Introduction to Lattice QCD





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Lecture 2: Fermion actions Outline



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- Doubling of "naive" fermions
- Wilson Fermions (WF)
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- 3 Staggered fermions (SF)
 - Symanzik's improvement program

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- The twisted mass Wilson action
- Chiral actions

Improved gauge actions Lüscher-Weisz Action

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Fermion Action

To discretize the Dirac action, Wilson replaced the derivative with the symmetrized difference and included appropriate gauge links to maintain gauge invariance

$$\bar{\psi}D\psi = \frac{1}{2a}\bar{\psi}(x)\sum_{\mu}\gamma_{\mu}[U_{\mu}(x)\psi(x+\hat{\mu}) - U^{\dagger}_{\mu}(x-\hat{\mu})\psi(x-\hat{\mu}).s$$

It is easy to see that one recovers the Dirac action in the limit $a \rightarrow 0$ by Taylor expanding the U_{μ} and $\psi(x + \hat{\mu})$ in powers of the lattice spacing a. Keeping only the leading term in a

$$\begin{aligned} &\frac{1}{2a}\bar{\psi}(x)\gamma_{\mu}\left[\left.\left(1+iagA_{\mu}(x+\hat{\mu})+\ldots\right)\left(\psi(x)+a\psi'(x)+\ldots\right)-\right.\right.\right.\\ &\left.\left.\left(1-iagA_{\mu}(x-\hat{\mu})\right)+\ldots\right)\left(\psi(x)-a\psi'(x)+\ldots\right)\right.\right.\right] \\ &= &\bar{\psi}(x)\gamma_{\mu}(\partial_{\mu}+\frac{a^{2}}{6}\partial_{\mu}^{3}+\ldots)\psi(x)\\ &\left.+ig\bar{\psi}(x)\gamma_{\mu}\left[A_{\mu}+\frac{a^{2}}{2}\left(\frac{1}{4}\partial_{\mu}^{2}A_{\mu}+(\partial_{\mu}A_{\mu})\partial_{\mu}+A_{\mu}\partial_{\mu}^{2}\right)+\ldots\right]\psi(x),\end{aligned}$$

which, to $O(a^2)$, is the kinetic part of the standard continuum Dirac action in Euclidean space-time. Thus one arrives at the simplest (called "naive") lattice action for fermions

$$S^{N} = m_{q} \sum_{x} \bar{\psi}(x)\psi(x) + \frac{1}{2a} \sum_{x} \bar{\psi}(x)\gamma_{\mu} \left[U_{\mu}(x)\psi(x+\hat{\mu}) - U_{\mu}^{\dagger}(x-\hat{\mu})\psi(x-\hat{\mu}) \right]$$
$$\equiv \sum_{x} \bar{\psi}(x)M_{xy}^{N}[U]\psi(y)$$

where the interaction matrix M^N is

$$\mathcal{M}_{i,j}^{N}[U] = m_q \delta_{ij} + \frac{1}{2a} \sum_{\mu} \left[\gamma_{\mu} U_{\mu}(i) \delta_{i,j-\mu} - \gamma_{\mu} U_{\mu}^{\dagger}(i-\mu), \delta_{i,j+\mu} \right]$$

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The Euclidean γ matrices are hermitian, $\gamma_{\mu} = \gamma^{\dagger}_{\mu}$, and satisfy $\{\gamma_{\mu}, \gamma_{\nu}\} = 2\delta_{\mu\nu}$. Non-relativistic representation

$$\vec{\gamma} = \begin{pmatrix} 0 & i\vec{\sigma} \\ -i\vec{\sigma} & 0 \end{pmatrix} , \quad \gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} , \quad \gamma_5 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$$

which is related to Bjorken and Drell conventions as follows: $\gamma_i = i\gamma_{BD}^i$, $\gamma_4 = \gamma_{BD}^0$, $\gamma_5 = \gamma_{BD}^5$. In this representation γ_1 , γ_3 are pure imaginary, while γ_2 , γ_4 , γ_5 are real.

The Taylor expansion showed that the discretization errors start at $O(a^2)$. For another simple illustration consider the inverse of the free-field propagator $m + i/a \sum_{\mu} \gamma_{\mu} \sin(p_{\mu} a)$. Set $\vec{p} = 0$ and rotate to Minkowski space ($p_4 \rightarrow iE$, *i.e.* $\sin p_4 a \rightarrow i \sinh E a$). Then, using the forward propagator (upper two components of γ_4), gives

 $m_q^{\text{pole}}a = \sinh Ea$

for the relation between the pole mass and the energy. This shows that, even in the free field case, the continuum relation $E(\vec{p} = 0) = m$ is violated by corrections that are $O(a^2)$.

Symmetries of Fermion Action

The invariance group of the fermion action under rotations in space and time is the hypercubic group. Full Euclidean invariance will be recovered only in the continuum limit. The action is invariant under translations by *a* and under $\mathcal{P}, \mathcal{C},$ and \mathcal{T} .

The *naive* action $\bar{\psi}_x M_{xy}^N \psi_y$ has the following global symmetry:

$\psi(x)$	\rightarrow	$e^{i heta}\psi(x)$
$\bar{\psi}(x)$	\rightarrow	$\bar{\psi}(\mathbf{x})e^{-i\theta}$

where θ is a continuous parameter. This symmetry is related to baryon number conservation and leads to a conserved vector current. For $m_q = 0$ the action is also invariant under

 $\psi(x) \rightarrow e^{i\theta\gamma_5}\psi(x)$ $\bar{\psi}(x) \rightarrow \bar{\psi}(x)e^{i\theta\gamma_5}$

It turns out that while the naive fermion action preserves chiral symmetry it also has the notorious fermion doubling problem. The chiral charges of these extra fermions are such as to exactly cancel the anomaly. In fact the analysis of S^N lead to a no-go theorem by Nielsen-Ninomiya that states that it is not possible to define a local, translationally invariant, hermitian lattice action that preserves chiral symmetry and does not have doublers.

Comments regarding fermion simulations

Generalization of stochastic evolution of path integrals for Bosons to Fermions involves significant new problems.

- The fundamental difference is the minus signs arising from the antisymmetry of fermions.
- The evolution operator e^{-βH} filters out the lowest state and therefore the symmetric state and not the antisymmetric unless a projection to the antisymmetric space is made.

Exact projection is done by writing the path integral in terms of Grassmann variables and integrating out the fermion fields resulting in the fermion determinant (see Lecture 1).

- The price is a non-local action, which has complicated dynamical quark simulations for two decades.
 ⇒ set *DetM* = 1, a simplification used in the past known as quenched approximation.
- In addition relativistic fermions suffer from the so called fermion doubling problem
- In non-relativistic systems with two-body potentials one makes use of the Hubbard-Stratonovich transformation to integrate the quadratic potential terms.

The problem of the sign of the resulting fermion determinant still remains hindering simulation of many fermion systems - the notorious fermion problem.

Doubling of "naive" fermions

In addition to the fermion sign problem we also encounter the so called doubling of fermions. Consider the simplest discretization of the Dirac equation

$$\begin{split} S_{F}^{\text{naive}} &= a^{4} \sum_{n} \left[m \bar{\psi}(n) \psi(n) + \frac{1}{2a} \sum_{\mu} \left(\bar{\psi}(n) \gamma_{\mu} U_{\mu}(n) \psi(n+a_{\mu}) - \bar{\psi}(n+a_{\mu}) \gamma_{\mu} U_{\mu}^{\dagger}(n) \psi(n) \right) \right] \\ &\rightarrow \int d^{4} x \left[m \bar{\psi}(x) \psi(x) + \frac{1}{2a} \sum_{\mu} \left(\bar{\psi}(x) \gamma_{\mu} (1 + igaA_{\mu}) (1 + +a\partial_{\mu}) \psi(x) - \bar{\psi}(x) (1 + a\partial_{\mu}) \gamma_{\mu} (1 - igaA_{\mu}) \psi(x) \right) \right] \\ &\rightarrow \int d^{4} x \bar{\psi}(x) \left[m + \gamma_{\mu} (\partial_{\mu} + igA_{\mu}) \right] \psi(x). \end{split}$$

To see the problem associated with S_F^{maive} we consider the associated Hamiltonian in one space-dimension for the free massless theory i.e. $U_{\mu} = 1$ and m = 0.



Although E_k has the correct dispersion relation for $k \to 0$ it has an extra node at the Brillouin zone \to for every physical mode k there is a degenerate unphysical mode $\frac{\pi}{a} - k$. In the partition function these count equally and lead to a factor Of 2 over-counting. Furthermore since $v = \frac{dE_k}{dk}$ the lattice mixes right and left moving

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Fermion doubling and chiral symmetry

The naive action:

$$S_{F}^{\text{naive}} = \bar{\psi} D \psi = \sum_{k} \bar{\psi}_{k} (m_{q} + i \sum_{\mu} \gamma_{\mu} \frac{\sin(k^{\mu} a)}{a}) \psi_{\mu}$$

leads to the inverse of the free field propagator $S^{-1}(p) = m_q + \frac{i}{a} \sum_{\mu} \gamma_{\mu} \sin k_{\mu} a$.

It has $2^4 = 16$ zeros within the Brillouin cell in the limit $m_q \rightarrow 0$.

The doubling problem is general and intimately related to simultaneously preserving chiral symmetry. The inclusion of the gauge fields does not solve the doubling problem.

Defining the momentum range of the Brillouin cell to be $(-\pi/a, \pi/a]$, the zeros lie at $p_{\mu} = 0$ and π/a . This proliferation holds under very general conditions specified by the Nielsen-Ninomiya or no-go theorem. Let us investigate the properties of these extra zero modes under chiral transformations: Define a set of 16 4-vectors $\Pi^A = \{(0,0,0,0), (\pi/a,0,0,0), \dots, (\pi/a,\pi/a,\pi/a,\pi/a)\}$ with $A = \{1,\ldots,16\}$, and consider the expansion of the massless propagator about these points. Then

$$S^{-1}(p, m = 0) = \frac{i}{a} \sum_{\mu} \gamma_{\mu} \sin p_{\mu} a = \frac{i}{a} \sum_{\mu} \gamma_{\mu} \sin(\Pi^{A} + k)_{\mu} a = \frac{i}{a} \sum_{\mu} \gamma_{\mu} S^{A}_{\mu} \sin k_{\mu} a$$
$$\equiv \frac{i}{a} \sum_{\mu} \tilde{\gamma}_{\mu} \sin k_{\mu} a,$$

where $S^A_{\mu} = \{+1, -1\}$ depending on whether the μ component of Π^A is $\{0, \pi/a\}$ and $\tilde{\gamma}_{\mu} = Y_A \gamma_{\mu} Y^{\dagger}_A$, $Y_A = \prod_{\mu} (\gamma_{\mu} \gamma_5)^{\pi^A_{\mu}}$ and π^A_{μ} are $\{0, 1\}$ depending on whether the momentum expansion in the μ direction is about 0 or π/a .

Now,
$$\tilde{\gamma}_5 = Y_A \gamma_5 Y_A^{\dagger} = S_1^A S_2^A S_3^A S_4^A \gamma_5 \equiv X^A \gamma_5$$
, with $X^A = \pm$

 \implies the sixteen species break up into two sets of 8 with chiral charge ± 1 , and render the theory anomaly-free. Consequently, this "naive" discretization is phenomenologically not acceptable.

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Now, $\tilde{\gamma}_5 = Y_A \gamma_5 Y_A^{\dagger} = S_1^A S_2^A S_3^A S_4^A \gamma_5 \equiv X^A \gamma_5$, with $X^A = \pm$.

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Wilson Fermions

One way out of the no-go theorem is to give up chiral symmetry and add a second derivative [Wilson 1974] In one-dimension the Wilson Hamiltonian is given

$$H_W = a \sum_{n} \bar{\psi} \left[\gamma_1 \frac{\psi(n+1) - \psi(n-1)}{2ia} - \frac{ra}{2i} \gamma_1 \gamma_0 \frac{\psi(n+1) - 2\psi(n) + \psi(n+1)}{a^2} \right]$$
$$= \sum_{k} \bar{\psi}_k^{\dagger} \left[\gamma_1 \frac{\sin(ka)}{a} - r \gamma_1 \gamma_0 \frac{\cos(ka) - 1}{ia} \right] \psi_k$$

with the energy spectrum

$$E_{K}^{2} = \left(\frac{\sin(ka)}{a}\right)^{2} + \left(\frac{r}{a}(\cos(ka) - 1)\right)^{2}$$
$$\stackrel{k \to 0}{\longrightarrow} \pm k \left(1 - \frac{k^{2}a^{2}}{6} + \cdots\right)$$
$$\stackrel{k \to \frac{\pi}{a}}{\longrightarrow} \pm \frac{2r}{a}$$

 \implies the mode for $k \rightarrow \frac{\pi}{a}$ becomes infinitely massive and decouples for $a \rightarrow a$.

Wilson action

The Wilson action in 4-dimensions is

$$S_{W} = a^{4} \sum_{n} \frac{1}{2a} \sum_{\mu} \left[\bar{\psi}(n)(r - \gamma_{\mu}) U_{\mu}(n) \psi(n + \mu) + \bar{\psi}(n + \mu)(r + \gamma_{\mu}) U_{\mu}^{\dagger}(n) \psi(n) \right] + a^{4} \sum_{n} \bar{\psi}(n) \left(m + \frac{4r}{a} \right) \psi(n) = a^{4} \sum_{n} \frac{1}{2a} \sum_{\mu} \left[\bar{\psi}(n)(r - \gamma_{\mu}) U_{\mu}(n) \psi(n + \mu) + \bar{\psi}(n + \mu)(r + \gamma_{\mu}) U_{\mu}^{\dagger}(n) \psi(n) \right] + a^{4} \sum_{n} \bar{\psi}(n) \left(m + \frac{4r}{a} \right) \psi(n) = a^{4} \sum_{n} \frac{1}{2a} \sum_{\mu} \left[\bar{\psi}(n)(r - \gamma_{\mu}) U_{\mu}(n) \psi(n + \mu) + \bar{\psi}(n + \mu)(r + \gamma_{\mu}) U_{\mu}^{\dagger}(n) \psi(n) \right] + a^{4} \sum_{n} \bar{\psi}(n) \left(m + \frac{4r}{a} \right) \psi(n) = a^{4} \sum_{n} \frac{1}{2a} \sum_{\mu} \left[\bar{\psi}(n)(r - \gamma_{\mu}) U_{\mu}(n) \psi(n + \mu) + \bar{\psi}(n + \mu)(r + \gamma_{\mu}) U_{\mu}^{\dagger}(n) \psi(n) \right] + a^{4} \sum_{n} \bar{\psi}(n) \left(m + \frac{4r}{a} \right) \psi(n) = a^{4} \sum_{n} \frac{1}{2a} \sum_{n}$$

and has only one fermion in the continuum limit.

The Wilson action breaks chiral symmetry through the *r*-term which acts as a mass term together with the non-zero value of m. Since this mass is not protected from renormalization we need to "fine tuned" to attain the mass we are interested in. Wilson's fix for doublers comes with a high price tag – a hard breaking of chiral symmetry at O(a).

 \Rightarrow for given g and r we determine the input quark mass so that so that $m_{\pi} = 0$ or $m_{\pi} = 140$ MeV. Define the hopping parameter κ as:

$$\kappa = \frac{1}{2ma+8r}$$

and rescale the fermion fields $\psi
ightarrow (2\kappa a^3)^{1/2}\psi$

$$S_W = \sum_n \left[\bar{\psi}(n)\psi(n) - \kappa \sum_\mu \left(\bar{\psi}(n)(1-\gamma_\mu)U_\mu(n)\psi(n+\mu) + \bar{\psi}(n+\mu)(1+\gamma_\mu)U_\mu^{\dagger}\psi(n) \right) \right]$$

where we have set r = 1.

$$m_q = \frac{1}{2a} \left(\frac{1}{\kappa} - \frac{1}{\kappa_{\rm cr}} \right)$$

where $\kappa_{\rm cr}$ is the value of κ for which $m_{\pi} = 0$.

Wilson propagator

The free propagator in momentum space for Wilson fermions is

$$S_F(p) = M_W^{-1}(p) = rac{a}{1 - 2\kappa \sum_{\mu} (r \cos p_{\mu} a - i \gamma_{\mu} \sin p_{\mu} a)}$$

Due to the dimension 5 operator (terms proportional to *r*) the 15 extra states at $p_{\mu}a = \pi$ get masses of order 2r/a.

The operator *M* satisfies the following relations:

The first two state that the "hermiticity" property of M^N is preserved. The second equation relates a quark propagator from $x \to y$ to the antiquark propagator from $y \to x$. This important identity, called hermiticity or γ_5 invariance, leads to a significant simplification in numerical calculations. The adjoint in S_F^{\dagger} is with respect to the spin and color indices at each site. The last relation shows that M^W is not anti-hermitian due to the Wilson r term.

The pole mass derived from the propagator is different from the bare mass and given by

 $m_q^{pole}a = r(\cosh Ea - 1) + \sinh Ea$.

This shows, as expected, that the discretization corrections in spectral quantities occur at O(a).

Properties of Wilson fermions

- The doublers are given a heavy mass, 2r/a, and decouple in the continuum limit.
- Chiral symmetry is broken explicitly. The derivation of axial Ward identities, using the invariance under the transformation ψ(x) → e^{iθγ5}ψ(x), ψ(x) = ψ(x)e^{-iθγ5} have the generic form

$$\left\langle \frac{\partial \delta S}{\partial \theta} \mathcal{O} \right\rangle = \left\langle \frac{\partial \delta \mathcal{O}}{\partial \theta} \right\rangle.$$

For WF, the variation of the action under an axial transformation is

$$\frac{\partial \delta S}{\partial \theta} = \partial_{\mu} A_{\mu} - 2mP + raX,$$

where *X* is an additional term coming from the variation of the Wilson *r* term.

 \implies in general, all relations based on axial WI will have corrections at order *ra* and involve mixing with operators that would normally be absent due to the chiral symmetry.

The quark mass gets both additive and multiplicative renormalization.

The zero of the quark mass is set by κ_{cr}. There are two ways to calculate κ_{cr} at any given a.

(i) Assume the chiral relation $M_{\pi}^2 \propto m_q$, calculate the pion mass as a function of $1/2\kappa$, and extrapolate it to zero. The value of κ at which the pion becomes massless is, by definition, κ_{cr} .

(ii) Calculate the quark mass through the ratio $\langle \partial_{\mu} A_{\mu}(x) P(0) \rangle / \langle P(x) P(0) \rangle$ (based on the axial Ward identity) as a function of $1/2\kappa$ and extrapolate to zero.

The two estimates can differ by corrections of O(a).

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• Calculation of the matrix element $\langle 0 | T[A_{\mu}V_{\nu}V_{\rho}] | 0 \rangle$ shows that the Adler-Bell-Jackiw (ABJ) anomaly of the singlet axial current is correctly reproduced in the continuum limit. An explicit 1-loop calculation shows that while each of the extra 15 states contribute terms proportional to *r*, the total contribution from all sixteen states is independent of *r* and equals the ABJ anomaly.

Properties of Wilson fermions

 The spin and flavor degrees of freedom are in one-to-one correspondence with continuum Dirac fermions.

 \implies the construction of interpolating field operators is straightforward, e.g. $\bar{\psi}\gamma_5\psi$ and $\bar{\psi}\gamma_i\psi$ are interpolating operators for pseudoscalar and vector mesons just as in the continuum.

- The Wilson term changes the discretization errors to O(a).
- Conserved Vector Current: The Wilson action is invariant under the global U(1) transformation $\psi(x) \rightarrow e^{i\theta} \psi(x), \bar{\psi}(x) \rightarrow \bar{\psi}(x) e^{-i\theta} \rightarrow \text{conserved Noether current:}$

$$\Delta^{\mu} V_{\mu}(n) = V_{\mu}(n) - V(n - \mu) = 0$$

$$V_{\mu}(n) = -\frac{1}{2}\bar{\psi}(n)(1-\gamma_{\mu})U)\mu(n)\psi(n+\mu) + \frac{1}{2}\bar{\psi}(n+\mu)(1+\gamma_{\mu})U_{\mu}^{\dagger}(n)\psi(n)$$

In many applications like decay constants one uses the local (flavor) currents defined by

$$V_{\mu}(x) = \bar{\psi}(x)\gamma_{\mu}\psi(x)$$

$$A_{\mu}(x) = \bar{\psi}(x)\gamma_{5}\gamma_{\mu}\psi(x),$$

which are not conserved, and consequently have associated non-trivial renormalization factors Z_V and Z_A which have to included when calculating matrix elements.

Staggered fermions (SF) in a nutshell

The 16-fold doubling problem of the naive fermion action can be reduced to 4 by distributing the spin components to the corners of the hypercube. The basic idea is to transform the fermion fields into a new representation for which the naive fermion action is diagonal in the Dirac indices i.e. produce N_D copies and then keep one of these copies so that the degeneracy is reduced to $16/N_D$.



Distribution of 2^d degrees of freedom on *d*-dimensional lattice (d = 2)

• Transformation: $\bar{\psi}(n) = \gamma_1^{n_1} \gamma_2^{n_2} \gamma_3^{n_3} \gamma_4^{n_4} \chi(n)$. Then e.g. the term $\bar{\psi}(n) \gamma_2 \psi(n + \mu_2)$ becomes

$$\begin{split} \bar{\chi}(n)\gamma_4^{n_4}\gamma_3^{n_3}\gamma_2^{n_2}\gamma_1^{n_1}\gamma_2\gamma_1^{n_1}\gamma_2^{n_2+1}\gamma_3^{n_3}\gamma_4^{n_4}\chi(n+\mu_2) \\ = (-1)^{n_0+n_1}\bar{\chi}(n)\chi(n+\mu_2) \end{split}$$

- Only partial lifting of the degeneracy: $16 \rightarrow 4$ leaving 4 "tastes" per physical flavor
- Flavor symmetry is broken \rightarrow mixing of tastes

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The staggered solutions χ for a given momentum k are the sum or difference of ψ_k and $\psi_{\frac{\pi}{a}-k}$. Thinning of the d.o.f corresponds to doubling the lattice spacing \rightarrow the maximum momentum is $\frac{\pi}{2a}$ and therefore there are no spurious modes from the end of the Brillouin zone.

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Staggered fermions

The action for staggered fermions:

$$S_{SF} = m_q \sum_n \bar{\chi}(n)\chi(n) + \frac{1}{2} \sum_{n,\mu} \bar{\chi}(n)\eta_{\mu}(n) (U_{\mu}(n)\chi(n+\hat{\mu}) - U_{\mu}^{\dagger}(x-\hat{\mu})\chi(n-\hat{\mu})) \equiv \sum_{n,m} \bar{\chi}(n)M_{nm}^{S}\chi(m)$$

with the matrix M^S given by

$$M^{S}[U]_{x,y} = m_{q}\delta_{xy} + \frac{1}{2} \sum_{\mu} \eta_{x,\mu} \left[U_{x,\mu}\delta_{x,y-\mu} - U_{x-\mu,\mu}^{\dagger}\delta_{x,y+\mu} \right].$$

The γ matrices are replaced by the phases $\eta_{x,\mu}$.

The different spin components of χ are decoupled as the phase factor $\eta_{\mu}(n)$ depends only on the site index and direction and do not have a spinor index.

 \implies drop the spin index on χ leaving only color degrees of freedom at each site.

This reduces the original 2^d-fold degeneracy of naive fermions by a factor of four.

- The mass term in M^S[U]_{n,m} is hermitian, while the D term is anti-hermitian, required to realize chiral symmetry.
- The SF action has translation invariance under shifts by 2a due to the phase factors η_μ(n). ⇒ in the continuum limit, the 16 degrees of freedom reduce to 4 copies of Dirac fermions.
- At finite a the gauge interactions break this flavor symmetry and the 16 degrees of freedom in the hypercube are a mixture of spin and flavor. This is one of the major drawbacks of staggered fermions.

Symanzik's improvement program

A simple example: Consider the symmetric discretization of the derivative of f'(x)

$$\frac{f(x+a)-f(x-a)}{2a} = f'(x) + a^3 C^{(3)}(x) + a^5 C^{(5)}(x) + \mathcal{O}(a^7)$$

where due to the symmetrized discretization only odd powers of *a* appear. Since $f(x \pm a) = f(x) \pm f'(x) + \frac{a^2}{2}f''(x) \pm \frac{a^3}{3!}f'''(x) + \mathcal{O}(a^4)$, we obtain $C^{(3)} = \frac{1}{2}f'''(x)$. For improvement of $\mathcal{O}(a^3)$ we use

$$\frac{f(x+a)-f(x-a)}{2a}+ca^{3}D^{(3)}[f](x)=f'(x)+\mathcal{O}(a^{4})$$

where $D^{(3)}[f]$ is a discretize expression of f'''. Taking:

$$D^{(3)}[f](x) = \frac{f(x+2a) - 2f(x+a) + 2f(x-a) - f(x-2a)}{2a^3}$$

and $c = -\frac{1}{6}$ the (a^3) -term is eliminated.

Improvement for QCD is done in an analogous way except than the determination of the coefficients is more involved. Like in the simple example we start by identifying a continuum expression for the correction terms ordering them according to their dimension. We write the associated effective action as

$$S_{\mathrm{eff}} = \int \mathrm{d}^4 x \left\{ \mathcal{L}_0(x) + a \mathcal{L}_1(x) + a^2 \mathcal{L}_2(x) + \ldots \right\},$$

where \mathcal{L}_0 denotes the continuum QCD Lagrangian and the \mathcal{L}_k 's, $k \ge 1$, are linear combinations of local operators of dimension 4 + k.

There are three independent dimension-5 operators that have the symmetries of the lattice action. Two of these can be absorbed in the original action resulting in a redefinition of the bare parameters.

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Introduction to Lattice QCD

Symanzik's improvement program

A simple example: Consider the symmetric discretization of the derivative of f'(x)

$$\frac{f(x+a)-f(x-a)}{2a} = f'(x) + a^3 C^{(3)}(x) + a^5 C^{(5)}(x) + \mathcal{O}(a^7)$$

where due to the symmetrized discretization only odd powers of *a* appear. Since $f(x \pm a) = f(x) \pm f'(x) + \frac{a^2}{2}f''(x) \pm \frac{a^3}{3!}f'''(x) + \mathcal{O}(a^4)$, we obtain $C^{(3)} = \frac{1}{2}f'''(x)$. For improvement of $\mathcal{O}(a^3)$ we use

$$\frac{f(x+a)-f(x-a)}{2a}+ca^{3}D^{(3)}[f](x)=f'(x)+\mathcal{O}(a^{4})$$

where $D^{(3)}[f]$ is a discretize expression of f'''. Taking:

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Introduction to Lattice QCD

The Sheikholeslami-Wohlert (clover) Action

For the improved action we thus obtain

$$S = S_{\text{Wilson}} + a^5 \sum_{x} c_{\text{sw}} \, \bar{\psi}(x) \frac{i}{4} \sigma_{\mu\nu} \widehat{F}_{\mu\nu}(x) \psi(x),$$

where $\hat{F}_{\mu\nu}$ is a lattice representation of the gluon field tensor. The product of the gauge field variables around a plaquette in the (μ, ν) -plane is equal to $1 + a^2 F_{\mu\nu} + \ldots$ in the classical continuum limit.

A symmetric definition of the lattice field tensor is hence given by

$$\widehat{F}_{\mu\nu}(x) = \frac{-1}{8a^2} \{Q_{\mu\nu}(x) - Q_{\nu\mu}(x)\}$$

with $Q_{\mu\nu}(x)$ being the sum of the plaquette loops: $Q_{\mu\nu}(n) = P_{\mu,\nu}(n) + P_{\nu,-\mu}(n) + P_{-\mu,-\nu}(n) + P_{-\nu,\mu}(n)$

To achieve the desired improvement, the coefficient c_{sw} multiplying the O(*a*) counterterm in the improved action should be chosen appropriately. The one-loop formula is

$$c_{\rm sw} = 1 + 0.2659g^2 + \mathcal{O}(g^4).$$

One also has techniques to compute c_{sw} non-perturbatively using numerical simulations.

The advantages of the clover action is that it is local and leaves perturbation theory tractable. Adding the clover term is only a \sim 15% overhead on Wilson fermion simulations.

However we need to also improve the operators.



Twisted mass fermions

Consider the continuum action for two-degenerate flavors:

$$S = \int d^4 x \bar{\chi}(x) \left(\gamma_{\mu} D_{\mu} [U] + m_0 + i \mu \gamma_5 \tau_3 \right) \chi(x)$$

The mass term can be written as $m_0 + i\mu\gamma_5\tau_3 = M e^{i\alpha\gamma_5\tau_3}$ with $\alpha = \tan^{-1}\left(\frac{\mu}{m_0}\right)$ and $M^2 = m_0^2 + \mu^2$. Perform axial transformation to the physical basis:

$$\psi(\mathbf{x}) = \mathbf{e}^{i\omega\gamma_5\frac{\tau_3}{2}}\chi(\mathbf{x}), \quad \bar{\psi}(\mathbf{x}) = \bar{\chi}(\mathbf{x})\,\mathbf{e}^{i\omega\gamma_5\frac{\tau_3}{2}}$$

The mass term transforms as $Me^{i(\alpha-\omega)\gamma_5\tau_3}$ and if $\alpha = \omega$ we recover the Dirac action

$$S = \int d^4x \, \bar{\psi}(x) \left(\gamma_\mu D_\mu[U] + M \right) \psi(x)$$

 \implies In the continuum the twisted mass action is equivalent to QCD but at finite *a* it provides an alternative discrete formulation.

Advantages:

- Automatic O(a) improvement at maximal twist
- Only one parameter to tune like with Wilson fermions, namely we tune the PCAC mass at smallest µ
 value to zero
- No additional operator improvement

Disadvantages:

- Explicit chiral symmetry breaking like for all Wilson-type actions
- Explicit breaking of isospin symmetry to $\mathcal{O}(a^2)$. In practise only π^0 receives large $\mathcal{O}(a^2)$ corrections

Chiral actions

Chiral symmetry at non-zero lattice spacing is realized if the Ginsparg-Wilson relation is satisfied

 $D\gamma_5 + \gamma_5 D = aD\gamma_5 D.$

This amounts to adding a contact term that vanishes in the continuum limit. Using *D* we can define a chiral rotation which reduces to the continuum one as $a \rightarrow 0$

$$\psi' = e^{i\theta\gamma_5\left(1-\frac{a}{2}D\right)}\psi, \quad \bar{\psi}' = \bar{\psi}' e^{i\theta\left(1-\frac{a}{2}D\gamma_5\right)}$$

leaving $L(\bar{\psi}, \psi) = \bar{\psi} D \psi$ invariant. Explicit construction of D is provided by:

Overlap operator:

$$D_{ov} = \frac{1}{a} \left[1 - \frac{A}{\sqrt{A^{\dagger}A}} \right], \quad A = 1 - aD_W$$

Left-handed

fermion

where D_W is the massless Wilson-Dirac operator. The main drawback is that its expensive.

Domain wall operator is defined on a 5-D lattice:

 $D_{DW}(n_1, s_1; n_2, s_2) = \delta_{s_1, s_2} D_W(n_1; n_2) + \delta_{n_1, n_2} D_{DW5}(s_1; s_2)$

where s_1 , s_2 denote the fifth direction. D_W is the 4-D Wilson Dirac operator. The link variables are define in 4-D as before and the operator D_{DW5} act in the 5th direction. Left and right handed fermions live on the opposite boundaries of the fifth dimension



Computational costs

Algorithmic improvements



Lattice size: 24^3x40 lattice \rightarrow number of d.o.f ~ $5x10^7$, dimension of fermion (sparse) matrix $D \sim 10^7$

Improved gauge actions:Lüscher-Weisz action

The leading order term in the expansion of all Wilson loops is $\mathcal{O}^{(4)} = \sum_{\mu\nu} F_{\mu\nu} F_{\mu\nu} F_{\mu\nu}$ and corrections begin at $\mathcal{O}(a^2) \Longrightarrow$ any lattice action written as a linear combination of Wilson loops will have the correct continuum limit with corrections at $\mathcal{O}(a^2)$.

There are three dimension 6 operators which in continuous notation are:

$$\begin{aligned} \mathcal{O}_1^{(6)} &= & \sum_{\mu,\nu} \mathrm{Tr} \left(D_\mu F_{\mu\nu} D_\mu F_{\mu\nu} \right) \,, \\ \mathcal{O}_2^{(6)} &= & \sum_{\mu,\nu,\rho} \mathrm{Tr} \left(D_\mu F_{\nu\rho} D_\mu F_{\nu\rho} \right) \,, \\ \mathcal{O}_3^{(6)} &= & \sum_{\mu,\nu,\rho} \mathrm{Tr} \left(D_\mu F_{\mu\rho} D_\nu F_{\nu\rho} \right) \,. \end{aligned}$$

Thus, classical improvement of the lattice action, *i.e.* removing the $O(a^2)$ term, can be achieved by taking a linear combination of the plaquette and these three six-link loops that have the expansion

$$\mathcal{L} = r^{(4)} \mathcal{O}^{(4)} + r_1^{(6)} \mathcal{O}_1^{(6)} + r_2^{(6)} \mathcal{O}_2^{(6)} + r_3^{(6)} \mathcal{O}_3^{(6)} + \dots ,$$

and Lüscher and Weisz have shown an elegant way of calculating the expansion coefficients $r_{\alpha}^{(d)}$ Their results are summarized in the Table.

Also there are only 3 six-link loops that one can draw on the lattice: Planar $\mathcal{L}_1^{(6)}$, twisted $\mathcal{L}_2^{(6)}$ and the L shaped $\mathcal{L}_3^{(6)}$.



Loop	r ⁽⁴⁾	$r_{1}^{(6)}$	$r_{2}^{(6)}$	$r_{3}^{(6)}$
$\mathcal{L}^{(4)}_{(6)}$	$-\frac{1}{4}$	1 24	0	0
$\mathcal{L}_{1}^{(6)}$	-2	56	0	0
$\mathcal{L}_{2}^{(6)}$	-2	$-\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$
$\mathcal{L}_{3}^{(6)}$	-4	$\frac{1}{6}$	Ó	$\frac{1}{2}$

The Lüscher-Weisz action

The lattice gauge action can be written as

$$\mathcal{S}_{g} \;=\; rac{6}{g^2} \left\{ c^{(4)}(g^2) \; \mathcal{L}^{(4)} + \sum_{i=1,3} c^{(6)}_i(g^2) \; \mathcal{L}^{(6)}_i
ight\}$$

in terms of the plaquette and the three 6-link loops with the renormalization condition: $c^{(4)}(g^2) + 8c^{(6)}_1(g^2) + 8c^{(6)}_2(g^2) + 16c^{(6)}_3(g^2) = 1$ so that in the continuum limit the action reduces to $F_{\mu\nu}F_{\mu\nu}/4$. Tree level improvement can be obtained by the choice

$$c^{(4)} + 20c^{(6)}_1 = 0; \quad c^{(6)}_2 = 0; \quad c^{(6)}_3 = 0$$

Choosing $c_3^{(6)} = 0$ one finds

$$c_1^{(6)} - c_2^{(6)} = -\frac{1}{12}$$

Quantum effects are included at one-loop needed to kill $O(a^2)$ at all length scales. Lüscher and Weisz derived the 1-loop improved action which has leading correction at $O(g^4a^4)$ and fixes

$$\begin{split} c_0^{(4)}(g^2) &= \frac{5}{3} + 0.2370g^2 \;, \;\; c_1^{(6)}(g^2) = -\frac{1}{12} - 0.02521g^2 \\ c_2^{(6)}(g^2) &= -0.00441g^2 \;, \;\; c_3^{(6)}(g^2) = 0 \;. \end{split}$$

for which the c_i normalization condition is satisfied.

The bottom line on the Lüscher-Weisz action is that since the coefficient $c_2^{(6)}$ is small, the action, to a very good approximation, can be improved by keeping just $\mathcal{L}^{(4)}$ and $\mathcal{L}^{(6)}_1$ as in the classical case. This 1-loop result can be mean-field improved without much effort.

Exercise: Conserved current for Wilson fermions

To derive the associated conserved current (for degenerate masses) we use the standard trick of calculating the variation of the action

$$\delta S = \kappa \sum_{x,\mu} \bar{\psi}(x)(\gamma_{\mu} - r)U_{\mu}(x)\psi(x+\hat{\mu})\exp(i\theta(x) - i\theta(x+\mu))$$

-
$$\kappa \sum_{x,\mu} \bar{\psi}(x+\mu)(\gamma_{\mu} + r)U_{\mu}^{\dagger}(x)\psi(x)\exp(i\theta(x+\mu) - i\theta(x))$$

which, to first order in θ , is

$$\begin{split} &-\sum_{\mathbf{x},\mu} \left[\bar{\psi}(\mathbf{x})(\gamma_{\mu}-r)U_{\mu}(\mathbf{x})\psi(\mathbf{x}+\hat{\mu}) \right. + \\ &\left. \bar{\psi}(\mathbf{x}+\mu)(\gamma_{\mu}+r) \; U_{\mu}^{\dagger}(\mathbf{x})\psi(\mathbf{x}) \right] \left[i \frac{\partial \theta}{\partial x_{\mu}} \right]. \end{split}$$

The conserved current, obtained after integration by parts, is

$$V^{c}_{\mu} = \bar{\psi}(x)(\gamma_{\mu} - r)U_{\mu}(x)\psi(x + \hat{\mu}) + \bar{\psi}(x + \mu)(\gamma_{\mu} + r)U^{\dagger}_{\mu}(x)\psi(x)$$

 V_{μ}^{c} is hermitian and reduces to the symmetrized version of the 1-link vector current for r = 0.