Topology, the Wilson flow and the HMC algorithm

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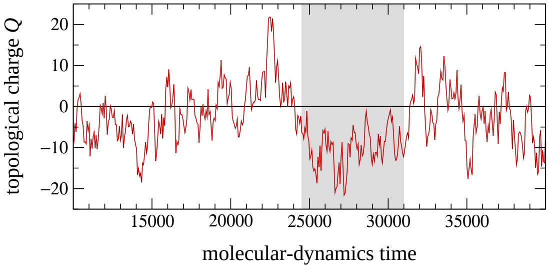

HMC, pure gauge

64×32^3

$a = 0.07$ fm

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Empirical facts

- The autocorrelation time of Q grows like a^{-5} or even more rapidly
- Little changes when the sea quarks are included in the simulations
- HMC, DD-HMC and link-update algorithms are all similarly ineffective

Del Debbio, Panagopoulos & Vicari '02

Schaefer, Sommer & Virotta '09

→ talk by Virotta

$\Rightarrow$ **at fixed physics, the effort for HMC simulations grows at least like a^{-10}**

In practice, simulations are often not that long

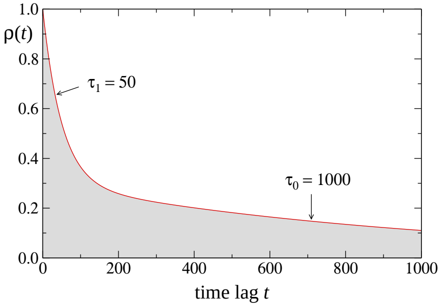
⇒ the calculated expectation values can be biased (by $1/V$-terms, for example) and

⇒ one may also totally underestimate their statistical errors

For illustration, consider an autocorrelation function

$$\rho(t) = |c_0|^2 e^{-t/\tau_0} + |c_1|^2 e^{-t/\tau_1} + \dots$$

such as



Easy case:

$$\tau_0 |c_0|^2 \lesssim \tau_1 |c_1|^2$$

Difficult case:

$$\tau_0 |c_0|^2 \gg \tau_1 |c_1|^2$$

Note: *Runs much longer than τ_0 are required to be able to control the situation*

- How exactly do the topological sectors emerge when $a \longrightarrow 0$?
- Which modes of the gauge field tend to be slowly updated?
- Is there a way to bypass the problem?

Wilson flow

Consider the flow equation

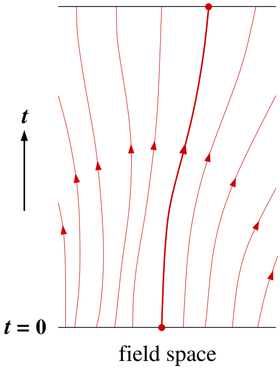
$$\dot{V}_t(x,\mu) = -g_0^2\{\partial_{x,\mu} S_{\mathrm{w}}(V_t)\} V_t(x,\mu)$$

$$V_t(x,\mu)|_{t=0} = U(x,\mu)$$

Properties

- ⋆ $\dot{S}_{\mathrm{w}} \leq 0 \Rightarrow$ the flow tends to smoothen the field and
- ⋆ is in fact generated by infinitesimal stout link-smearing steps

  Morningstar & Peardon '04
- ⋆ The global existence of the flow is rigorously guaranteed



Wilson flow in QED

Continuum flow equation

$$\dot{B}_\mu = D_\nu G_{\nu\mu} \quad \Rightarrow \quad t = [\text{length}]^2$$

Solution in the abelian case

$$B_\mu(t,x) = \int \mathrm{d}^4y\, K_t(x-y) A_\mu(y) + \text{gauge terms}, \qquad K_t(z) = \frac{\mathrm{e}^{-\frac{z^2}{4t}}}{(4\pi t)^2}$$

i.e. $B = A$ smoothed over a range $\boldsymbol{\sqrt{8t}}$

$$\langle B_{\mu_1}(t,x_1)\ldots B_{\mu_n}(t,x_n)\rangle = e_0^n \int \mathrm{d}^4y_1 \ldots \mathrm{d}^4y_n\, K_t(x_1-y_1)\ldots K_t(x_n-y_n)$$

$$\times \underbrace{G_0(y_1,\ldots,y_n)_{\mu_1\ldots\mu_n}}_{\text{bare photon } n\text{-point function}} + \text{g.t.}$$

Renormalization

$$G_0 = Z_3^{n/2} G_{\rm R} \quad e_0 = Z_3^{-1/2} e_{\rm R} \quad \Rightarrow \quad e_0^n G_0 = e_{\rm R}^n G_{\rm R}$$

In other words

$B_\mu(t,x)$ is a renormalized smooth gauge field for $t > 0$

(up to its gauge dof)

Note, for example, that

$$\lim_{t\to\infty} t^2 \langle G_{\mu\nu} G_{\mu\nu} \rangle = \frac{3e_{\rm R}^2}{32\pi^2}$$

$\Rightarrow$ the renormalized charge $e_{\rm R}$ can be "measured" in this way

Wilson flow in QCD

Define

$$E = \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu}$$

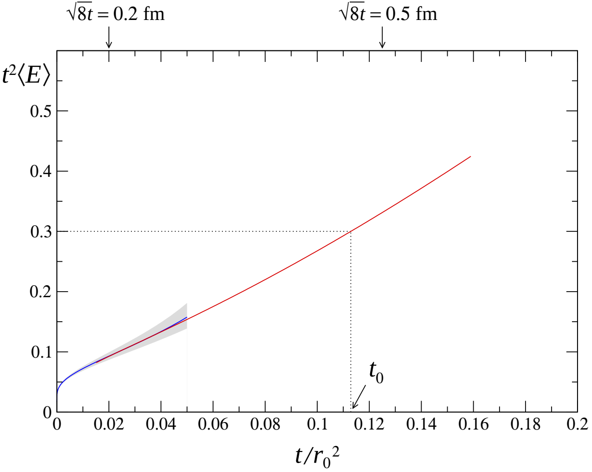
To 1-loop order

$$\langle E \rangle = \frac{3}{4\pi t^2} \alpha(q) \{1 + k_1 \alpha(q) + \ldots\}$$

$$q = (8t)^{-1/2}, \qquad k_1 = 1.0978 + 0.0075 \times N_\mathrm{f} \qquad (\overline{\mathrm{MS}} \text{ scheme})$$

turns out to be a renormalized quantity!

Beyond perturbation theory ...



Pure gauge, 100 cnfg

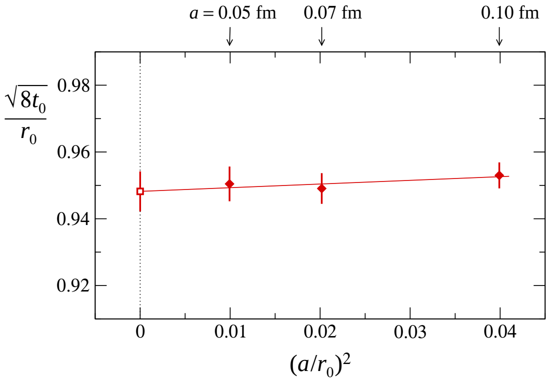
96×48^3

$a = 0.05$ fm

Definition of t_0:

$$t^2 \langle E \rangle \big|_{t=t_0} = 0.3$$

Scaling behaviour



⇒ *Little doubt remains that the Wilson flow maps the gauge field to a renormalized smooth field as in QED*

How do the topological sectors emerge?

Consider the transformation $U \to V = V_{t_0}$

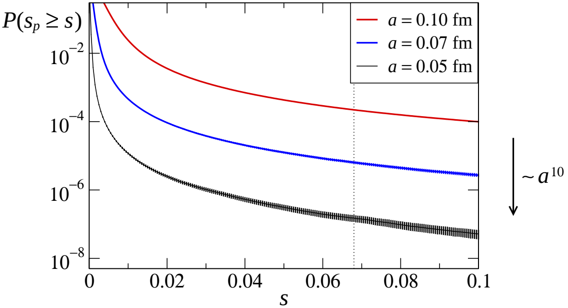
$$\int \mathrm{D}[U] \ldots \mathrm{e}^{-S(U)} = \int \mathrm{D}[V] \ldots \mathrm{e}^{-\tilde{S}(V)}$$

$$\tilde{S}(V) = S(U) + \frac{16 g_0^2}{3a^2} \int_0^{t_0} \mathrm{d}t \, S_{\mathrm{w}}(V_t)$$

$\Rightarrow$ large values of

$$s_p = \mathrm{Re}\,\mathrm{tr}\{1 - V(p)\}, \qquad V(p) =$$

are strongly suppressed as $a \to 0$



The submanifold of fields V satisfying

$$s_p < 0.067 \text{ for all } p$$

divides into topological sectors ML '82, Phillips & Stone '86

$\Rightarrow$ **the probability to be "between the sectors" decreases roughly like a^6 !**

Autocorrelation times

SU(3) theory, HMC algorithm, $\tau = 2$, $P_{\rm acc} = 83\%$

t/t_0	$\tau_{\rm int}[Q]$	$\tau_{\rm int}[Q^2]$	$\tau_{\rm int}[E]$
0.2	65(5)	30(2)	22(1)
0.4	67(5)	32(2)	34(2)
0.8	68(6)	33(2)	43(3)

48×24^3, $a = 0.1$ fm

$\tau_{\rm int}[s_p] = 9$ [MD time]

0.2	614(90)	284(34)	53(4)
0.4	615(90)	286(34)	68(5)
0.8	615(90)	286(34)	85(6)

64×32^3, $a = 0.07$ fm

$\tau_{\rm int}[s_p] = 7$

$\tau_{\rm int}[Q]$: $\sim a^{-6}$ $\qquad$ $\tau_{\rm int}[E]$: $\sim a^{-2}$

Open boundary conditions

Periodic in space, but not in time

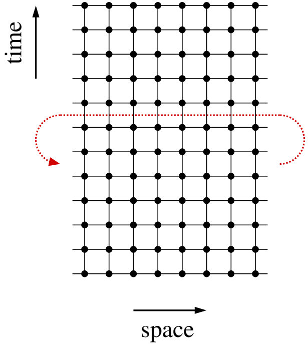
Amounts to Neumann b.c.

$$F_{0k}(x) = 0 \quad \text{at} \quad x_0 = 0, T$$

in the continuum theory

⇒ Field space becomes connected, i.e. instantons can move in and out

⇒ Simulations should not get trapped anymore



However . . .

	$\tau_{\text{int}}[Q]$	$\tau_{\text{int}}[Q^2]$	$\tau_{\text{int}}[E]$	
periodic	68(6)	33(2)	43(3)	48×24^3, $a = 0.1$ fm
open	61(6)	27(2)	36(3)	

periodic	615(90)	286(34)	85(6)	64×32^3, $a = 0.07$ fm
open	384(56)	155(20)	75(6)	

$\Rightarrow$ Visible improvement, but scaling is still $\sim \boldsymbol{a^{-5}}$

$\Rightarrow$ Slowdown is partly caused by other effects

Conclusions

The "wall" is still there, but looks less daunting than a year ago

- ⋆ *Wilson flow = interesting tool for studying the continuum limit in QCD*
- ⋆ *In particular, one can now understand how the topological sectors emerge*
- ⋆ *With open b.c., the barriers between the sectors disappear*

The challenge is to find algorithms that move V_t (at, say, $t = t_0$) rapidly through field space