Updating fermionic actions

- Fermions are Grassmann-fields - difficult to directly repesent numerically!
- However - action is quadratic in ψ's (or, of the form $\bar{\psi} M \psi$)
  - ⇒ can be integrated over; only bosonic fields remain!
- General method - Hybrid Monte Carlo (HMC)

Molecular dynamics

- As a warm-up, let us consider "equation of motion" for scalar field ϕ, with action $S(\phi)$ in fictitious, "update" time. $\phi \in R$
Let us introduce canonical momenta π for ϕ, and define

$$H = \frac{1}{2} \sum_x p_x^2 + S(\phi)$$ (in lattice units)

Now the Hamiltonian equations of motion are

$$\begin{cases} \dot{p}_x = -\dfrac{\partial H}{\partial \phi_x} = -\dfrac{\partial S}{\partial \phi_x} \\ \dot{\phi}_x = p_x \end{cases}$$

This preserves H, i.e. $\dot{H} = 0$.

This is the standard real-time <u>molecular dynamics</u> or classical equation of motion, if we identify $S(\phi)$ as the potential $V(\phi)$.

- Consider

$$\int dp\, d\phi\; e^{-H[p,\phi]} = c \int d\phi\, e^{-S[\phi]}$$

because the Gaussian integral over p_x is trivial.

- How to generate p, ϕ with correct weight?

Consider the following update cycle:

1) Generate new p_x from Gaussian distribution

2) Evolve p, ϕ using e.o.m. for fixed time T

3) Repeat from 1)

1) + 2) together satisfies detailed balance:

1) trivially, because p-update directly gives correct distribution

2) Evolution preserves H. Because e.o.m. preserves phase space volume (Liouville), the final p, ϕ-configuration is as likely as the initial one.

$\Rightarrow$ molecular dynamics w. <u>momentum refresh</u> gives correct distribution $e^{-H[p,\phi]}$ or $e^{-S[\phi]}$.

This is a general update for continuous d.o.f's, and can be applied to spin or gauge theory. However, usually overrelaxation + heat bath is more efficient.

- Detailed balance relies on exact (expensive) solution of the eqn. Difficult to achieve numerically!

$\Rightarrow$ Hybrid Monte Carlo:

a) get p_x from $e^{-\frac{1}{2}p_x^2}$

b) Use reversible but not necessarily exact evolution

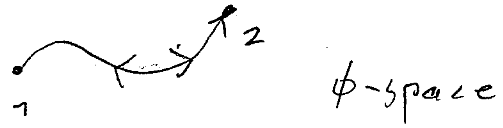
c) Accept/reject with $p_{acc.} = \min(1, e^{-\Delta H})$

$\Delta H = H_{END} - H_{START}$

- If rejected, restore $\phi \leftarrow \phi_{START}$ and go back to a)
- If accepted, $\phi \leftarrow \phi_{END}$ and go to a)

Reversibility means the following:

- Start w. ϕ_1, p_1
- evolve $(\phi_1, p_1) \to (\phi_2, p_2)$ length T
- flip $p_2 \to -p_2$
- evolve again $(\phi_2, -p_2) \to (\phi_1, -p_1)$ length T
  retrace steps!



Because of reversibility $\times$ acc/rej. the update obeys detailed balance; Metropolis acceptance

$$\frac{W((p_1, \phi_1) \to (p_2, \phi_2))}{W((-p_2, \phi_2) \to (-p_1, \phi_1))} = e^{H_1 - H_2}$$

(Note: $-p$ does not matter, because $P(p) = P(-p)$)

- Simplest reversible update:

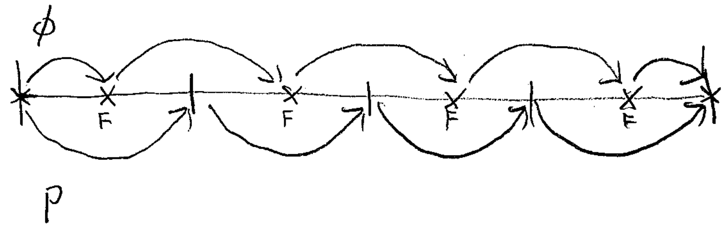
Leapfrog

- One update step from $\tau = n\delta\tau$ to $\tau = (n+1)\delta\tau$:
  a) $\phi_{\tau+\frac{1}{2}\delta\tau} = \phi_\tau + \frac{1}{2}\delta\tau\, p_\tau$
  b) calculate force: $F_{\tau+\frac{1}{2}\delta\tau} = -\frac{\partial S}{\partial \phi_{\tau+\frac{1}{2}\delta\tau}}$
  c) $p_{\tau+\delta\tau} = p_\tau + \delta\tau\, F_{\tau+\frac{1}{2}\delta\tau}$
  d) $\phi_{\tau+\delta\tau} = \phi_{\tau+\frac{1}{2}\delta\tau} + \frac{1}{2}\delta\tau\, p_{\tau+\delta\tau}$
- Reversible.

Full HMC-leapfrog update:

1. Generate p_x from Gaussian distr.
2. Update $(p,\phi)_\tau \to (p,\phi)_{\tau+\delta t}$
3. Repeat 2 until $\tau = T$
4. Accept/Reject
5. Go to 1.

One trajectory: $\delta\tau = \frac{T}{4}$



Note that successive ϕ and p can be put together

- General method

Fermion action is of form

$$S_F = \bar{\psi}_x M_{xy} \psi_y \qquad M = M(U)$$

Now $\int d\psi \, d\bar{\psi} \, e^{-S_F} = \det M(U)$

Thus, fermions "just" modify the gauge action!

Properties of $\det M$:

- M γ_5-hermitean: $M^\dagger = \gamma^5 M \gamma^5$ (Wilson, clover)

$\Rightarrow \det M^\dagger = \det(\gamma^5 M \gamma^5) = \det(M \gamma_5 \gamma_5) = \det M$

$\Rightarrow \det M \in \mathbb{R}$.

- Det M is finite, and thus in principle computable. However, it is very expensive!

We can bosonize it with pseudofermions χ, χ^+:

$$\det M = \int d\chi d\chi^* \, e^{-\chi^+ M^{-1} \chi}$$

However, this converges only if M is positive, i.e. all eigenvalues λ have $\mathrm{Re}\,\lambda > 0$. In general, $\chi^+ M^{-1} \chi$ is complex.

However, let us assume we have 2 degenerate mass fermions:

$$\int d\psi_1 d\bar\psi_1 \, d\psi_2 d\bar\psi_2 \, e^{-\bar\psi_1 M \psi_1 - \bar\psi_2 M \psi} = (\det M)^2$$

Because $\det M^+ = \det M$ (γ_5-hermiticity), we get

$$(\det M)^2 = \det M^+ \det M = \det(M^+ M)$$

$M^+ M$ is Hermitean, with all $\lambda \underset{(=)}{>} 0$

if $=0$: zero mode, very difficult!

$$\Rightarrow \underline{\det M^+ M = \int d\chi d\chi^+ \, e^{-\chi^+ (M^+ M)^{-1} \chi}}$$

Integral converges.

Full path integral

$$\underline{\int DU d\chi d\chi^+ \, e^{-S_G - \chi^+ (M^+ M)^{-1} \chi}}$$

Action is non-local

- Can be updated w. HMC:
- Fields $U_\mu(x)$ and $\chi(x)$ $(\chi^\dagger(x))$ $\chi^a_\alpha(x)$ ← colour, ← Dirac
- χ easy to obtain (for a given U and M):
  - pull $\xi^a_\alpha(x)$ from Gaussian, $\underline{p(\xi) \propto e^{-\xi^\dagger \xi}}$
  - Now $\chi = M^\dagger \xi$ is from distr. $e^{-\chi^\dagger (M^\dagger M)^{-1} \chi}$
- Introduce momenta $H_\mu(x)$ for $U_\mu(x)$, so that

$$\underline{\dot{U}_\mu(x) = i H_\mu(x) U_\mu(x)} \quad \text{or} \quad \underline{U_\mu(x, \tau+\delta\tau) = e^{i H_\mu \delta\tau} U_\mu(x,\tau)}$$

$H = h^a \lambda^a$, λ generator of $SU(N)$

- Force term: $\dfrac{\partial S}{\partial U}$? what does this mean ?

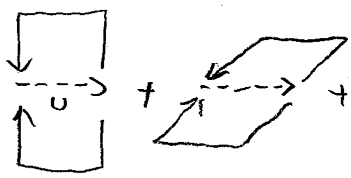
Recall that $U_{\tau+\delta\tau} = e^{i\omega^a \lambda^a} U_\tau$, thus

$$\underline{\dot{h}^a_\mu(x) = -\frac{\partial S}{i \partial \omega^a_\mu(x)}} = \underline{- S(U_\mu(x) \to \lambda^a U_\mu(x))}$$

- Those 2 equations are used in the trajectory.
- $H \equiv \frac{1}{2} \sum_{x,\mu} \mathrm{Tr}\, H^2_\mu(x) + S$ is conserved

- $$\frac{\partial S_{Gauge}}{(\delta U_\mu(x))^a} = -\beta \, \mathrm{Tr}\left[\lambda_a U_\mu(x) V_\mu(x)\right]$$

  where $V_\mu(x) = \sum'$ "staples" connecting to U,

  i.e. $V =$  + (4th dim.)

- $$\frac{\partial S_{fermion}}{(\partial U_\mu(x))^a} = \frac{\partial}{\partial U} \chi^\dagger (M^\dagger M)^{-1} \chi =$$

  $$= \left[(M^\dagger M)^{-1}\chi\right]^\dagger \frac{\partial (M^\dagger M)}{\partial U} \left[(M^\dagger M)^{-1}\chi\right]$$

  $$= \xi^\dagger \left[\frac{\partial M^\dagger}{\partial U} M + M^\dagger \frac{\partial M}{\partial U}\right] \xi$$

- $\frac{\partial M}{\partial U}$ is straightforward for Wilson; messier for Clover.

- $\xi = [M^\dagger M]^{-1}\chi$ is the <u>expensive bit</u>.

  standard inversion routine : <u>conjugate gradient</u>

- Finally, the full HMC update :
  1) pull H, ξ from Gaussian; $\chi = M^\dagger \xi$
  2) Use eqm to update U, H (χ fixed!)
  3) acc/rej with $P_{acc} = \max(1, e^{-\Delta H})$