ETH zürich

QUANTUM SIMULATIONS OF GAUGE THEORIES

Fermions on the Lattice

Author
Roshni Sahoo

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Declaration of originality

The signed declaration of originality is a component of every semester paper, Bachelor's thesis, Master's thesis and any other degree paper undertaken during the course of studies, including the respective electronic versions.

Lecturers may also require a declaration of originality for other written papers compiled for their courses.

I hereby confirm that I am the sole author of the written work here enclosed and that I have compiled it in my own words. Parts excepted are corrections of form and content by the supervisor.

Title of work (in block letters):

FERMIONS ON THE LATTICE

Authored by (in block letters):

For papers written by groups the names of all authors are required.

Name(s):	**First name(s):**
SAHOO	ROSHNI

With my signature I confirm that

- I have committed none of the forms of plagiarism described in the 'Citation etiquette' information sheet.
- I have documented all methods, data and processes truthfully.
- I have not manipulated any data.
- I have mentioned all persons who were significant facilitators of the work.

I am aware that the work may be screened electronically for plagiarism.

Place, date	**Signature(s)**
Zürich, 11.12.23	Roshni Sahoo

For papers written by groups the names of all authors are required. Their signatures collectively guarantee the entire content of the written paper.

Contents

1 Introduction

Quantum Chromodynamics (QCD) is the theory of quarks and gluons or, in other words, the theory of *strongly* interacting particles and fields. Gluons are the elementary particles responsible for mediating the interaction between quarks. QCD is a non-Abelian gauge theory with SU(3) gauge symmetry, i.e., the Lagrangian is invariant under SU(3) gauge transformations. The strong coupling constant decreases at high energy scales, known as asymptotic freedom. In the low-energy regime, the coupling constant increases to a point where the perturbative series no longer converges, and non-perturbative methods such as lattice QCD have to be used. In this regime, quarks form bound states (baryons and mesons) whose masses cannot be determined using perturbative techniques. Thus, lattice QCD becomes extremely important for understanding the theory at low energies. This report describes two algorithms widely used to simulate QCD at low energies and then discusses their limitations and the recent advancements to improve their performance.

2 Lattice Quantum Chromodynamics

To obtain the lattice path integral for QCD, we need to discretize the continuum Euclidean action. This section reviews the basic formulas in lattice QCD, followed by a description of dynamical fermions that then leads to a discussion of algorithms for simulating dynamical fermions in section 3.

2.1 Lattice Path Integral

The action for QCD (in Euclidean space) in the continuum case is given by

$$S_E = \int d^4x \big[\bar{\psi}(x)\left(\gamma_\mu(\partial_\mu + igA^a_\mu T^a) + m\mathbb{1}\right)\psi(x) \; + \; \frac{1}{4}G^{(a)}_{\mu\nu}G^{(a)}_{\mu\nu}\big] \tag{1}$$

The Euclidean action can be divided into the fermionic action and gauge action.

$$S_F = \int d^4x\, \bar{\psi}(x)(\gamma_\mu(\partial_\mu + igA^a_\mu T^a) + m\mathbb{1})\psi(x), \qquad S_G = \int d^4x\, \frac{1}{2}Tr[G_{\mu\nu}G_{\mu\nu}] \tag{2}$$

To do numerical simulations of QCD, the Euclidean action must be discretized such that,

$$x \longrightarrow n \in \Lambda = \{n = (n_1, n_2, n_3, n_4), \quad n_i = 1, ..., (N-1)\}$$

Lattice Gauge Action
QCD has the internal symmetry of rotations in the colour space. So, the action has to be invariant under such rotations, and this enforces the introduction of link variables (gauge fields) $U_\mu(n)$ on

the lattice. The link variables are elements of the SU(3) groups and invariant under this symmetry. The gauge action is constructed as follows,

$$S_G[U] = \frac{2}{g^2} \sum_{n\in\Lambda} \sum_{\mu<\nu} Re\, tr[\mathbb{1} - U_{\mu\nu}(n)] \tag{3}$$

$U_{\mu\nu}$ is called a *plaquette* which is a product of only 4 link variables,

$$U_{\mu\nu} = U_\mu(n)\, U_\nu(n+\hat{\mu})\, U_{-\mu}(n+\hat{\mu}+\hat{\nu})\, U_{-\nu}(n+\hat{\nu})$$

Lattice Fermion Action

The discretized fermion action in the presence of gauge fields is,

$$S_F[\psi,\bar{\psi},U] = a^4 \sum_{n\in\Lambda} \bar{\psi}(n)\Big(\sum_{\mu=1}^{4} \gamma_\mu \frac{U_\mu(n)\psi(n+\hat{\mu}) - U_{-\mu}(n)\psi(n-\hat{\mu})}{2a} + m\psi(n)\Big) \tag{4}$$

The naive fermion action can also be written in the following format,

$$S_F[\psi,\bar{\psi},U] = a^4 \sum_{n,m\in\Lambda} \sum_{a,b,\alpha,\beta} \bar{\psi}(n)^a_\alpha D(n|m)^{ab}_{\alpha\beta} \psi(m)^b_\beta \tag{5}$$

$$D(n|m)^{ab}_{\alpha\beta} = \sum_{\mu=1}^{4} (\gamma_\mu)_{\alpha\beta} \frac{U_\mu(n)_{ab}\delta_{n+\hat{\mu},m} - U_{-\mu}(n)_{ab}\delta_{n-\mu,\hat{m}}}{2a} + m\delta_{\alpha\beta}\delta_{ab}\delta_{n,m} \tag{6}$$

$D(n|m)$ is the naive Dirac operator on the lattice. However, this naive discretization of the fermion action results in 15 additional unphysical degrees of freedom called *doublers*. Wilson and Staggered fermions are implemented to remove these doublers.

The Wilson's Dirac operator on the lattice is,

$$D^W(n|m)^{ab}_{\alpha\beta} = \Big(m + \frac{4}{a}\Big)\delta_{\alpha\beta}\delta_{ab}\delta_{n,m} - \frac{1}{2a}\sum_{\mu=\pm1}^{\pm4} (\mathbb{1}-\gamma_\mu)_{\alpha\beta}\, U_\mu(n)_{ab}\delta_{n+\mu,\hat{m}} \tag{7}$$

The doublers have reduced from 16 to 1 in the Wilson's Dirac operator. Whereas, in the case of Staggered/ Kogut-Susskind fermions [1, 2], the doublers (or flavours) reduce from 16 to 4 while preserving chiral symmetry, which is not preserved in the case of Wilson fermions. The staggered Dirac operator is as follows:

$$D^{st}(n|m) = m\delta_{n,m} + \sum_{\mu=1}^{4} \eta_\mu(n) \frac{U_\mu(n)\delta_{n+\hat{\mu},m} - U_{-\mu}(n-\hat{\mu})\delta_{n-\hat{\mu},m}}{2a} \tag{8}$$

where η_μ are the staggered sign functions introduced because of performing a staggered transformation to eliminate γ_μ in the naive Dirac operator.

The Euclidean correlators as a lattice path integral can then be written as,

$$\langle O_2(t)O_1(0)\rangle = \frac{1}{Z}\int \mathcal{D}[\bar{\psi},\psi]\,\mathcal{D}[U]\, e^{-S_F[\bar{\psi},\psi,U]} e^{-S_G[U]}\, O_2[\bar{\psi},\psi,U]\, O_1[\bar{\psi},\psi,U] \tag{9}$$

The partition function is then,

$$Z = \int \mathcal{D}[\bar{\psi}, \psi]\, \mathcal{D}[U]\, e^{-S_F[\bar{\psi},\psi,U]} e^{-S_G[U]} \tag{10}$$

This completes the brief overview of lattice QCD, and now we will delve into some essential concepts crucial for simulating fermions on the lattice.

2.2 Fermion Determinant

Fermions obey fermi-statistic, meaning that one must use Grassman (anti-commuting) numbers for quark fields. Considering only the fermionic part of the path integral,

$$Z_F[U] = \int \mathcal{D}[\bar{\psi}, \psi]\, e^{-S_F[\bar{\psi},\psi,U]} \tag{11}$$

The fermion path integral Z_F can be rewritten as a determinant with some algebra,

$$Z_F = \det[D] \tag{12}$$

where D is the massive Dirac operator on the lattice. We have essentially integrated out the quarks from the partition function in equation (11). This is crucial for simulating QCD on a computer.

For 1 u and 1 d quark the partition function in equation (11) takes the form,

$$Z = \int \mathcal{D}[U]\, e^{-S_G[U]}\, \det[D_u]\, \det[D_d] \tag{13}$$

To perform Monte Carlo simulations for fermions, Z has to be used as a weight for the distribution of gauge fields. This is problematic because the fermion determinant is a function of the gauge fields U and must be computed for every new gauge configuration created. The Dirac operator is a huge matrix with $12|\Lambda|$ rows and columns, so this number is huge for very large lattices. So, to avoid computing the fermion determinant, the first simulations of QCD were done using the quenched approximation in which the determinant was set to unity. This approximation has a major drawback as it neglects the quark vacuum loops because the determinant becomes 1 in the limit $m \longrightarrow \infty$, and the quarks can no longer be generated from the vacuum as particle-antiparticle pairs. Thus, there is a need for ***dynamical quarks*** [3] to simulate QCD as opposed to *quenched quarks*, and one has to take into account the fermion determinant in the partition function.

2.3 Dynamical Fermions

For the partition function Z in equation (13) to act as a suitable weight for Monte Carlo sampling, the fermion determinant has to be real and nonnegative. In general, chiral symmetry along with γ_5-hermiticity [4] ensures that $\det[D]$ is real and positive. Wilson fermions explicitly break chiral symmetry, so the determinant could take on negative values. On the other hand, Staggered

fermions preserve chiral symmetry and obey γ_5-hermiticity; thus, the determinant is always real and nonnegative (strictly positive for nonzero quark masses). To circumvent this problem, it is assumed that the u and d quarks are mass-degenerate so that,

$$\det[D_u]\det[D_d] = \det[D_{ud}]^2 = \det[D_{ud}D_{ud}^\dagger]$$

where D_{ud} takes the average mass of u and d quarks. However, in the case of a chiral, γ_5-hermitian Dirac operator like the Staggered operator, odd powers of the determinant can also lead to a suitable weight for MC evaluations.

Pseudofermions

The fermion determinant can be expressed as a Gaussian integral over bosonic fields with the same degrees of freedom as fermionic fields, thus the term 'pseudofermions'. Suppose $\phi(n) = \phi_R + i\phi_I$ is a complex scalar (bosonic) field. So, as before, for two mass degenerate u and d quarks,

$$\det[DD^\dagger] = \pi^{-N}\int \mathcal{D}[\phi_R]\mathcal{D}[\phi_I]\, e^{-\phi^\dagger(DD^\dagger)^{-1}\phi} \tag{14}$$

$$\int \mathcal{D}[\bar{\psi}]\mathcal{D}[\psi]\, e^{-\bar{\psi}_u D\psi_u - \bar{\psi}_d D\psi_d} = \pi^{-N}\int \mathcal{D}[\phi_R]\mathcal{D}[\phi_I]\, e^{-\phi^\dagger(DD^\dagger)^{-1}\phi}$$

In this particular formulation, the determinant must be positive to ensure the convergence of the bosonic Gaussian integrals.

Effective Fermion Action

The fermion determinant can be rewritten as an extra term added to the gauge action in the partition function, hence called 'effective action'. This transformation relies on the fact that a positive Dirac operator D can be written as an exponential trace of the logarithm of D.

$$\det[D] = \exp(\mathrm{tr}[\ln(D)]) = \exp(-S_F^{eff}) \tag{15}$$

Thus, this formulation is valid for either an even number of degenerate mass Wilson fermions or any (even or odd) number of Kogut-Susskind fermions.

3 Algorithms for Lattice QCD Simulations

Simulation of pure SU(3) gauge theory can be done using standard Monte Carlo algorithms by generating gauge field configurations U_n, distributed with probability $P_S = \frac{1}{Z}\exp(-S_G[U_n])$. A sequence of gauge field configurations is generated using Markov chains, and this process is called Markov Chain Monte Carlo (MCMC). Any Markov process will converge to a fixed equilibrium point given that P_S is ergodic and satisfies the detailed balance. The advancement from one field configuration to the next is done using the Metropolis algorithm. The Metropolis algorithm has two steps to it - 1) Choose a new gauge configuration with some selection probability P_C. 2) Accept or reject the new configuration with probability P_A such that,

$$P_A(U \to U') = \min\Big(1, \frac{P_S(U')P_C(U' \to U)}{P_S(U)P_C(U \to U')}\Big)$$

And finally, 3) Repeat the steps from the beginning. Once the gauge configurations are generated, the goal is to compute the expectation value of some operator $\langle O \rangle$. The mean $\bar{O}$ is accurate up to $\mathcal{O}(1/\sqrt{N})$ as $N \to \infty$, where N is the total number of configurations. The Wilson gauge action is an extremely local quantity, i.e., every link variable is coupled to other link variables in its neighbourhood.

To perform simulations including dynamical fermions, the gauge field configurations have to be distributed according to the probability $P_S = \frac{1}{Z}\, e^{-(S_G[U] - S_F^{eff}[U])}$, and standard Monte Carlo techniques cannot be used because the effective fermion action is highly nonlocal. This means that every time you compute the change in the total action to generate a new gauge configuration, you must consider all link variables, i.e., the state of the whole system. To tackle this problem, people came up with the idea of using the hybrid molecular dynamics/Langevin algorithm. Two such algorithms - the Hybrid Monte Carlo and the R algorithm for simulating QCD are reviewed in detail in the following sections.

3.1 Hybrid Monte Carlo

The Hybrid Monte Carlo [5] (HMC) uses hybrid molecular dynamics and a leapfrog algorithm for integration. The entire system evolves with the equations of motion dependent on a fictitious time variable, also known as computer time τ. The equations of motion are solved to update the gauge fields at all lattice sites parallelly, followed by a Metropolis accept/reject step. New configurations must be taken with a relatively high probability that doesn't depend too strongly on the system's volume. Secondly, the correlations between consecutive configurations should be as small as possible.

As done by the original authors of the HMC, we consider two mass degenerate u and d quarks. The HMC uses that the fermion determinant can be rewritten as bosonic Gaussian integral as in equation (14). Taking two mass degenerate quarks guarantees that the bosonic integral will converge, while also allowing us to generate the pseudofermion fields from a global heat bath. The partition function is now as follows,

$$Z = \int \mathcal{D}[U]\mathcal{D}[\phi^\dagger]\mathcal{D}[\phi]\, e^{-S_G[U]}\, e^{-\phi^\dagger (DD^\dagger)^{-1}\phi} = \int \mathcal{D}[U]\mathcal{D}[\phi^\dagger]\mathcal{D}[\phi]\, e^{-S} \tag{16}$$

To do Hamiltonian dynamics, we introduce the momenta $P_\mu(n)$ conjugate to gauge link variables $U_\mu(n)$, which are traceless and hermitian matrices. P is generated from the Gaussian distribution $\exp\frac{1}{2}(-\mathrm{tr}[P^2])$, this is known as momenta refreshment. P and U are evolved in time τ using the Hamiltonian,

$$\mathcal{H}(U,P) = \frac{1}{2}\mathrm{tr}[P^2] + S_G[U] + \phi^\dagger (DD^\dagger)^{-1}\phi \tag{17}$$

$$U = \exp\left(i\sum_{a=1}^{9-1} \omega^a T^a\right) \equiv \exp(iQ), \qquad P_\mu(n) = \sum_{a=1}^{8} P_\mu^a(n) T^a \tag{18}$$

$$\mathrm{tr}(P^2) = \sum_{n,\mu} \mathrm{tr}(P_\mu(n)^2) = \sum_{n,\mu,a} (P_\mu^a(n))^2$$

The field configurations are generated with probability,

$$P_S = \frac{1}{Z} \exp(-\mathcal{H}) \qquad \text{with} \qquad Z = \int \mathcal{D}[U]\mathcal{D}[\phi^\dagger]\mathcal{D}[\phi]\mathcal{D}[P]\, e^{-\mathcal{H}} \tag{19}$$

The pseudofermion fields ϕ are generated using Gaussian random numbers R from the distribution $\exp(-RR^\dagger)$ and then determining,

$$\phi = D^\dagger[U]R \tag{20}$$

During the molecular dynamics steps, the pseudofermion field is kept fixed. Since gauge links are elements of the SU(3) group, the conjugate momenta are the real variables $P_\mu^a(n)$ conjugate to the real variables ω^a. Thus, there are eight such conjugate variables for each link because a takes N^2-1 values. The field configurations are then evolved in time τ using the Hamiltonian equations of motion. To get the equations of motion, you must take the derivative of $\mathcal{H}$ w.r.t. Q and P.

$$\dot{Q} = \frac{\partial \mathcal{H}}{\partial P} = P \tag{21}$$

$$\dot{P} = -\frac{\partial \mathcal{H}}{\partial Q} = \sum_{a=1}^{8} T^a \left(-\frac{\partial S_G[U]}{\partial \omega^a} + \phi^\dagger (DD^\dagger)^{-1} \Big(D \frac{\partial D^\dagger}{\partial \omega^a} + \frac{\partial D}{\partial \omega^a} D^\dagger \Big) (DD^\dagger)^{-1} \phi \right) = F[U,\phi] \tag{22}$$

$F[U,\phi]$ is called the force term, and it lies in the algebra $\mathfrak{su}(3)$. For every iteration of the HMD, one has to compute the derivative of D and the inverse of $DD^\dagger$. The force term calculation is the most expensive part of the algorithm, where one has to find the solution of a set of equations of the form,

$$\chi = (DD^\dagger)^{-1}\phi$$

which is done using iterative solvers such as the conjugate gradient (CG). The Hamiltonian equations of motion are usually solved using the leapfrog integration scheme, which takes the configurations $\{U, P\}$ to $\{U', P'\}$. The MD trajectory must be area-preserving and reversible to satisfy the detailed balance. The leapfrog algorithm is area-preserving and, thus, a suitable candidate for the integration. For a given initial gauge configuration U_0, generate 8 real conjugate momenta variables P_0.

Initial half-step:

$$P(\delta\tau/2) = P(0) - \frac{\delta\tau}{2} F[U,\phi]_{U_0}$$

$n = \tau_0/\delta\tau$ full steps in U and $n-1$ full steps in P, where τ_0 is the amount of time you let the system evolve according to Hamilton's equations.

Intermediate steps:

$$U(\tau+\delta\tau) = \exp[i\delta\tau P(\tau+\delta\tau/2)]\, U(\tau)$$

$$P(\tau+\delta\tau) = P(\tau-\delta\tau/2) - (\delta\tau) F[U,\phi]_{U(\tau)}$$

Final half-step:

$$P(\tau_0) = P(\tau_0 - \delta\tau/2) - \frac{\delta\tau}{2} F[U,\phi]_{U(\tau_0)}$$

Numerical integration is not exact, and so, discretization errors are introduced of $\mathcal{O}(\delta\tau^2)$ in the half-steps and $\mathcal{O}(\delta\tau^3)$ in the full-steps.

At the end of the MD trajectory, the new configurations $\{U', P'\}$ now must be accepted or rejected with probability P_A. This is the Metropolis acceptance step of the algorithm.

$$P_A = \min\Big(1, e^{-\delta\mathcal{H}}\Big), \qquad \delta\mathcal{H} = \mathcal{H}(U', P') - \mathcal{H}(U, P) \tag{23}$$

This essentially means that you must pick a random number $r \in (0, 1]$ and accept the new configuration if $r < e^{-\delta\mathcal{H}}$. The leapfrog integration scheme is inexact and introduces discretization errors because it takes finite step size $\delta\tau$ during the evolution. The Metropolis accept/reject step corrects these errors, making the HMC an exact algorithm.

3.2 R Algorithm

The R algorithm [6] is another algorithm for simulating dynamical fermions that utilizes a molecular dynamics/Langevin algorithm. The critical difference is that the fermion determinant is not rewritten as bosonic Gaussian integrals but as an exponential trace logarithm, as shown in equation (15). To understand the algorithm, let's write down the partition function for real scalar field q and real conjugate momenta variable p.

$$\begin{aligned} Z &= \int \mathcal{D}[q]\mathcal{D}[p]\, e^{-\frac{1}{2}p^2}\, e^{-S_o(q)}\, [\det(D^\dagger D]^{N_f/4} \\ S &= S_o(q) - \frac{N_f}{4}\mathrm{tr}[\ln(D^\dagger D)] \end{aligned} \tag{24}$$

D is the staggered Dirac operator. Thus, the fourth root of the fermion determinant reduces the four tastes to a single quark. The determinant is raised to the power N_f, the number of quark flavours. Rewriting the determinant as bosonic integrals over pseudofermions and implementing the HMC algorithm is not possible as it is difficult to evaluate the nth root of the matrix or its derivative. Thus, the R algorithm is better suited for such calculations.

The molecular dynamics equations required for evolving the q and p fields are,

$$\dot{q} = p, \qquad \dot{p} = -\frac{\partial S_o}{\partial q} + \frac{N_f}{4}\mathrm{tr}\left[\frac{1}{D^\dagger(q)D(q)}\frac{\partial[D^\dagger(q)D(q)]}{\partial q}\right] = -\frac{\partial V(q)}{\partial q} \tag{25}$$

$\dot{p}$ includes a trace, which is problematic because the inverse matrix has to be explicitly calculated in each MD step. Instead, the the $(D^\dagger D)^{-1}$ is replaced by a noisy estimator [7]. The inverse matrix

can be replaced by the projection operator,

$$P_{i,j}^{R_0} = X_i^{R_0} X_j^{R_0 *} \tag{26}$$

$$X^{R_0} = \frac{1}{D^\dagger D} D^\dagger(q) R$$

$$\dot{p}^{R_0} = -\frac{\partial S_o}{\partial q} + \frac{N_f}{4} X^{R_0 *} \frac{\partial [D^\dagger(q) D(q)]}{\partial q} X^{R_0} = -\frac{\partial V(q)^{R_0}}{\partial q} \tag{27}$$

where R is a vector of Gaussian random numbers. This is equivalent to an auxiliary noise field,

$$\phi_{noise} = D^\dagger R$$

$$X^{R_0} = (D^\dagger D)^{-1} \phi_{noise} \tag{28}$$

The key difference between this auxiliary noise field and the pseudofermion field in the HMC algorithm is that the noise field is updated in each molecular dynamics time step instead of keeping it constant for all the time steps for a particular update of the fields. Doing so introduces an error of $\mathcal{O}(\delta\tau^2)$ which then leads to an overall error of $\mathcal{O}(\delta\tau)$ in measured quantities and this is undesired. The noise errors can be made $\mathcal{O}(\delta\tau^3)$ by making a small change to the noisy estimator X^{R_0}.

Suppose we know $q(t)$ and $p(t)$, and we want to find and compute their values after time step $\delta\tau$.

$$q(\tau + \delta\tau) = q(\tau) + (\delta\tau)\, p(\tau + \delta\tau/2) + \mathcal{O}(\delta\tau^3) \tag{29}$$

$$p(\tau + \delta\tau) = p(\tau) - (\delta\tau) \frac{\partial V^R(\tau + \delta\tau/2)}{\partial q} + \mathcal{O}(\delta\tau^3) \tag{30}$$

To calculate $p(\tau + \delta\tau)$, you need to calculate the force term by making a conjugate gradient calculation to obtain,

$$X^R(\tau + \frac{1}{2}\delta\tau) = \frac{1}{D^\dagger(\tau + \frac{1}{2}\delta\tau) D(\tau + \frac{1}{2}\delta\tau)} D^\dagger \left[\tau + \left(\frac{1}{2} - \frac{N_f}{8} \right) \delta\tau \right] R \tag{31}$$

Then, to get $q(\tau + \delta\tau)$,

$$q(\tau + \delta\tau) = q(\tau) + (\delta\tau) \left(\frac{p(\tau) + p(\tau + \delta\tau)}{2} \right) + \mathcal{O}(\delta\tau^3) \tag{32}$$

Note that the noise estimator has been modified so that the auxiliary field ϕ_{noise} is refreshed at an asymmetric time within each time-step, depending on the number of fermions N_f. This gives the overall integration scheme errors of $\mathcal{O}(\delta\tau^3)$ at the cost of making the integration non-area preserving and non-reversible. This makes it impossible to add a Metropolis accept/reject step at the end of the update to correct for the step-size errors incurred during the MD evolution. So, the $\mathrm{R}[\mathrm{R}^0]$ algorithm is expected to have errors of $\mathcal{O}(\delta\tau^2)[\mathcal{O}(\delta\tau)]$ in measured quantities.

For a given gauge configuration $U(\tau)$ and newly refreshed momenta $P(\tau)$ from the Gaussian distribution $\exp(-\frac{1}{2}\mathrm{tr}[P^2])$. We want to use n molecular dynamics steps and find the new configurations $U(\tau + n\delta\tau)$ and $P(\tau + n\delta\tau)$.

Step 1: Generate intermediate U

$$U\left[\tau+\delta\tau\left(\frac{1}{2}-\frac{N_f}{8}\right)\right]=\exp\left[i\delta\tau\left(\frac{1}{2}-\frac{N_f}{8}\right)P(\tau)\right]U(\tau)$$

Step 2: Generate the noise field with Gaussian random vectors R

$$\phi_{noise}=D^\dagger\left[\tau+\delta\tau\left(\frac{1}{2}-\frac{N_f}{8}\right)\right]R$$

Step 3: Update U at midpoint

$$U\left[\tau+\frac{\delta\tau}{2}\right]=\exp\left[i\delta\tau\frac{N_f}{8}P(\tau)\right]U\left[\tau+\delta\tau\left(\frac{1}{2}-\frac{N_f}{8}\right)\right]$$

Step 4: Compute X

$$X=\frac{1}{D^\dagger(\tau+\frac{1}{2}\delta\tau)D(\tau+\frac{1}{2}\delta\tau)}\,\phi_{noise}$$

Step 5: Compute $\dot{P}(\tau+\delta\tau/2)$
Step 6: Compute $P(\tau+\delta\tau)$

$$P(\tau+\delta\tau)=P(\tau)+(\delta\tau)\dot{P}(\tau+\delta\tau/2)$$

Step 7: Unless this is the last MD step, compute

$$U\left[\tau+\delta\tau\left(1-\frac{N_f}{8}\right)+\delta\tau\right]=\exp\left[i\delta\tau\left(\frac{1}{2}-\frac{N_f}{8}\right)P(\tau+\delta\tau)\right]U\left[\tau+\frac{\delta\tau}{2}\right]$$

In the last iteration, leave the loop after step 6 and compute $U(\tau+n\delta\tau)$:

$$U(\tau+n\delta\tau)=\exp\left[i\frac{\delta\tau}{2}\,P(\tau+n\delta\tau)\right]U\left[\tau+(n-\frac{1}{2})\delta\tau\right]$$

This completes the analysis for the R algorithm for dynamical fermions in the presence of gauge fields.

3.3 Limitations & Improvements

Simulating dynamical quarks in the chiral limit is a big challenge as the cost of simulations rapidly increases with decreasing fermion mass as a result of the large condition number $\kappa(D)$ of the Dirac operator D [8]. This increases the number of iterations in the conjugate gradient solver for the inverse of the Dirac operator, which is a large sparse matrix. So, generally, simulations are done for quarks of much heavier masses, and then an extrapolation to the chiral limit is done [9]. As we reach the chiral limit, the step size must be reduced to maintain a constant acceptance rate at the

cost of many Dirac matrix inversions. A simple modification of the pseudofermion action in the HMC algorithm was proposed by Hasenbusch [10] to increase the step size still maintaining a fixed acceptance rate. This is known as 'mass preconditioning'. The idea is to split the pseudofermion action in equation 14 by first rewriting the determinant as,

$$\det[D(U)D^{\dagger}(U)] = \det[\tilde{D}(U)\tilde{D}^{\dagger}(U)]\ \det\left[\frac{1}{\tilde{D}(U)}D(U)D^{\dagger}(U)\frac{1}{\tilde{D}^{\dagger}(U)}\right] \tag{33}$$

where $\tilde{D}(U)$ is the fermion determinant of a heavier quark mass, thereby having a smaller hopping parameter (and condition number). The fermionic action is also split into two parts with two pseudofermions (bosonic) fields ϕ and χ as follows,

$$S = \phi^{\dagger}(\tilde{D}(U)\tilde{D}^{\dagger}(U))^{-1}\phi + \chi^{\dagger}(\tilde{D}(U)D(U)^{-1})\chi \tag{34}$$

The condition number of the Dirac matrices $\tilde{D}$ and $\tilde{D}D^{-1}$ is reduced as compared to D, allowing an increase in the step size $\delta\tau$ results in fewer inversions of Dirac matrices during a given molecular dynamics trajectory. Hasenbuch reported a net gain in the performance by a factor of 2 for their largest value of the hopping parameter for the simulation of 2 mass degenerate quarks.

The limitation of the R algorithm is that it suffers from step-size errors, making it an inexact algorithm. Moreover, it cannot be made exact very easily using a Metropolis acceptance test as its integration scheme is neither area-preserving nor reversible, which violates the detailed balance. An alternative algorithm that cannot only simulate arbitrary flavours of fermions but is also exact is the Rational Hybrid Monte Carlo (RHMC) [11, 12]. The fermion determinant is rewritten as bosonic integrals over pseudofermion field ϕ such that the fermion action $S_F = \phi_l D_l^{-(1/2)}\phi_l + \phi_s^{\dagger} D_s^{-(1/4)}\phi_s$. The square and fourth root Dirac matrices are replaced with rational approximations, and the rest of the algorithm is the same as the HMC.

4 Conclusion

This report explored two basic algorithms that have played a pivotal role in lattice QCD simulations - the Hybrid Monte Carlo and the R algorithm, both of which have advantages and disadvantages. Some algorithmic advancements that speed up computations for the HMC, such as preconditioning and the Rational Hybrid Monte Carlo for exact simulations of an arbitrary number of quark flavours, were outlined. Significant progress has been made in recent decades in algorithmic advancements aimed at reducing the computational costs of dynamical fermions and towards more realistic simulations of QCD. Progress is constantly being made in lattice QCD to better understand the theory of strong interactions at low-energy scales.

References

Gattringer, C., & Lang, C. B. (2010a). More about lattice fermions. In *Quantum chromodynamics on the lattice: An introductory presentation* (pp. 243–266). Springer Berlin Heidelberg. https://doi.org/10.1007/978-3-642-01850-3_10

Kogut, J., & Susskind, L. (1975). Hamiltonian formulation of wilson's lattice gauge theories. *Physical Review D*, *11*(2), 395.

Gattringer, C., & Lang, C. B. (2010b). Dynamical fermions. In *Quantum chromodynamics on the lattice: An introductory presentation* (pp. 185–211). Springer Berlin Heidelberg. https://doi.org/10.1007/978-3-642-01850-3_8

Mohler, D., & Schaefer, S. (2020). Remarks on strange-quark simulations with wilson fermions. *Physical Review D*, *102*(7), 074506.

Duane, S., Kennedy, A. D., Pendleton, B. J., & Roweth, D. (1987). Hybrid monte carlo. *Physics letters B*, *195*(2), 216–222.

Gottlieb, S., Liu, W., Toussaint, D., Renken, R. L., & Sugar, R. L. (1987). Hybrid-molecular-dynamics algorithms for the numerical simulation of quantum chromodynamics. *Phys. Rev. D*, *35*, 2531–2542. https://doi.org/10.1103/PhysRevD.35.2531

Batrouni, G. G., Katz, G. R., Kronfeld, A. S., Lepage, G. P., Svetitsky, B., & Wilson, K. G. (1985). Langevin simulations of lattice field theories. *Phys. Rev. D*, *32*, 2736–2747. https://doi.org/10.1103/PhysRevD.32.2736

Clark, M., & Kennedy, A. (2007a). Accelerating dynamical-fermion computations using the rational hybrid monte carlo algorithm with multiple pseudofermion fields. *Physical review letters*, *98*(5), 051601.

Fukaya, H. (2008). The chiral limit in lattice qcd. *The Origin of Mass and Strong Coupling Gauge Theories*. https://doi.org/10.1142/9789812790750_0019

Hasenbusch, M. (2001). Speeding up the hybrid monte carlo algorithm for dynamical fermions. *Physics Letters B*, *519*(1-2), 177–182.

Horváth, I., Kennedy, A., & Sint, S. (1999). A new exact method for dynamical fermion computations with non-local actions. *Nuclear Physics B-Proceedings Supplements*, *73*(1-3), 834–836.

Clark, M., & Kennedy, A. (2007b). Accelerating dynamical-fermion computations using the rational hybrid monte carlo algorithm with multiple pseudofermion fields. *Physical review letters*, *98*(5), 051601.