crafting the change of variables for HMC

Xiao-Yong Jin - Argonne National Laboratory - July 28, 2026 - Lattice 2026 - UMD

change of variables and HMC

- for a partition function with a change of variables, $\theta = f(\phi)$

$$Z = \int e^{-S(\theta)} d\theta = \int |\det J_f(\phi)| \, e^{-S(f(\phi))} d\phi = \int e^{-S_{\text{eff}}(\phi)} d\phi$$

- sample the effective action in HMC with the variable ϕ

$$S_{\text{eff}}(\phi) = S(f(\phi)) - \ln |\det J_f(\phi)|$$

- with the gradient

$$\partial_\phi S_{\text{eff}}(\phi) = J_f(\phi)^T S'(f(\phi)) - \partial_\phi \ln |\det J_f(\phi)|$$

2D U(1) lattice gauge

- Wilson plaquette gauge action, with θ the phase angle of the gauge link

$$S(\theta) = -\beta \sum_x \cos \Phi_x$$

- with the principle plaquette angle

$$\Phi_x = \left[\theta_{0,x} + \theta_{1,x+\hat{0}} - \theta_{0,x+\hat{1}} - \theta_{1,x}\right]_{2\pi} \in [-\pi, \pi)$$

- topological charge

$$Q(\theta) = \frac{1}{2\pi} \sum_x \Phi_x$$

local change of variables for 2D U(1)

local maps of scalar analytic Jacobians

- option 1: change a single link depending on the two plaquette

$$\chi = \frac{\phi_+ + \phi_-}{2}, \qquad \xi = \frac{\phi_+ - \phi_-}{2}, \qquad \eta = g(\xi;\chi) \qquad \Phi_+ = \chi + \eta, \qquad \Phi_- = \chi - \eta, \qquad \Delta = \eta - \xi$$

$$\theta_{\text{sel}} = \vartheta_{\text{sel}} + \Delta, \qquad \det J_{\text{link}} = g_\xi, \qquad g_\xi \equiv \frac{\partial g}{\partial \xi} > 0$$

  - a special case is the stout smearing step, or gradient flow step

$$g(\xi;\chi) = \xi - 2\rho \cos\chi \, \sin\xi \qquad g_\xi = 1 - 2\rho \cos\chi \cos\xi = 1 - \rho\left(\cos\phi_+ + \cos\phi_-\right) \geq 1 - 2|\rho| > 0$$

- option 2: change 4 links that surround a plaquette

$$\Phi_c = g(\phi_c), \qquad \Delta = \Phi_c - \phi_c \qquad \theta_j = \vartheta_j + \frac{\Delta}{4}, \qquad j = 0,1,2,3$$

$$\Phi_j = \phi_j - \frac{\Delta}{4}, \qquad \det J_{\text{plaq}} = g'(\phi_c)$$

- option 3: consider all 5 plaquette values to change those 4 links (not shown in this talk)

target effective action
what to optimize?

- lower barrier
  - Hamiltonian dynamics may move around the phase space
- smooth
  - small force, small force gradient, reduced integration error in MD
- look at the force and force gradient on the mapped & un-mapped links
- $\ln g'$ lowers action barrier, dynamic range $g' \sim 0$ to e^S
- circular map constraint: $\int_{-\pi}^{\pi} g'(x)dx = g(\pi) - g(-\pi) = 2\pi$, and symmetry $g'(-x) = g'(x)$

mapping one link → force on neighbors

$$\delta S_{\text{eff}} = F_\xi \, \delta\xi + F_\chi \, \delta\chi$$

$$(\delta\xi, \delta\chi) = (\delta\vartheta, 0) \quad \Longrightarrow \quad F_{\text{mapped}} = F_\xi$$

$$(\delta\xi, \delta\chi) = \frac{1}{2}(\pm\delta\vartheta, \delta\vartheta) \quad \Longrightarrow \quad F_{\text{unmapped}} = \frac{1}{2}(F_\chi \pm F_\xi)$$

$$K_{\max} \equiv \max_i \left| \lambda_i\left(\nabla_\vartheta F \right) \right|$$

analytic target effective action

- option 1: make the effective action a scale of the original, reduced β

$$S_{\text{eff}}(\phi) = \alpha S(\theta) + C$$

- option 2: mostly lower the barrier of the original action
  - generic exponential suppression

$$S_{\text{eff}} = S - De^{-2\kappa(1-z)} \quad z_{\text{link}} = \frac{1 - \cos\chi\cos\xi}{2} \quad z_{\text{plaq}} = \frac{1 - \cos\Phi}{2}$$

  - only change the link depending on the 2 plaquettes

$$S_{\text{eff}} = S - D(1 - r_+ r_-) \quad r_\pm = 1 - e^{-\kappa(1+\cos\phi_\pm)}$$

parameterize the map $g(x)$, and optimize

- a scalar circle map, $g(x + 2\pi) = g(x) + 2\pi$, $g'(x) > 0$ for all x
- we parameterize $g'(x)$ in practice, to match the target effective action
  - analytical form of the first and second derivatives
  - maximal flexibility, yet still cheap to compute
- possible parmeterization
  - squared Fourier series, or squared interpolating cubic spline
  - Fejer series, a special Fourier, non-negative kernel by construction
  - B-spline with non-negative basis, cheaper than series to evaluate ⟵ this talk
- direct repeating map helps with numerical stability, eg. for 3 steps, $g = g_{1/3} \circ g_{1/3} \circ g_{1/3}$

code, QEX, autodiff

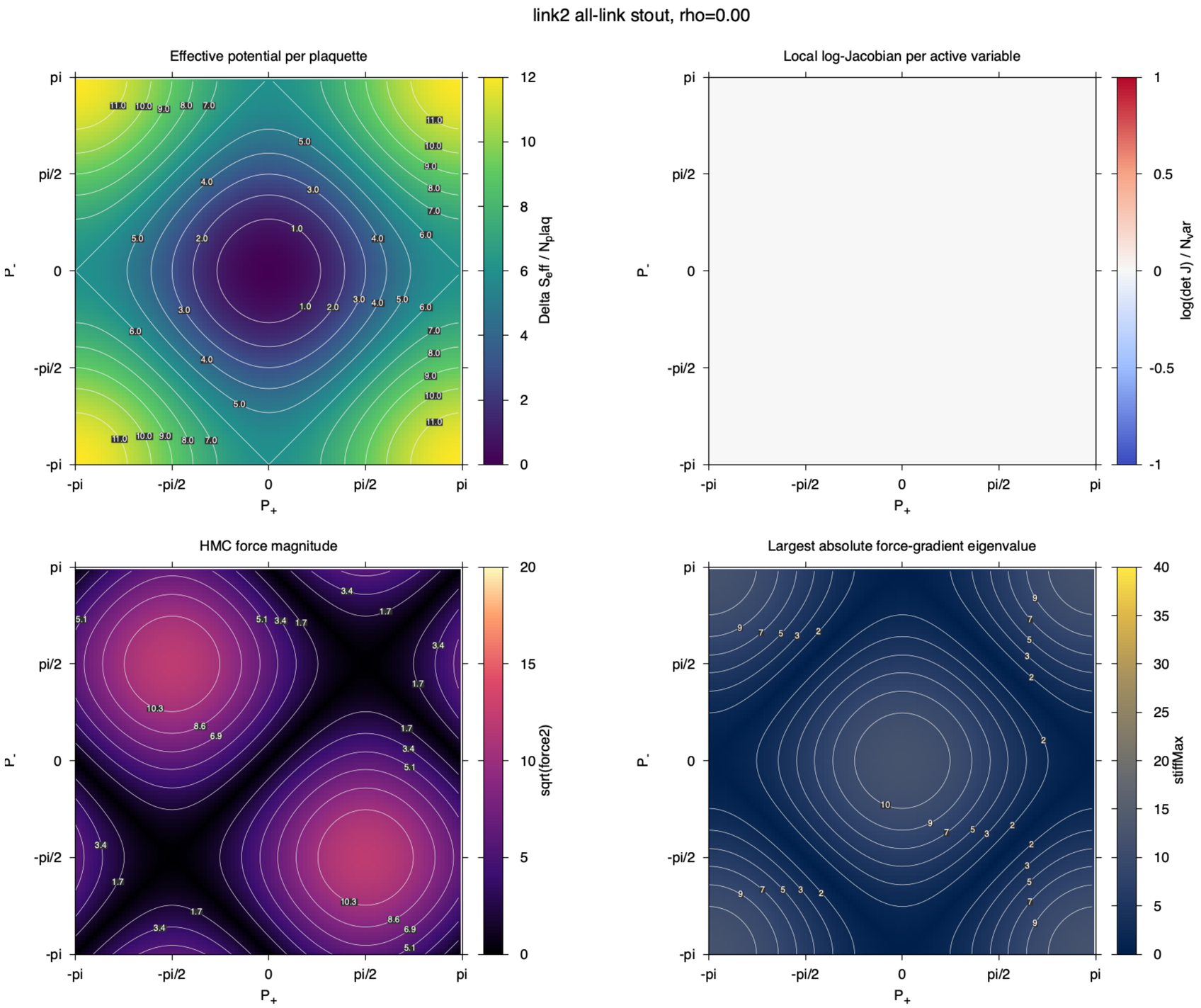
- implementation in QEX, with autodiff https://github.com/jcosborn/qex/tree/devel/src/experimental/ft2du1

```
proc mulggb(zb: Gvalue, z: Gvalue, i: int, input: Gvalue): Gvalue =
  let x = Ggauge(z.inputs[0])
  let y = Ggauge(z.inputs[1])
  let upstream = requireUpstream(zb, "g*g backward", Ggauge)
  if i == 0: result = upstream * y.adj
  x.adj * upstream
proc mulggf(v: Gvalue) =
  let x = Ggauge(v.inputs[0])
  let y = Ggauge(v.inputs[1])
  let z = Ggauge(v)
  z.mapGaugeSites(x.gval[mu] * y.gval[mu])
let mulgg = Gfunc(forward: mulggf, backward: mulggb, name: "g*g")
proc `*`*(x: Ggauge, y: Ggauge): Ggauge =
  graphNode(sameShapeGaugeNodeLike(x, y, "g*g"), @[Gvalue(x), Gvalue(y)], mulgg, "g*g")
```

```
let grt = initGraphRuntime()
grt.graphDebug = true

let x = toGvalue(grt, 0.0)
let y = toGvalue(grt, 0.0)
let w = x - 2.0
let v = w + y
let z = v * (-v) / w
let dzdy = z.grad y

let a = 1.1
let b = 3.7
let c = 1.3

x.update a
y.update b

echo "z = ", z
echo "dzdy = ", dzdy

y.update c

echo "z = ", z
echo "dzdy = ", dzdy
```

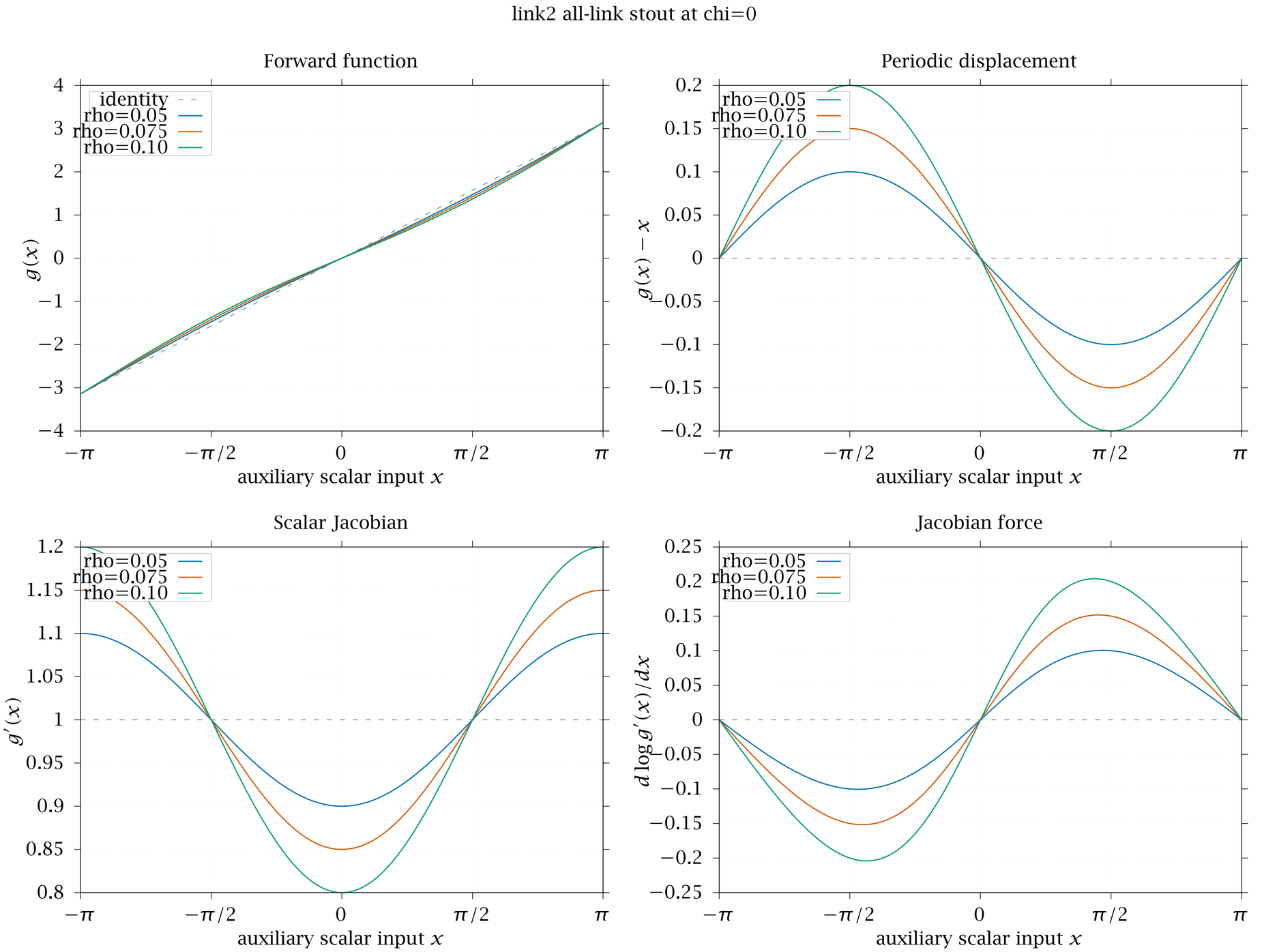
identity map
single link

- $\beta = 6$ 2D U(1) action
- effective action
- force on the link
- force gradient



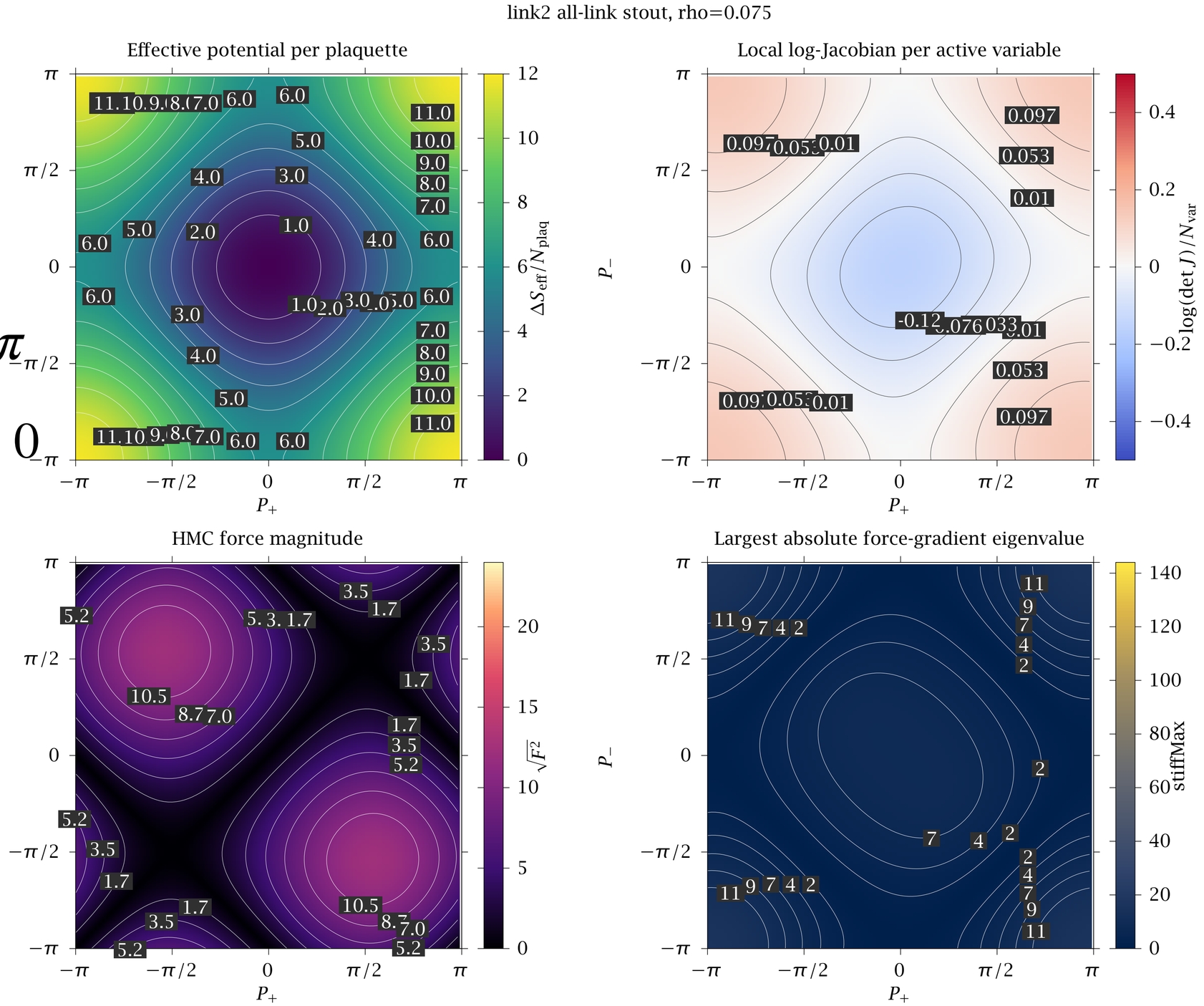
stout step
single link

- smooth
- numerically stable



stout step
single link

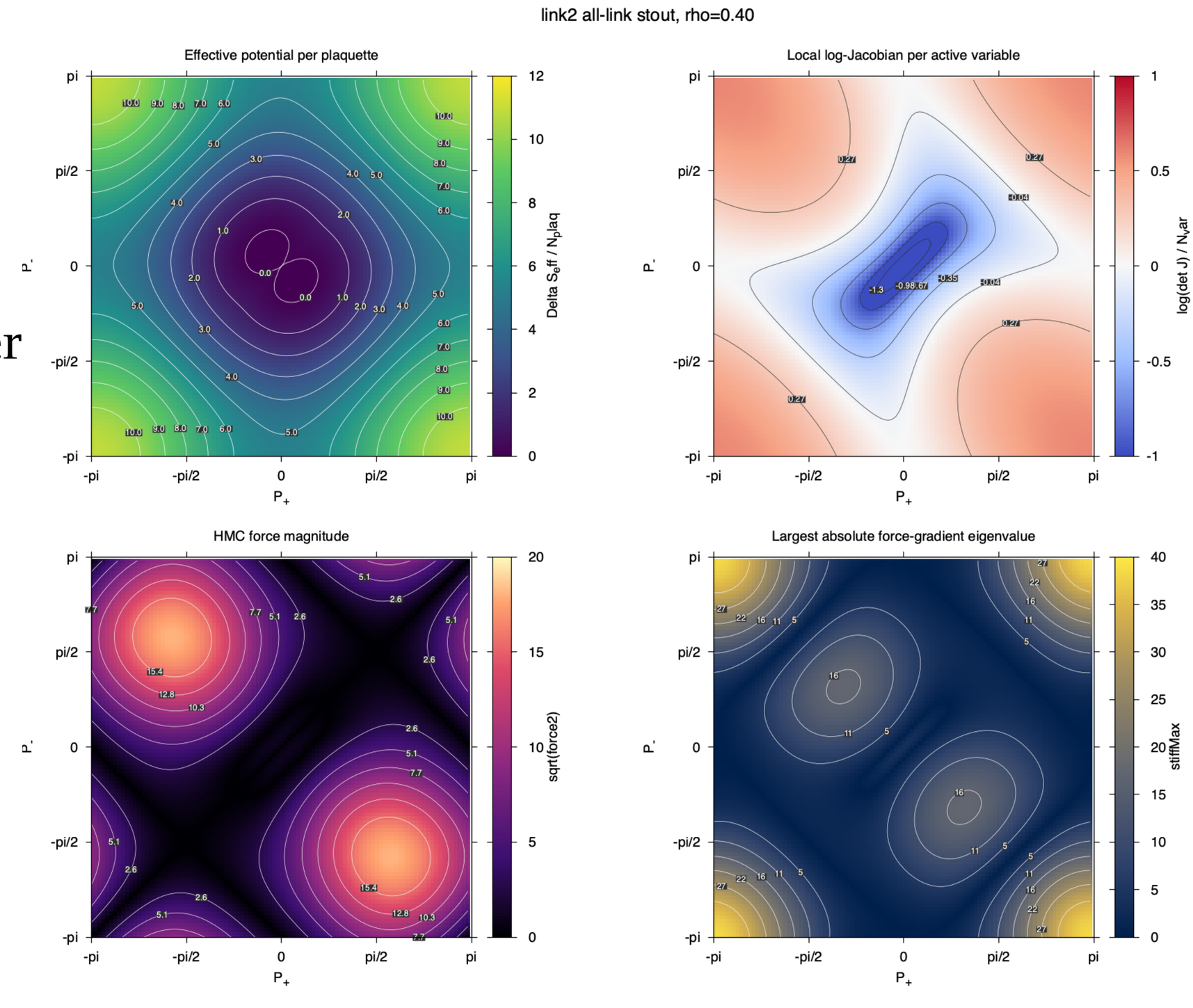
- lower the action at $\pm\pi$
- increase the action at 0
- increase the force
- increase the force gradient



stout step

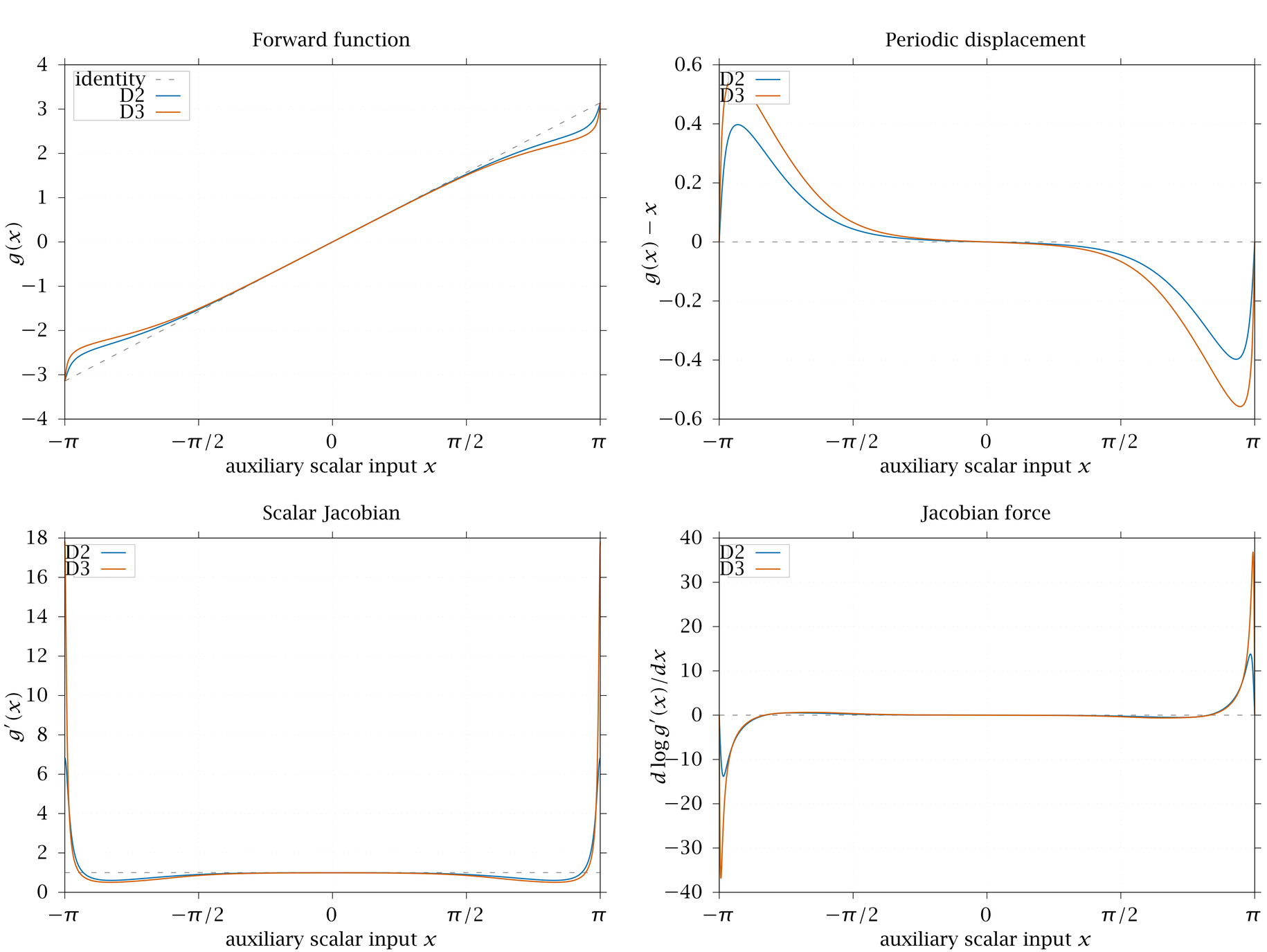
$\rho = 0.4$

- slight distorted center
- larger max force
- larger max force gradient
- flatter within $\pm\frac{\pi}{4}$



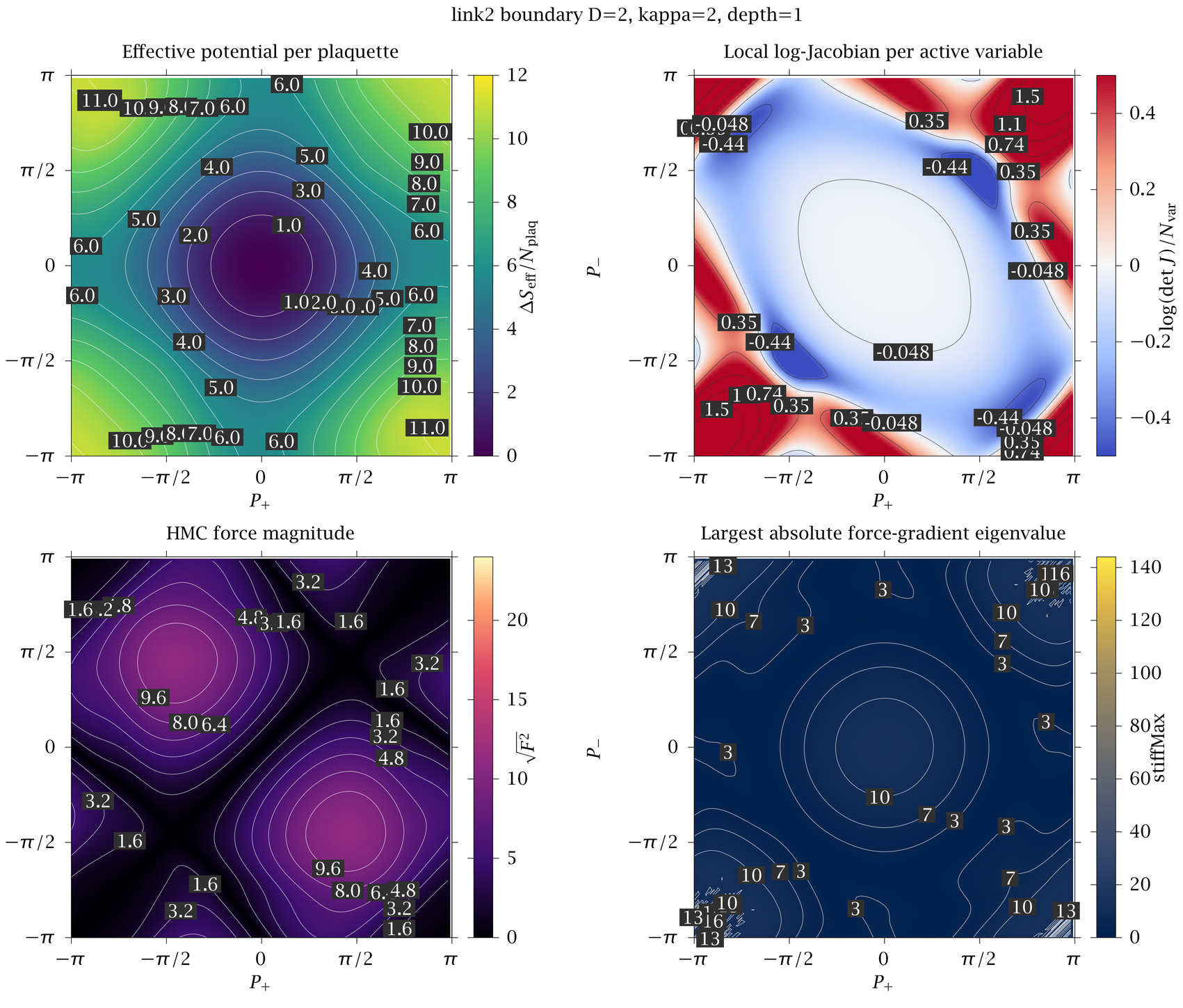
single link
D=2 and 3

- large jacobian, force near the boundary



single link
D=2

- small change in the center
- lower barrier
- lower force
- larger force gradient at the corner



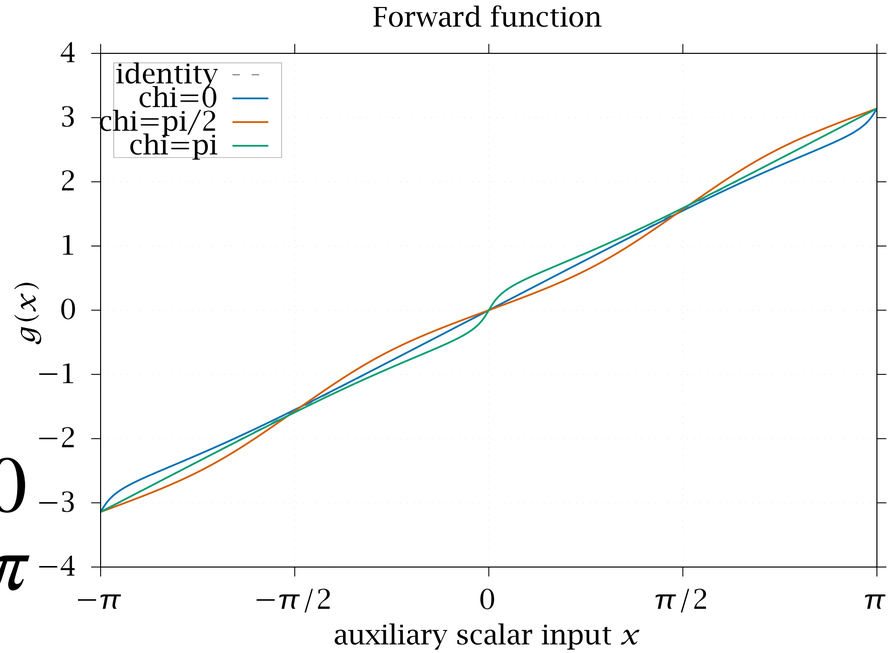
single link
stronger map

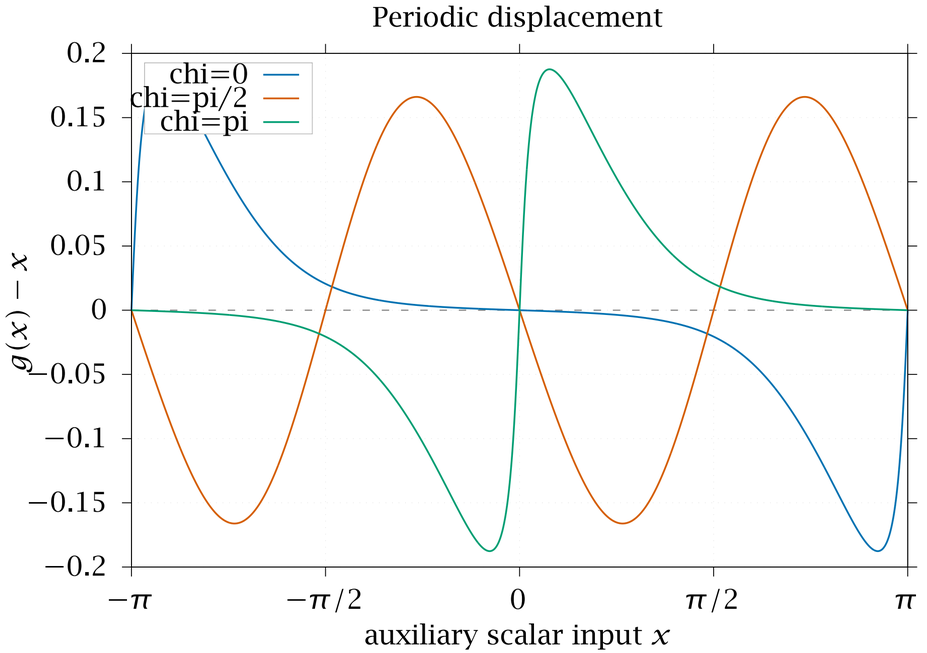
- large g' spikes
  at $\xi = \pm\pi, \chi = 0$
  at $\xi = 0, \chi = \pm\pi$

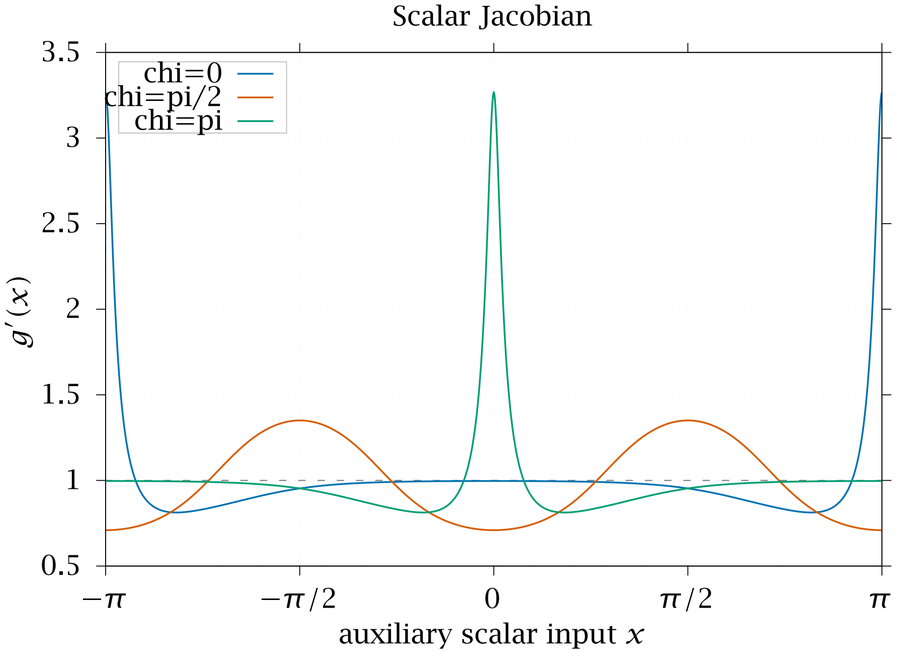
$$\chi = \frac{\phi_+ + \phi_-}{2}$$

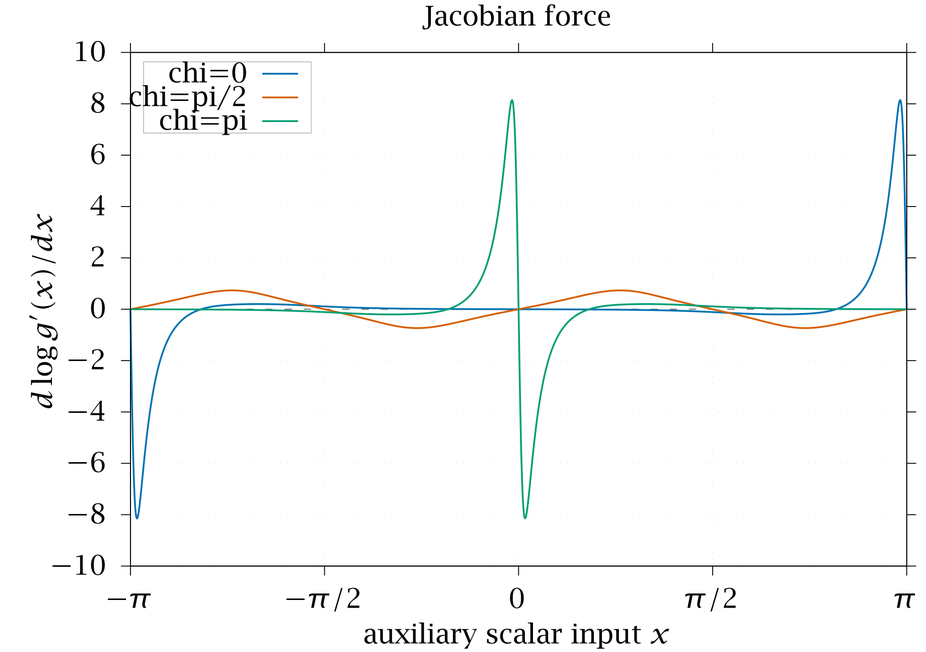
$$\xi = \frac{\phi_+ - \phi_-}{2}$$

$$\eta = g(\xi;\chi)$$



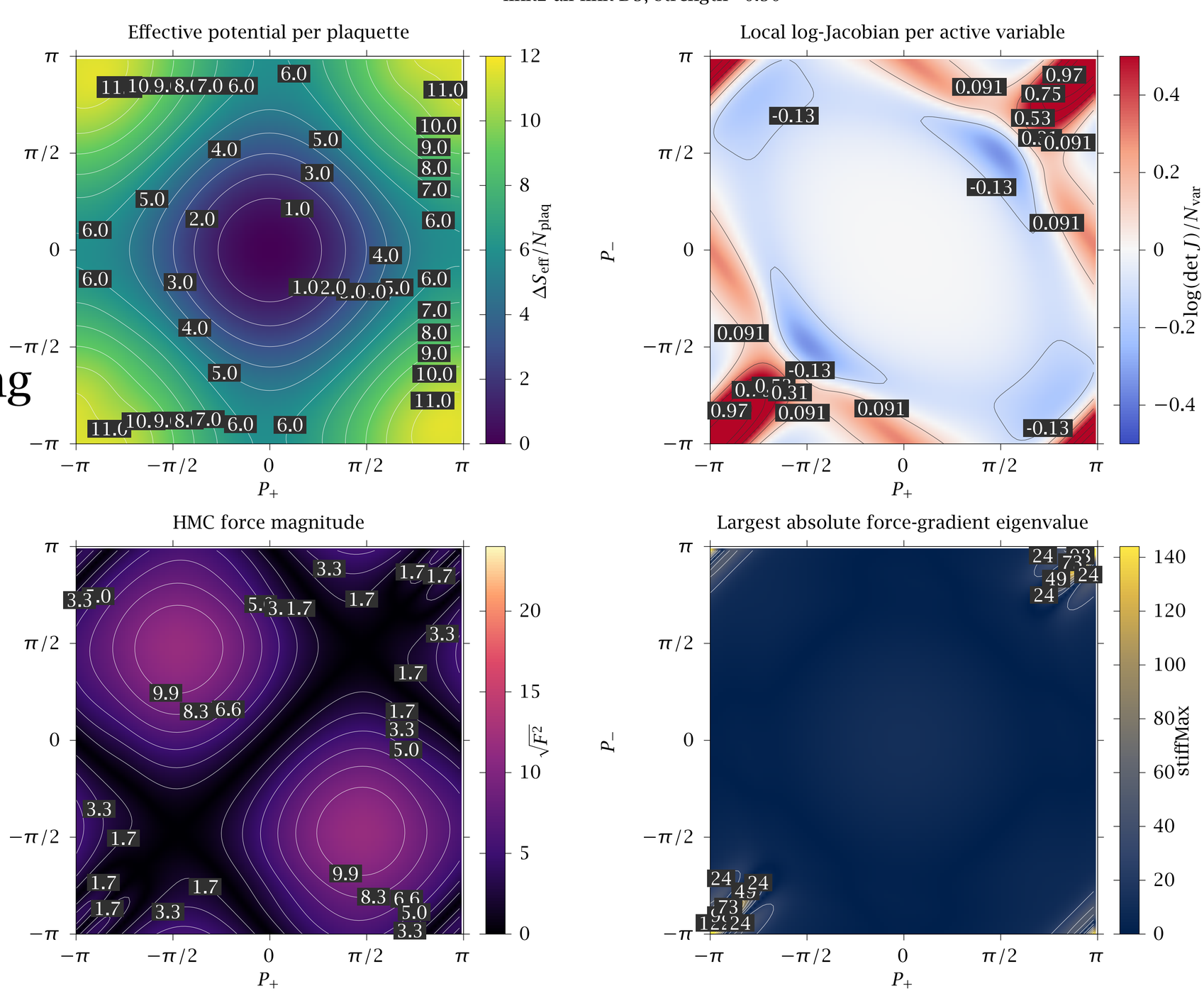




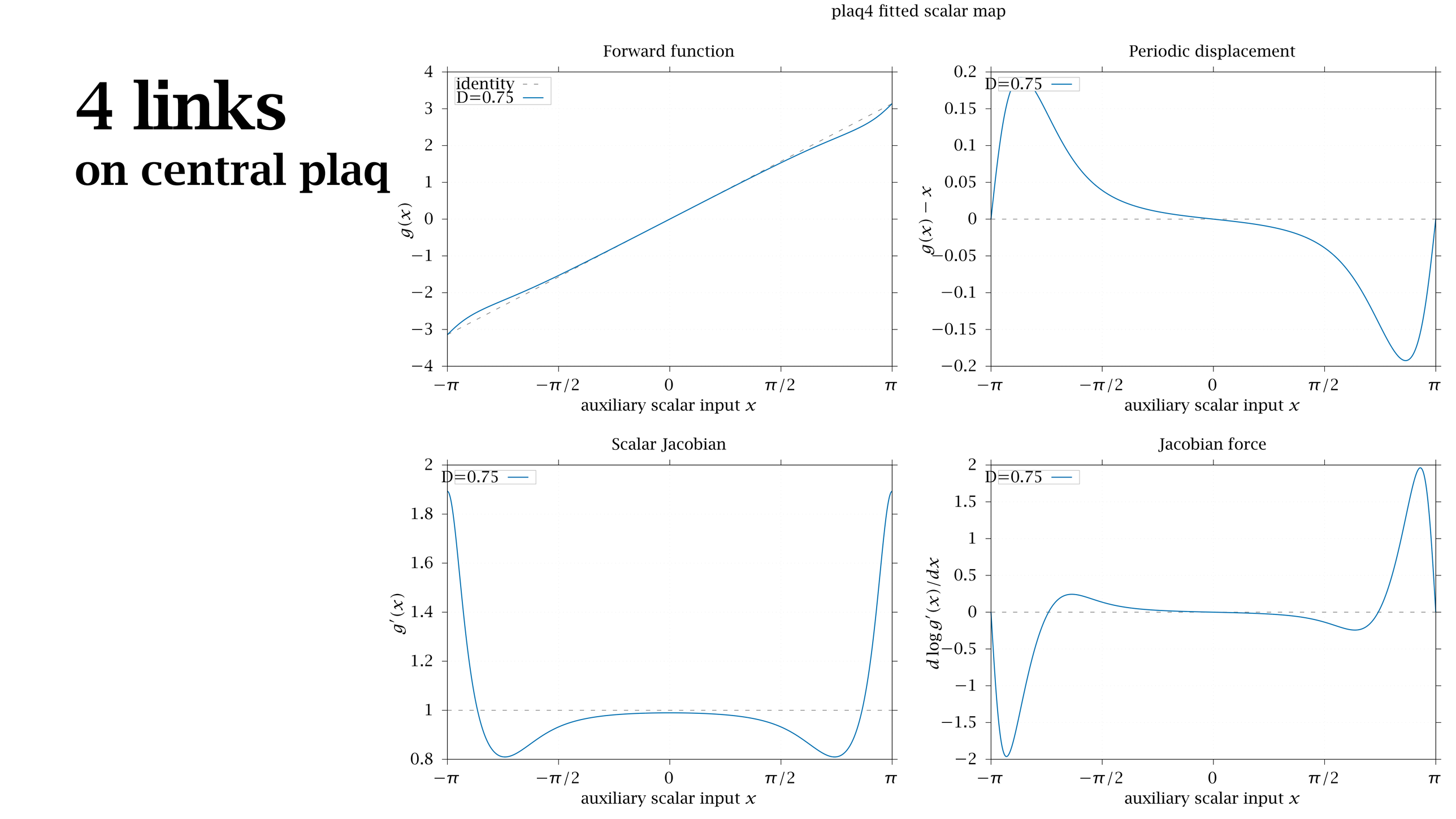


single link
stronger map

- Jacobian peak at corners, corresponding to the large spikes
- lower action barrier
- lower force
- large spikes in force gradient at corners

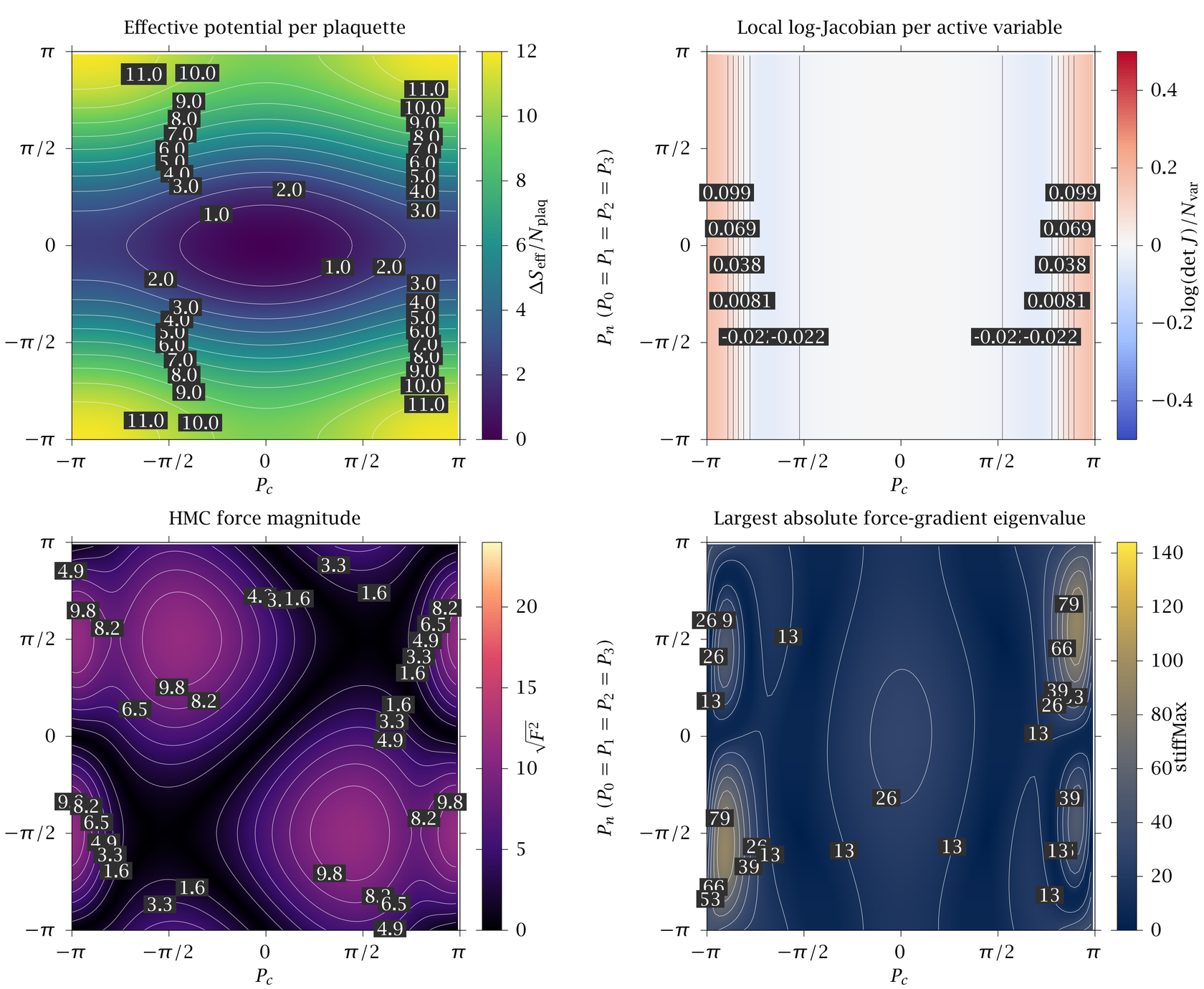


4 links
on central plaq



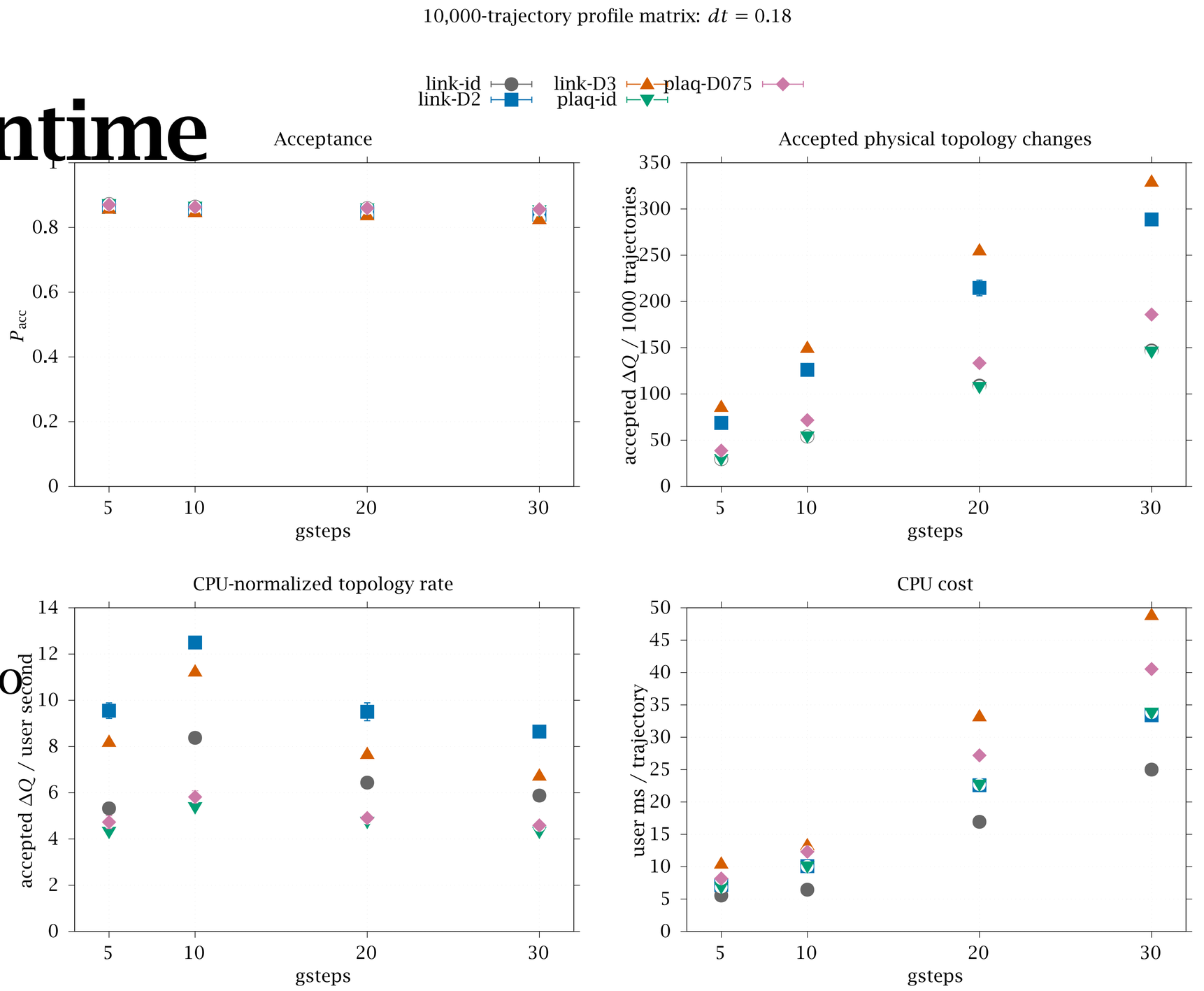
4 links
map of central plaq

- lower barrier for the central plaqutte at $\pm\pi$
- lower force
- larger force gradient at 0 and $\pm\pi$



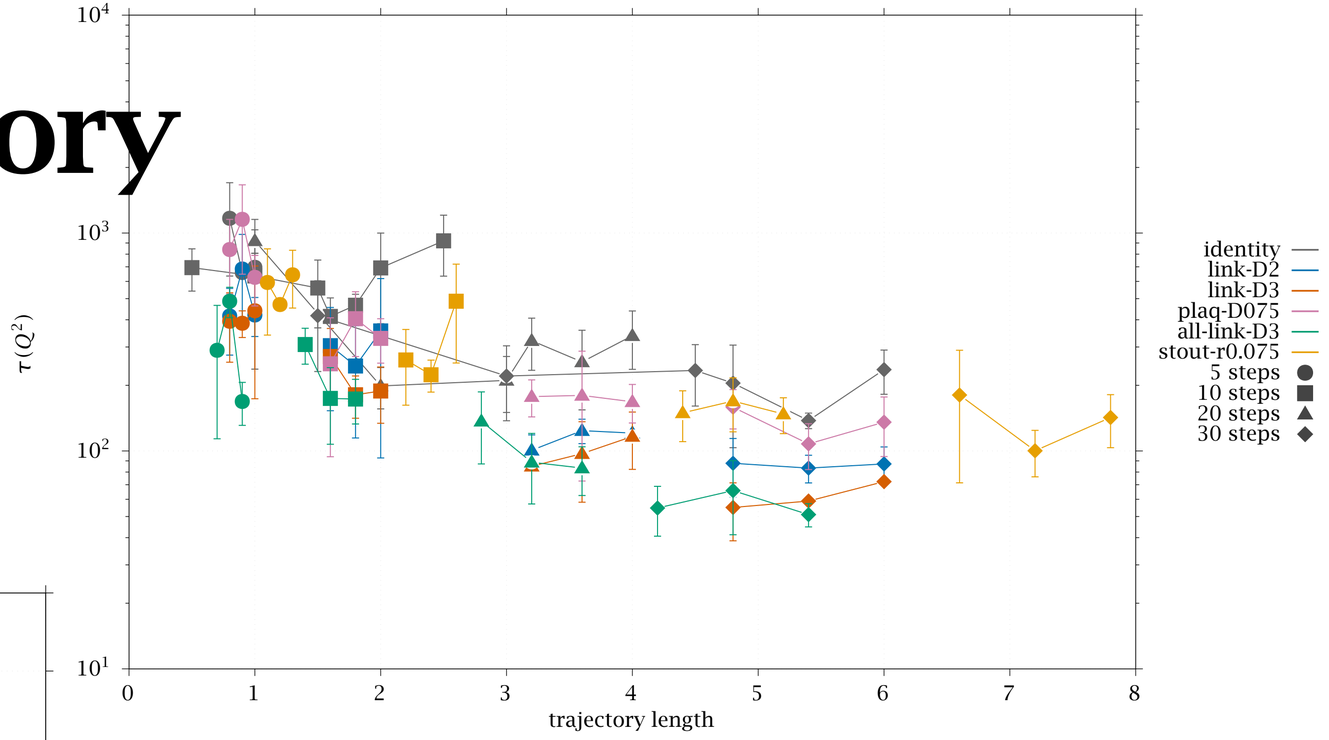
steps and runtime

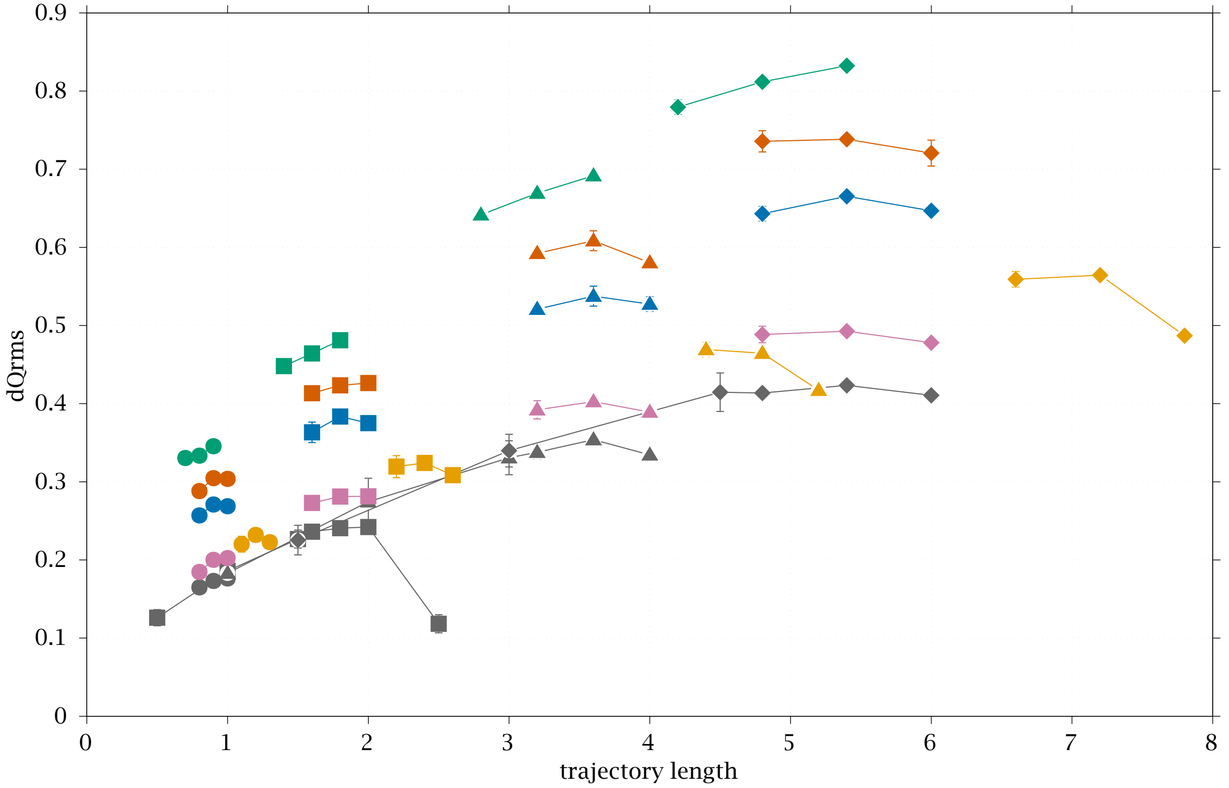
- run on laptop
- not optimized
- relative cost meaningful
- D=2 and 3 applied to 1/4 of all links



tuning HMC trajectory

- 64×64, 2D U(1), $\beta = 6$





- D=2 and 3 applied to 1/4 of all gauge links
- integrated autocorrelation length noisy
- Q changes improved

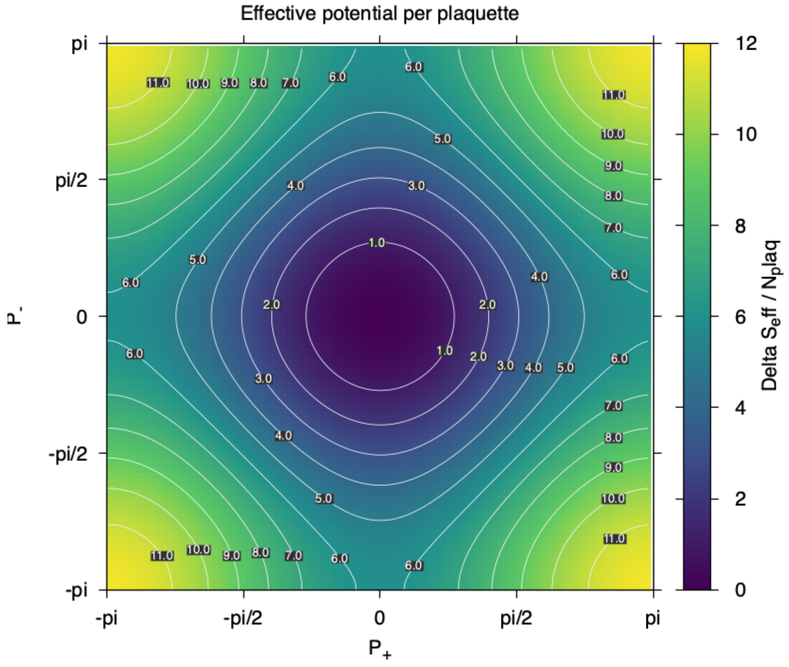
next

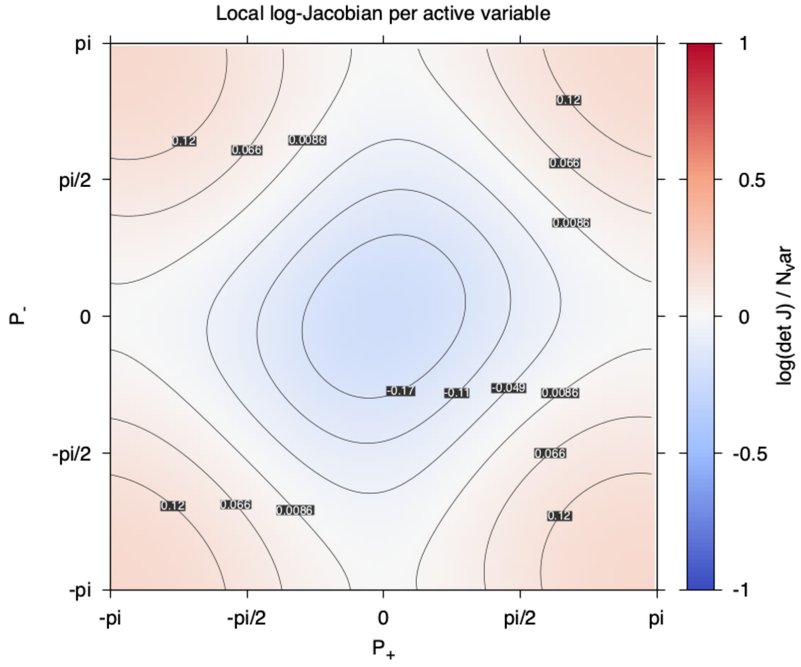
- need to understand the source of large force gradient
- make the effective action more smooth everywhere
- tune B-spline directly with some loss function
- extend to 4D SU(3)

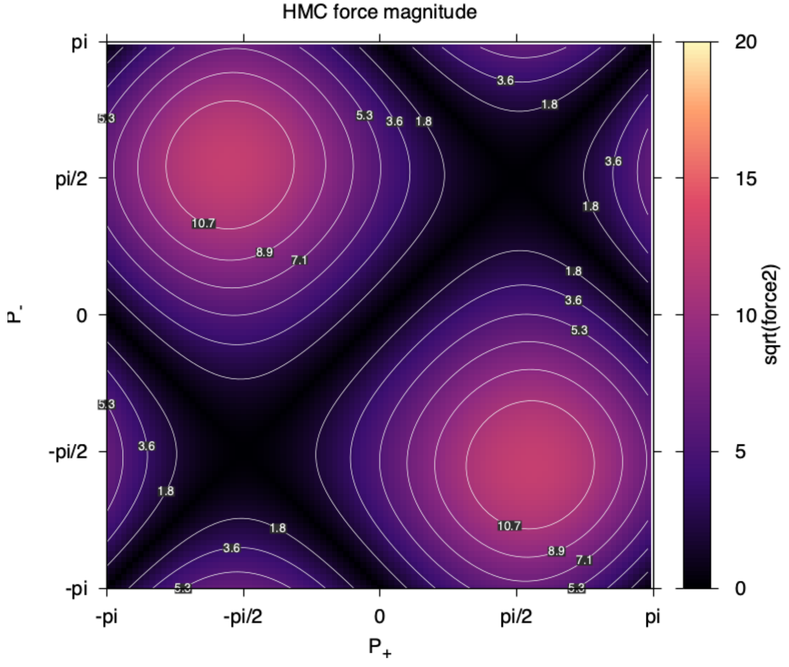
acknowledgment

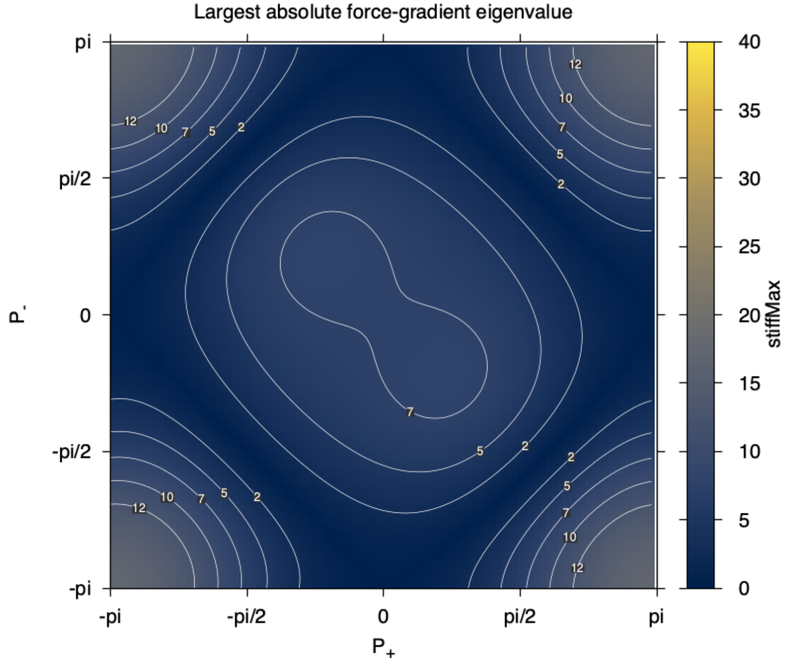
- supported by SciDAC-5 funded by the U.S. Department of Energy
- thanks James Osborn for insightful discussions
- claude opus 4.8 and gpt 5.6 sol verified maths and refactored/wrote substantial portion of the implementation in QEX

link2 all-link stout, rho=0.10

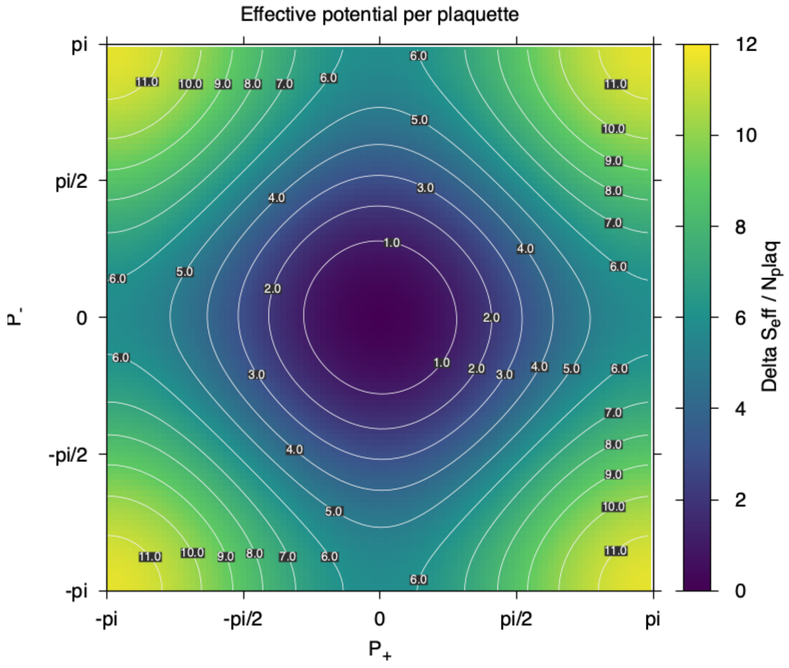


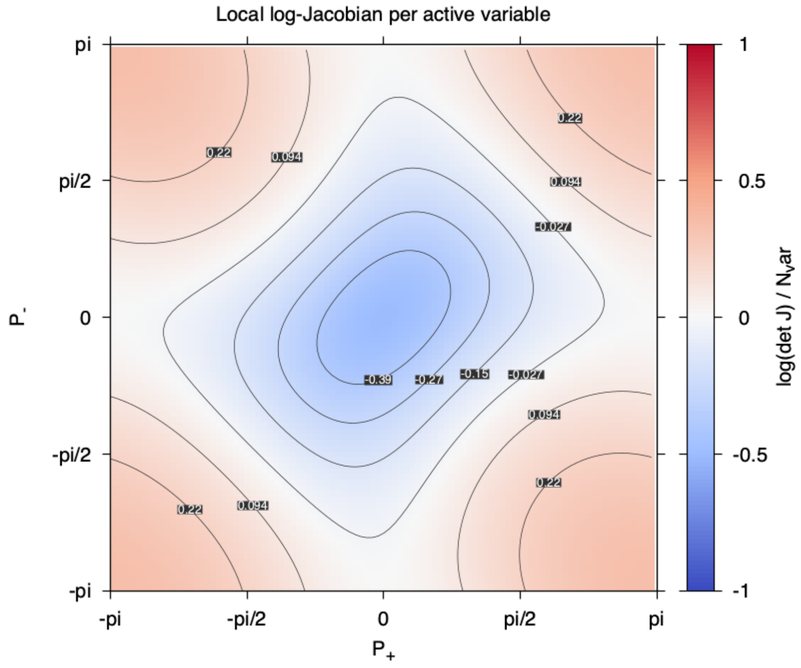


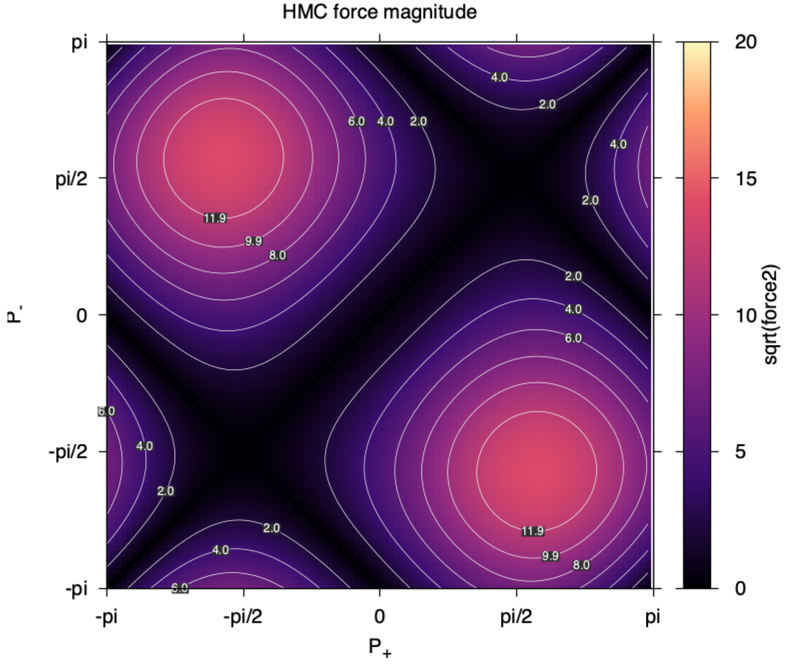


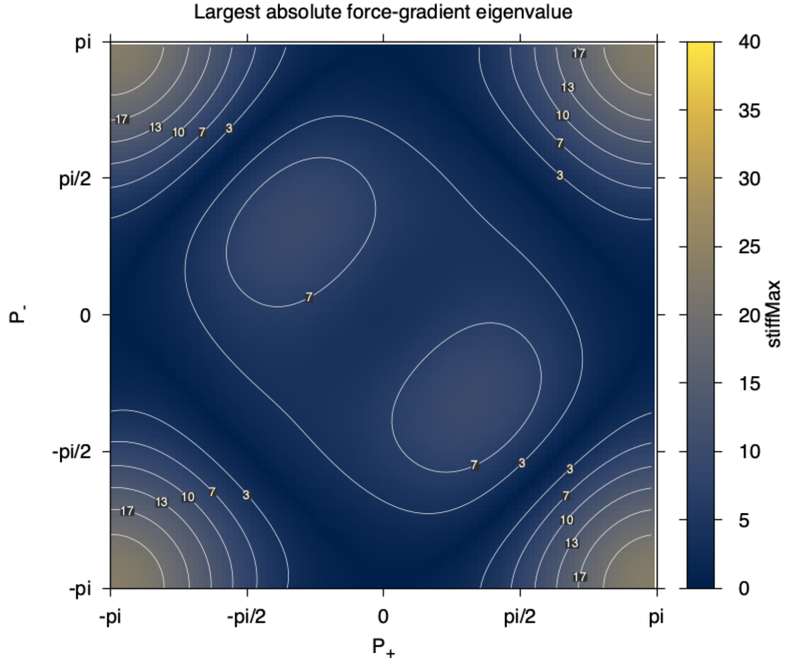


link2 all-link stout, rho=0.20









link2 all-link stout, rho=0.30