Computing the density of states with the global Hybrid Monte Carlo

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Outline

Motivations

- Monte-Carlo simulations are very effective for observables that can be written as expectation values over a probability measure.

$$\widehat{O} = \langle O \rangle \tag{1}$$

- They are not as efficient when they deal with free energies or partition functions. [1]

- They are not suitable for system with complex action.

[1] P. de Forcrand, M. D'Elia, and M. Pepe, Phys.Rev.Lett.86, 1438

The density of states

- Let us consider an euclidean quantum fied theory

$$Z = \int [D\phi] e^{-\beta S[\phi]} \tag{2}$$

The density of states

$$\rho(S) = \int [D\phi] \delta(S[\phi] - S) \tag{3}$$

- Which leads to

$$\langle O \rangle = \frac{\int \rho(S) O(S) e^{-\beta S}}{\int \rho(S) e^{-\beta S}} \tag{4}$$

Analytic support function

- The basic idea is to multiply the usual probability density by a strongly localized function
- The natural choice being a gaussian

$$\langle\langle f(S)\rangle\rangle_{a,S0,\sigma} = \frac{1}{Z}\int_{-\infty}^{+\infty} f(S)\rho(S)e^{-aS}e^{-\frac{(S-S_0)^2}{\sigma^2}}dS \qquad (5)$$

with

$$Z = \int_{-\infty}^{+\infty} \rho(S)e^{-aS}e^{-\frac{(S-S_0)^2}{\sigma^2}}dS \qquad (6)$$

- We can choose $f(S) = \Delta S = S - S_0$

$$\langle\langle \Delta S \rangle\rangle_{a,S_0,\sigma} = \frac{1}{Z}\int_{-\infty}^{+\infty} (S - S_0)\rho(S) e^{-aS} e^{-\frac{(S-S_0)^2}{\sigma^2}} dS \qquad (7)$$

- It is possible to expand the r.h.s. in power of σ

$$\langle\langle \Delta S \rangle\rangle_{a,S_0,\sigma} = c\sigma^2 \left(\left.\frac{d\rho}{dS}\right|_{S_0} - a\rho(S_0) \right) + \mathcal{O}(\sigma^6) \qquad (8)$$

Fundamental relation

Fundamental relation between $\langle\langle \Delta S \rangle\rangle_{a,S_0,\sigma}$ and the coefficients a

$$\langle\langle \Delta S \rangle\rangle_{a,S_0,\sigma} = 0 \rightarrow a = \left.\frac{d \log(\rho(S))}{ds}\right|_{S_0} + \mathcal{O}(\sigma^5) \qquad (9)$$

- The DoS can be constructed from the a coefficients

$$\rho(S) = \rho_0 \left(\prod_{k=1}^{N-1} e^{a_k \sigma} \right) e^{a_N (S - S_N) + \mathcal{O}(\sigma^5)} \qquad (10)$$

- The problem to compute the DoS is reduced to finding the root of $\langle\langle \Delta S \rangle\rangle_{a,S_0,\sigma}$ solved by Robbins-Monro 1952

The probability weight

- In order to compute $\langle\langle \Delta S \rangle\rangle_{a,S_0,\sigma}$ the weight that needs to be sampled is

$$W(S[\phi], S_0, \sigma, a) \propto e^{-aS} e^{-\frac{(S-S_0)^2}{\sigma^2}} = e^{-U[\phi,S_0,\sigma,a]} \quad (11)$$

Definition of a potential energy

$$U[\phi, S_0, \sigma, a] = \frac{(S[\phi] - S_0)^2}{\sigma^2} + aS[\phi] \quad (12)$$

- Which is analytic and can be used to define the Hamiltonian evolution of the HMC.

The HMC

- The Hamiltonian is given by

$$H\left[p_i,\phi_i\right] = \sum_i \frac{p_i p_i}{2} + aS\left[\phi\right] + \frac{\left(S\left[\phi\right] - S_0\right)^2}{\sigma^2}, \qquad (13)$$

where S is the usual action.

The force

$$f_i = -\frac{\partial H}{\partial \phi_i} = -\frac{\partial S}{\partial \phi_i}\left(a + \frac{2}{\sigma^2}(S - S_0)\right) \qquad (14)$$

- The Hamiltonian evolution can be performed with the standard leapfrog method.

The HMC

- Usual metropolis step at the end of the Hamiltonian evolution
- The acceptance can be tuned to be as high as wanted changing the integration step
- During thermalization the forces are very big while they became much smaller once the action is close to S_0.
- The integration needs to be adaptive
- Can be combined with replica exchange method, see next seminar by B. Lucini

Application to the energy momentum tensor in Yang-Mills

- The energy momentum tensor $T_{\mu\nu}$ is the current of the traslational symmetry.
- When the regulator of the theory preserves traslational invariance it does not renormalize.
- In pure gauge theory is given by

$$T_{\mu\nu} = \frac{1}{g^2}\left\{ F_{\mu\alpha}F_{\nu\alpha} - \frac{1}{4}\delta_{\mu\nu}F_{\alpha\beta}F\alpha\beta \right\} \tag{15}$$

- On the lattice translational symmetry is broken and it needs to be renormalized

$$T_{\mu\nu} = Z_T \left\{ T^{[1]}_{\mu\nu} + z_t T^{[3]}_{\mu\nu} + z_s \left(T^{[2]}_{\mu\nu} - \langle T^{[2]}_{\mu\nu} \rangle \right) \right\} \tag{16}$$

The energy momentum tensor on the lattice

- Using shifted boundary condition

$$A(L_0, \mathbf{x}) = A(0, \mathbf{x} - L_0 \boldsymbol{\xi}) \tag{17}$$

it is possible to write Ward Identities[2] that fix the normalization constant

Determination of Z_T

$$Z_T(\beta) = \frac{f(\beta, L_0, \boldsymbol{\xi} - a\hat{k}L_0) - f(\beta, L_0, \boldsymbol{\xi} + a\hat{k}L_0)}{2a} \frac{1}{\langle T^{[1]}_{0k}(\beta)\rangle_{\boldsymbol{\xi}}} \tag{18}$$

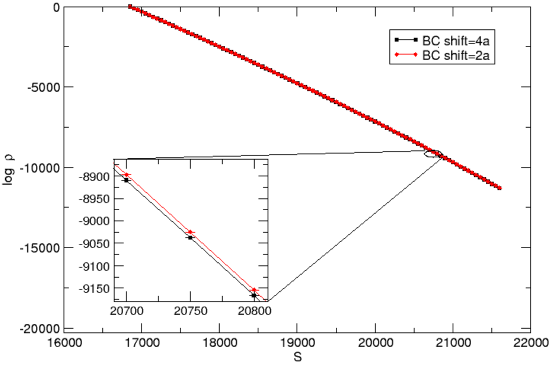
where

$$f(\beta, L_0, \boldsymbol{\xi}) = \frac{\log \int dS e^{(-\beta S)} \rho(S)}{V} + c \tag{19}$$

[2] L. Giusti and M. Pepe Phys. Rev. D 91, 114504

The DoS in SU(2)

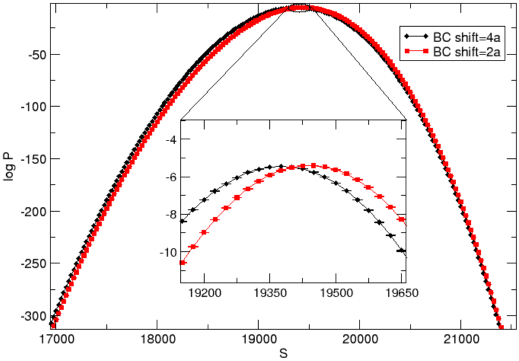
Computation time 48 hours per point, but covers a range of β.



$$\text{Vol} = 12^3 x3 \text{ and shift} = \left(\frac{4}{3}, 0, 0\right), \ \left(\frac{2}{3}, 0, 0\right)$$

The probability density in SU(2)

$$\Delta f = \frac{1}{V}\left[\log\left(\int dS e^{-\beta S}\rho_{\xi}(S)\right) - \log\left(\int dS e^{-\beta S}\rho_{\xi'}(S)\right)\right] = 0.002319(21)$$



β=2.36869, vol $= 12^3 x3$ and shift $= \left(\frac{4}{3}, 0, 0\right), \left(\frac{2}{3}, 0, 0\right)$

Conclusions

- We presented an algorithm to compute the DoS using the global Hybrid Montecarlo
- The method seems to be very efficient in pure $SU(N)$ Yang-Mills
- Computations of the energy momentum tensor and thermodynamics properties are in progress

  Future developments
- Inclusion of fermions which is straightforward