{-1}$$

- with the Wilson parameter r taken to be 1 here
- gauge field link in the adjoint representation

$$[V_\mu(x)]_{ab} \equiv 2Tr\left[U_\mu^\dagger(x)T^a U_\mu(x)T^b\right] = \left[V_\mu^*(x)\right]_{ab} = \left[V_\mu^T(x)\right]_{ab}^{-1}$$

- the generators T^a in the $SU(2)$ case

$$T^a = \frac{1}{2}\tau^a$$

the majorana fermions

- the majorana fermions

$$\lambda = \lambda^{\mathcal{C}} = \mathcal{C}\bar{\lambda}^{T}$$

(with the charge conjugation matrix $\mathcal{C}$)

- with the rescaled fermion fields

$$\lambda \rightarrow \sqrt{\frac{1}{2\kappa}}\lambda$$

- with Majorana fields constructed from the dirac fields

$$\lambda^{1} = \frac{1}{\sqrt{2}}\left(\phi + \mathcal{C}\bar{\phi}^{T}\right), \; \lambda^{2} = \frac{1}{\sqrt{2}}\left(-\phi + \mathcal{C}\bar{\phi}^{T}\right)$$

the pseudofermion representation

- defining the fermion matrix

$$Q_{x,y}\,[U] \equiv \delta_{x,y} - \kappa \sum_{\mu} [\delta_{y,x+\hat{\mu}}(1+\gamma_\mu)V_\mu(x) + \delta_{y+\hat{\mu}}(1-\gamma_{y+\hat{\mu}})V_\mu^T(y)]$$

- leads to a compactly representation of S

$$S_f = \frac{1}{2}\sum_{xy} \overline{\lambda}(x) Q_{x,y} \lambda(y)$$

- it´s not feasible to simulate Grassmann fields directly, because $e^{-S_F} = e^{-\bar{\phi}D\phi}$ is not positive $\rightarrow$ poor importance sampling
- we therefore integrate out the fermion fields to obtain the fermion determinant

$$\int [d\lambda]\, e^{-S_f} = \int [d\lambda]\, e^{-\frac{1}{2}\overline{\lambda}Q\lambda} = \pm\sqrt{\det Q}$$

the Pfaffian

- a unique definition of the path integral is given by

$$\int [d\lambda]\, e^{-\frac{1}{2}\overline{\lambda} Q \lambda} = \int [d\lambda]\, e^{-\frac{1}{2}\overline{\lambda} \mathcal{M} \lambda} = Pf\,[\mathcal{M}]$$

- the complex antisymmetric matrix $\mathcal{M}$ is defined as

$$\mathcal{M} = \mathcal{C} Q = -\mathcal{M}^T$$

- $\mathcal{M}$ has the same determinant as Q. $Pf\,[\mathcal{M}]$ is the so-called Pfaffian of $\mathcal{M}$

$$\begin{aligned} pf(\mathcal{M}) &\equiv \frac{1}{N!2^N} \epsilon_{\alpha_1\beta_1\ldots\alpha_N\beta_N} \mathcal{M}_{\alpha_1\beta_1} \ldots \mathcal{M}_{\alpha_N\beta_N} \\ &= \int [d\lambda_i]\, e^{-\frac{1}{2}\lambda_\alpha \mathcal{M}_{\alpha\beta} \lambda_\beta} \end{aligned}$$

with $1 \leq \alpha\beta \leq 2N$ and the totally antisymmetric tensor ϵ.

- note the sign problem of the theory

the discrete equation of motion

- move the configuration through configuration space $\longrightarrow$ in each step all field variables are updated by computing their trajectory through a coupled set of equations of motions
- generate a sequence of p, U with the correct probability distribution:
  - update $p_\mu(x)$ using Gaussian random noise
  - update ϕ using Gaussian random noise via $\phi = D^\dagger \eta$
  - evolve p, U according to the Hamiltonian

$$H\left[p, U, \phi\right] \equiv \frac{1}{2}p^2 + S_g[U] + S_f[U]$$

  - accept/reject the final configuration p', U' with probability

$$P_{accept} = \min(1, \mathrm{e}^{-(H[p',U']-H[p,U])})$$

the leapfrog trajectory

- the discrete Hamilton equations of motion dictate the following update for p and U

$$\begin{aligned} T_U(\delta\tau) : U &\rightarrow \mathrm{e}^{i\delta\tau p} U \\ T_p(\delta\tau) : p &\rightarrow p + \delta\tau F \end{aligned}$$

- with the force F due to the variation of the gauge field

$$F = -\frac{\delta H}{\delta U} = F_g[U] + F_f[U]$$

- in detail a step in $U_{x\mu}$

$$U'_{x\mu} = U_{x\mu} e^{\sum_{j=1}^{3} i\Delta\tau T_j p_{x\mu j}}$$

- and p

$$p'_{x\mu j} = p_{x\mu j} - D_{x\mu j}\Delta\tau S[U]$$

the fermionic force

- in here we have

$$D_{x\mu j}\Delta\tau S_f[U] = D_{x\mu j}\left(\Delta\tau\frac{1}{2}\sum_{x'y'}\overline{\lambda}(x')Q_{x',y'}\lambda(y')\right)$$

- with the now known fermion matrix

$$Q_{x',y'}[U] \equiv \delta_{x',y'} - \kappa\sum_{\mu'}\left[\delta_{y',x'+\hat{\mu}}(1+\gamma_{\mu'})V_{\mu'}(x')\right.$$
$$\left.+\delta_{y'+\hat{\mu}}(1-\gamma_{y'+\hat{\mu}})V^T_{\mu'}(y')\right]$$

- and gauge field link in the adjoint representation

$$\left[V_{\mu'}(x')\right]_{ab} \equiv 2\mathrm{Tr}\left[U^\dagger_{\mu'}(x')T^aU_{\mu'}(x')T^b\right]$$

- we get

$$D_{x\mu j}\left[V_{\mu'}(x')\right]_{ab} = 2\epsilon_{bjk}\left[V_{\mu'}(x')\right]_{ak}$$

the gauge force

- gauge part

$$D_{x\mu j} S_g [U] = D_{x\mu j} \beta \sum_{x'} \sum_{\mu'\nu'} \left[1 - \frac{1}{N_c} \mathrm{ReTr} U_{\mu'\nu'}(x') \right]$$

- with the derivative

$$D_{x\mu j} f(U_{x\mu}) = \frac{\partial}{\partial \alpha} f\left[\mathrm{e}^{i2\alpha T_j} U_{x\mu} \right]_{\alpha=0}$$

- note that the gauge part is taken in the fundamental representation while in the fermionic part the adjoint representation is used

the leapfrog integration scheme

- one observes that $F_g[U] \gg F_f[U]$
- introduce two time steps:
  - a short one associated with the large but cheap gauge force $F_g[U]$
  - a long one associated with the small, but expensive fermionic force $F_f[U]$
- moreover, the fermionic force can be split into two or more pieces and put on different time scales according to their size

$$T(\Delta\tau) = T_P\left(\frac{\Delta\tau}{2}\right) T_U(\Delta\tau)\, T_P\left(\frac{\Delta\tau}{2}\right)$$

- split the force such that the most expensive piece contributes the least

multiple time scales

- in case of the hamiltonian, we have

$$H[p,U] = \frac{1}{2}p^2 + \sum_{i=1}^{k} S_i[U] \quad (k \geq 1)$$

for a trajectory with length τ, we define decreasing time steps

$$\Delta\tau_i = \frac{\Delta\tau_{i+1}}{N_i} = \frac{\tau}{N_k N_{k-1} \cdots N_i}$$

with N_i = step number, $(0 \leq i \leq k)$, $(\Delta\tau_{k+1} \equiv \tau)$

sexton-weingarten higher order integrator

- let us define

$$T_0(\Delta\tau_0) = T_{S_0}\left(\frac{\Delta\tau_0}{2}\right) T_U(\Delta\tau_0) T_{S_0}\left(\frac{\Delta\tau_0}{2}\right)$$

- and for $i = 1, 2, \ldots, k$

$$T_i(\Delta\tau_i) = T_{S_i}\left(\frac{\Delta\tau_i}{2}\right)\left\{T_{i-1}\left(\Delta\tau_{i-1}\right)\right\}^{N_{i-1}} T_{S_i}\left(\frac{\Delta\tau_i}{2}\right)$$

- sexton-weingarten

$$T_0(\Delta\tau_0) =$$

$$T_{S_0}\left(\frac{\Delta\tau_0}{6}\right) T_U\left(\frac{\Delta\tau_0}{2}\right) T_{S_0}\left(\frac{2\Delta\tau_0}{3}\right) T_U\left(\frac{\Delta\tau_0}{2}\right) T_{S_0}\left(\frac{\Delta\tau_0}{6}\right)$$

- improvements of HMC

polynomial filtering

- the polynomial approximation relies on

$$|\det Q|^{N_f} = \left[\det (Q^\dagger Q)\right]^{\frac{N_f}{2}} \approx \lim_{n\to\infty} \left[\det P(\tilde{Q}^2)\right]^{-1}$$

  with $\tilde{Q}^2 = Q^\dagger Q$
- where the polynomial $P_n(x)$ satisfies

$$\lim_{n\to\infty} P_n(x) = x^{-\frac{N_f}{2}} \quad \text{for} \quad x \in [\epsilon, \lambda]$$

- and

$$\epsilon \leq \min \operatorname{spec}(Q^\dagger Q)$$
$$\lambda \geq \max \operatorname{spec}(Q^\dagger Q)$$

- the approximation covers the UV part of $\tilde{Q}^2$
- only a low order polynomial is needed, since ϵ is large
- $P(x)$ is easy to invert and yealds a large force contribution

single step approximation

- using roots of the polynomial r_j

$$P_n(Q^\dagger Q) = P_n(\tilde{Q}) = r_0 \prod_{j=1}^{n} (\tilde{Q}^2 - r_j)$$

whith $r_j \equiv \rho^* \rho \equiv (\mu_j + i\nu_j)^2$, it follows

$$P_n(\tilde{Q}) = r_0 \prod_{j=1}^{n} ((\tilde{Q} - \rho_j^*)(\tilde{Q} - \rho_j))$$

- the multi-boson representation of the fermion determinant

$$r_0 \prod_{j=1}^{n} (\det(\tilde{Q} - \rho_j^*)(\tilde{Q} - \rho_j))^{-1}$$

$$\propto \int \mathcal{D}[\Phi] e^{-\sum_{j=1}^{n} \sum_{xy} \Phi_j^\dagger(y) \left[(\tilde{Q}-\rho_j^*)(\tilde{Q}-\rho_j)\right]_{xy} \Phi_j(x)}$$

two-step polynomial approximation

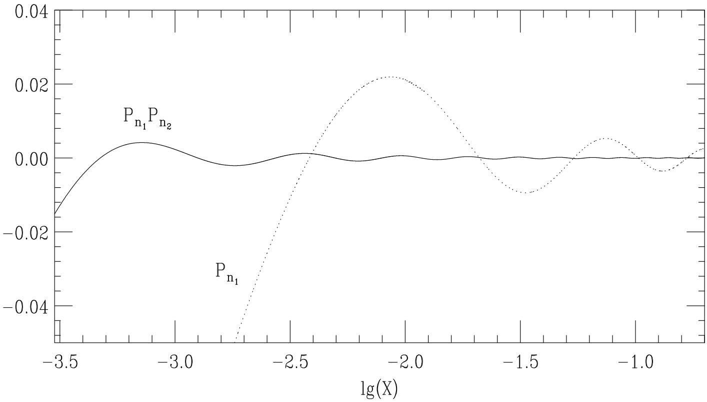
- problem: small fermion masses
  $\rightarrow$ hugh condition-number $\frac{\lambda}{\epsilon} \sim \mathcal{O}(10^4 - 10^6)$
- the key:

$$\lim_{n_2 \to \infty} P_{n_1}^{(1)}(x) P_{n_2}^{(2)}(x) = x^{-\frac{N_f}{2}}$$

- we get

$$|\det(Q)|^{N_f} \simeq \frac{1}{\det P_{n_1}^{(1)}(\tilde{Q}^2) \det P_{n_2}^{(2)}(\tilde{Q}^2)}$$

comparison of polynomial orders



- relative deviation of the successive polynomial approximation

the noisy correction in detail

- using the correction, first one has to generate a complex gaussian random vector η according to the normalized gaussian distribution

$$d\rho(\eta) = \frac{\mathrm{e}^{-\eta^\dagger P^{(2)}_{n_2}(\tilde{Q}^2)\eta}}{\int \mathcal{D}[\eta]\mathrm{e}^{\eta^\dagger P^{(2)}_{n_2}(\tilde{Q}^2)\eta}}$$

- and then accept the change of the gauge fiels $[U] \to [U']$ with the probability measure

$$P_{NC} = \min\left(1, e^{-\eta^\dagger\left(P^{(2)}_{n_2}(\tilde{Q}[U']^2) - P^{(2)}_{n_2}(\tilde{Q}[U]^2)\right)\eta}\right)$$

- the needed noisy estimator η is easily obtained from a simpel gaussian distributed vector η'

$$d\rho(\eta') = \frac{\mathrm{e}^{-\eta^\dagger \eta'}}{\int \mathcal{D}[\eta']\mathrm{e}^{-\eta'^\dagger \eta'}} \text{ and } \eta = P^{(2)}_{n_2}(\tilde{Q}^\dagger)^{-\frac{1}{2}}\eta'$$

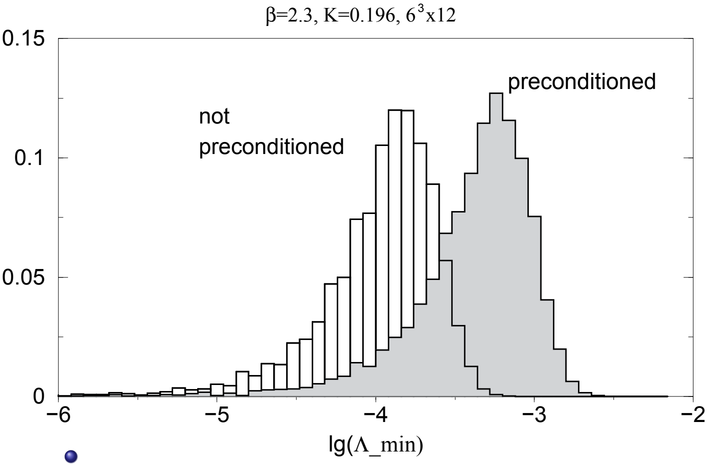
matrix preconditioning

- preconditioning decreasing the condition number $\frac{\lambda}{\epsilon}$ by even-odd preconditioning
- decompose the fermion matrix $\tilde{Q}$ in subspaces, containing the odd, respectively the even points of the lattice

$$\tilde{Q} = \gamma_5 Q = \begin{pmatrix} \gamma_5 & -\kappa\gamma_5 M_{oe} \\ -\kappa\gamma_5 M_{eo} & \gamma_5 \end{pmatrix}$$

- for the fermion determinant we have

$$\det \tilde{Q} = \det \hat{Q}, \text{ with } \hat{Q} \equiv \gamma_5 - K^2 \gamma_5 M_{oe} M_{eo}$$



- distribution of the smallest eigenvalues of the squared preconditioned fermion matrix $\tilde{Q}^2$ versus the non-preconditioned one

speed up the code: determinant breakup

- use the factorization of the fermionic determinant in several factors, also allowing for some "fractional" number of flavours

$$|\det(\tilde{Q})|^{N_f} = \left[|\det(\tilde{Q}^2)|^{\frac{N_f}{2n_B}}\right]^{n_B}$$

- measurement correction: reweighting

$$\lim_{n_4\to\infty} P^{(1)}_{n_1}(x)P^{(2)}_{n_2}(x)P^{(4)}_{n_4}(x) \text{ with } P^{(4)}_{n_4}(x) = \frac{1}{\sqrt{P^{(2)}_{n_2}}}$$

- after reweighting, the expectation value of a quantity A is given by

$$\langle A\rangle = \frac{\left\langle A\exp\left\{\eta^\dagger\left[1-P^{(4)}_{n_4}(Q^\dagger Q)\right]\eta\right\}\right\rangle_{U,\eta}}{\left\langle \exp\left\{\eta^\dagger\left[1-P^{(4)}_{n_4}(Q^\dagger Q)\right]\eta\right\}\right\rangle_{U,\eta}}$$

the polynomials

- $$P^{(1)}_{n_1} \simeq \frac{1}{x^\alpha}$$
- $$P^{(2)}_{n_2} \simeq \frac{1}{P^{(1)}_{n_1}(x)x^\alpha}$$
- $$P^{(4)}_{n_4}(x) = \frac{1}{\sqrt{P^{(2)}_{n_2}(x)}}$$

some results

- some results from the SUSY simulation

energy after conj. momenta:	1.526861e+03
energy after scalar fields:	7.600982e+03
energy after gauge fields:	5.581101e+03
energies: 5.581101e+03, 5.581198e+03	diff= -9.690565e-02
Noisy correction exponent for kapNum=0:	6.465429e+01
Average absolute value of DeltaH:	1.287792e+00
Average exponential of DeltaH:	9.879714e-01
Average acceptance rate in HMC-Trajectory:	5.000000e-01
Average absolute value of gauge force:	1.978851e+00
Average maximal value of gauge force:	8.895543e+00
Average absolute value of quark force:	5.223487e-01
Average maximal value of quark force:	3.770504e+00
Average acceptance rate of NoisyCorr:	0.000000e+00
Average exponential of NoisyCorr:	6.384178e+01

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