ETH zürich

FERMIONS ON THE LATTICE

Dynamical Fermions

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Outline

- **Fermion Determinant**
- **Dynamical Fermions**
  - Pseudofermions
  - Effective Fermion Action
- **Algorithms**
  - Hybrid Monte Carlo
  - R
  - Limitations & Improvements

Fermion Determinant

- Rewrite fermionic partition function as a determinant

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

$$Z = \int \mathcal{D}[U]\; e^{-S_G[U]}\, \det[D]$$

Dirac Operator

- Field configurations distributed according to

$$P_S = \frac{1}{Z} e^{-S_G[U]} \det[D]$$

- Quenched approximation: $\det[D] \rightarrow 1$
- Need to use ***dynamical quarks***
- $\det[D]$ must be real and non-negative

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

2 mass degenerate quarks

Dynamical Fermions

Pseudofermions

$$\phi(n) = \phi_R + i\phi_I$$

Complex Scalar Field

$$\det\left[DD^\dagger\right] = \int \mathcal{D}[\bar{\psi}]\mathcal{D}[\psi]\, e^{-\overline{\psi_u}D\psi_u} e^{-\overline{\psi_d}D\psi_d} \propto \int \mathcal{D}[\phi_R]\mathcal{D}[\phi_I]\, e^{-\phi^\dagger\left(DD^\dagger\right)^{-1}\phi}$$

Gaussian Integral over fermionic fields $\longrightarrow$ Gaussian Integral over bosonic fields

Dynamical Fermions

Effective Fermion Action

$$\det\left[DD^{\dagger}\right] = \exp\left(\mathrm{tr}\left[\ln\left(DD^{\dagger}\right)\right]\right) = \exp(-S_F^{eff})$$

- Valid for even number of mass degenerate Wilson fermions & any number of Staggered fermions
- Effective fermion Action is highly nonlocal, change of action involves all link variables
- Use hybrid molecular dynamics for simulations

Simulations

Pure SU(3) gauge theory $$Z = \int \mathcal{D}[U]\, e^{-S_G[U]}$$

- Generate gauge configurations distributed with probability

$$P_S = \frac{1}{Z}\exp(-S_G[U])$$

- Sequence of gauge field configurations generated using Markov chain (MCMC)
- Advancement from $U \to U'$ done using Metropolis algorithm
  - Accept/reject new configuration with probability

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

Hybrid Monte Carlo

- The HMC [1] algorithm is based on pseudofermion field concept

$$Z = \int \mathcal{D}[\phi^\dagger]\mathcal{D}[\phi]\,\mathcal{D}[U]\,e^{-S_G[U]}\;\;e^{-\phi^\dagger\left(DD^\dagger\right)^{-1}\phi}$$

Hamiltonian: $$\mathcal{H}(U,P) = \frac{1}{2}tr[P^2] + S_G[U] + \phi^\dagger\left(DD^\dagger\right)^{-1}\phi$$

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

$$U = \exp\left(i\sum_{a=1}^{8}\omega^a T^a\right) \equiv \exp(iQ)$$

$$\mathrm{P}_\mu(n) = \sum_{a=1}^{8} P_\mu^a(n)T^a$$

Conjugate momenta

- Generating pseudofermion fields ϕ using vector of Gaussian rand numbers R from $\exp\left(-RR^{\dagger}\right)$

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

- Field configurations evolve with computer time τ
- Molecular Dyamics equations:

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

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

Force term

- Calculate $F[U,\phi]$ in every MD step

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

- Solve MD equations using Leapfrog Integration Scheme to take $U \to U'$
  - Area- preserving & reversible trajectory

- Metropolis acceptance test: $P_A = \min(1, \mathrm{e}^{-\delta\mathcal{H}})$

R Algorithm

- R algorithm [2] is based on the effective fermion action

$$Z = \int \mathcal{D}[q]\mathcal{D}[p]\, \mathrm{e}^{-\frac{1}{2}p^2}\, e^{-S_o(q)} \left[\det\left(D^\dagger D\right)\right]^{\frac{N_f}{4}}$$

Reduces 4 flavours to a single one

- D is Staggered Dirac operator
- Works for any number of quark flavours N_f

$$\mathrm{S} = \mathrm{S_o(q)} - \frac{\mathrm{N_f}}{4}\mathrm{tr}\left[\ln\left(D^\dagger D\right)\right]$$

- MD equations:

$$\dot{q} = p$$

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

- Don't calculate trace of inverse Dirac matrix explicitly
- Replace $\left(D^\dagger D\right)^{-1}$ with a noisy estimator

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

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

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

- Noise field is updated in every time step of MD evolution
- Pseudofermion field is kept constant for a given MD trajectory in HMC
- $\mathcal{O}(\delta\tau)$ errors in measured quantities – undesired!
- Get $\mathcal{O}(\delta\tau^2)$ errors by making small change to X^{R_0}

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

- Noise field is refreshed at an asymmetric time step dependent on N_f
  - Makes MD trajectory non area-preserving & non-reversible
  - Cannot add Metropolis accept/reject step at the end
- R algorithm is an inexact algorithm

Limitations & Improvements

- The HMC is an exact algorithm but only applicable to even number of mass degenerate Wilson fermions or 4 flavours of Staggered fermions
- The R algorithm is an inexact algorithms applicable to any number of fermion flavours of either type
- Alternative: Rational Hybrid Monte Carlo [3,4] for 2+1 flavours:

$$S_F = \phi_l D_l^{-\left(\frac{1}{2}\right)} \phi_l + \phi_s D_s^{-\left(\frac{1}{4}\right)} \phi_s$$

- Mass-preconditioning [5] to speed up HMC,

$$S = \phi^\dagger \left(\tilde{D}\tilde{D}^\dagger\right)^{-1} \phi + \chi^\dagger \left(\tilde{D} D^{-1}\right)^{-1} \chi$$

Dirac operator of heavier quark

  - Can increase step size $\delta\tau$, fewer matrix inversions per MD trajectory

R Algorithm Steps

- For given $U(\tau)$ generate newly refreshed momenta $P(\tau)$
- Generate intermediate U

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

- Generate noise field

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

- Compute U at mid point
- Compute X

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

- Compute $\dot{P}\left(\tau+\frac{\delta\tau}{2}\right)$
- Compute $\dot{P}(\tau+\delta\tau)=P(\tau)+(\delta\tau)\,\dot{P}\left(\tau+\frac{\delta\tau}{2}\right)$
- Compute U at next intermediate point, unless this is the last time step
- After last time step, compute $U(\tau+n\delta\tau)$ where n is number of MD steps

Thank you for listening ☺

References

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