Field-Transformation HMC algorithm

Luchang Jin ljin.luchang@gmail.com

University of Connecticut / RIKEN BNL Research Center

$$U = \mathscr{F} V \tag{1}$$

$$\int \mathscr{D} U \exp\left(-S(U)\right) \mathscr{O}(U)$$
$$= \int \mathscr{D} V \det\left(\mathscr{F}_* = \frac{\partial U(V)}{\partial V}\right) \exp\left(-S(\mathscr{F} V)\right) \mathscr{O}(\mathscr{F} V) \tag{2}$$
$$= \int \mathscr{D} V \exp\left(-S_{\rm FT}(V)\right) \mathscr{O}(\mathscr{F} V) \tag{3}$$

Hybrid Monte Carlo (HMC) algorithm

- Standard algorithm to generate gauge configurations in lattice QCD simulations.

$$\langle \mathscr{O}(U) \rangle_{\rm QCD} = \frac{1}{\mathscr{Z}} \int \mathscr{D} U \exp\left(-S(U)\right) \mathscr{O}(U) \tag{4}$$

where S is the action, e.g. $S_{\rm Wilson} = \beta \sum_P \mathrm{Re} \frac{1}{3} \mathrm{tr}(1 - U_P)$.

- We evolve a system with the following Hamiltonian

$$H = \sum_i \frac{1}{2} \pi_i^2 + S(U) \tag{5}$$

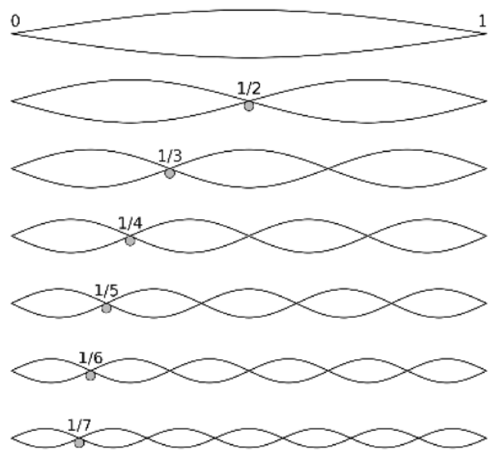
Every trajectory, we reinitialize the canonical momentum π_i with independent Gaussian random numbers of uniform width. After enough trajectories, the gauge field U will follow the desired distribution.

- With dynamical fermions

$$\int \mathscr{D} U \mathscr{D} \phi \exp\left(-S(U) - \phi^\dagger \frac{1}{D^\dagger D(U)} \phi\right) \tag{6}$$

Critical slowing down

- When the lattice spacing is small, QCD configuration has a lot of short wave-length, perturbative modes.



- These modes will oscillate with frequencies inversely proportion to the amplitudes of the modes. As an example, for a simple harmonic oscillator system

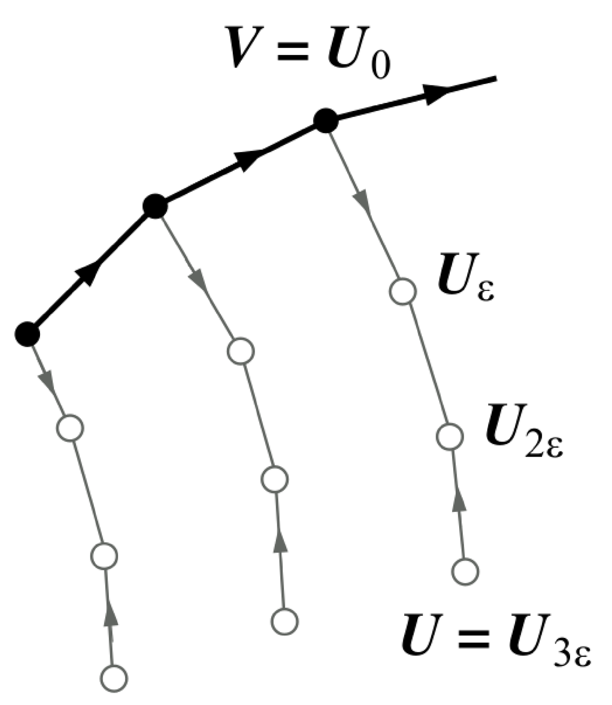
$$H_{\rm SHO} = \frac{1}{2} p^2 + \frac{1}{2} \omega^2 x^2 = \frac{1}{2} p^2 + \frac{1}{2} \frac{1}{A^2} x^2. \tag{7}$$

For QCD, the amplitudes of the modes is proportion to the wavelength of the modes.

Question: How far should we integrate the system to decorrelate?
Answer: Depends on the wavelength - disaster!

– Peter Boyle

Lüscher's trivializing map



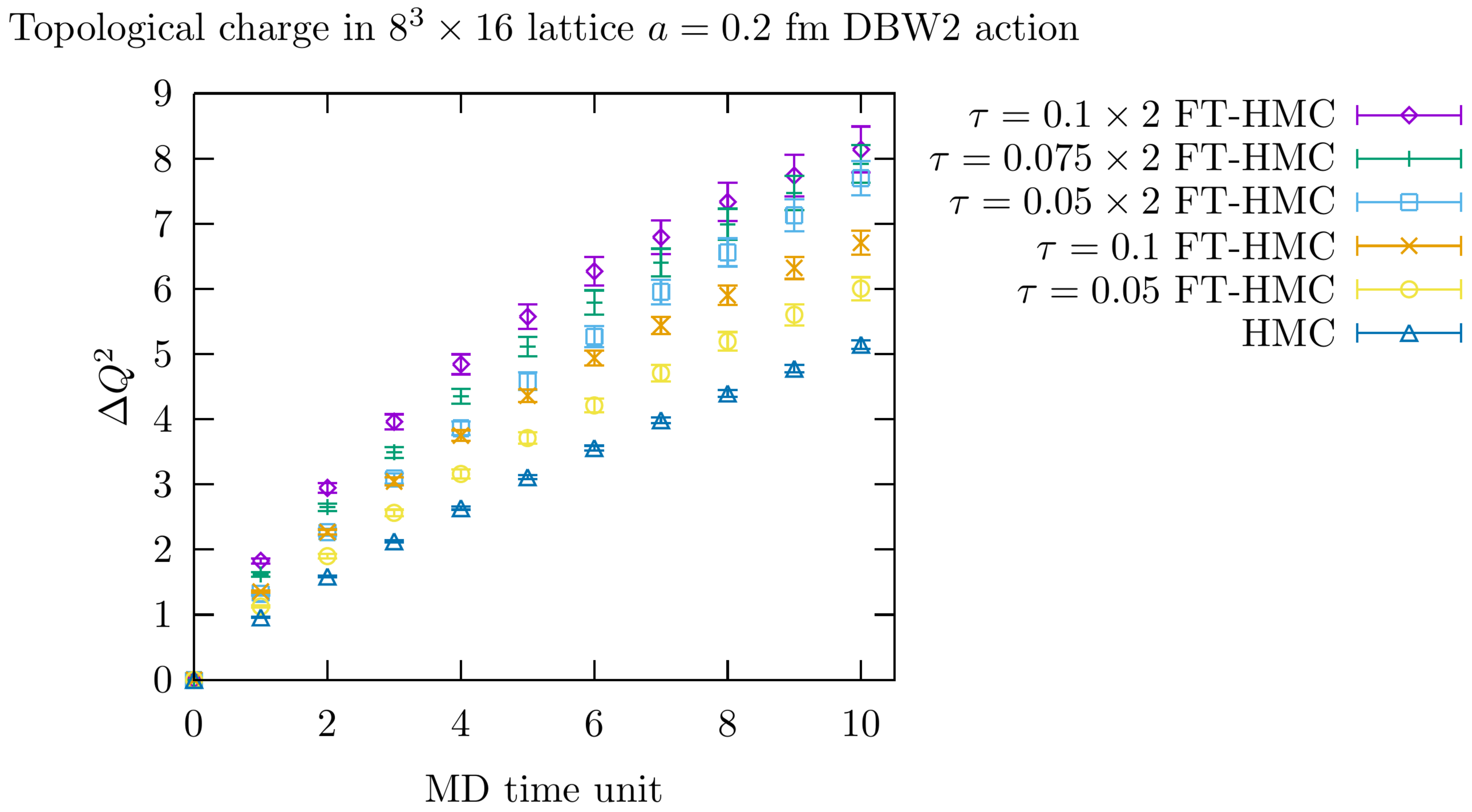
In Ref [1], M. Lüscher showed that

- There are field transformations that which trivializing the theory. That is, the action after the transformation is constant.

$$S_{\rm FT}(V) = S\left(\mathscr{F}(V)\right) - \ln \det \mathscr{F}_*(V) \tag{8}$$

- The Wilson flow trivializes the Wilson action pure gauge theory when β is small. One can calculate the trivializing transformation order by order perturbatively as an expansion in β.
- Use the (approximate) trivializing transformation in HMC may reduce auto-correlation. Concrete algorithm and formulas are given.

Numerical test on pure gauge QCD (4D)



Use discrete Wilson flow as the field transformation (Stout smearing). The flow time is τ.

Field transformation HMC with dynamical fermions

$$\int \mathscr{D} U \mathscr{D} \phi \exp\left(-S(U) - \phi^\dagger \frac{1}{D^\dagger D(U)} \phi\right)$$
$$= \int \mathscr{D} V \mathscr{D} \phi \det(\mathscr{F}_*) \exp\left(-S(\mathscr{F} V) - \phi^\dagger \frac{1}{D^\dagger D(\mathscr{F} V)} \phi\right) \tag{9}$$

The force in HMC transform in the following way:

$$F(U) = -\frac{\partial}{\partial U}\left(S(U) + \phi^\dagger \frac{1}{D^\dagger D(U)} \phi\right) \tag{10}$$

$$F_{\rm FT}(V) = F(\mathscr{F} V) \mathscr{F}_* + \frac{\partial}{\partial V} \det(\mathscr{F}_*) \tag{11}$$

Outlook

- Test the algorithm with dynamical fermions.
- Analytical calculation of the trivializing map to higher orders.
- Machine learn the transformation (many emerging works).
  - MIT group has constructed a machine learned transformation which approximately trivialize the QCD gauge field. [2].
  - Xiao-Yong Jin's talk at 13:45 Thu. Machine learn the transformation for FT-HMC in 2D U(1) case.
  - Sam Foreman's poster on 2D U(1) FT-HMC with machine learned transformations.

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References

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[2] D. Boyda, G. Kanwar, S. Racanière, D. J. Rezende, M. S. Albergo, K. Cranmer, D. C. Hackett and P. E. Shanahan, Phys. Rev. D **103**, no.7, 074504 (2021) doi:10.1103/PhysRevD.103.074504 [arXiv:2008.05456 [hep-lat]].