# 1 Hamiltonian Monte Carlo, code tests

### Energy conservation in HMC potential kinetic energy -1000 -2000

Figure 1: Action, kinetic term and Hamiltonian vs integration step;  $(p,q)=(1,1); n=20; g=-2.5; L=100; \tau=0.0001;$  time: 5s.

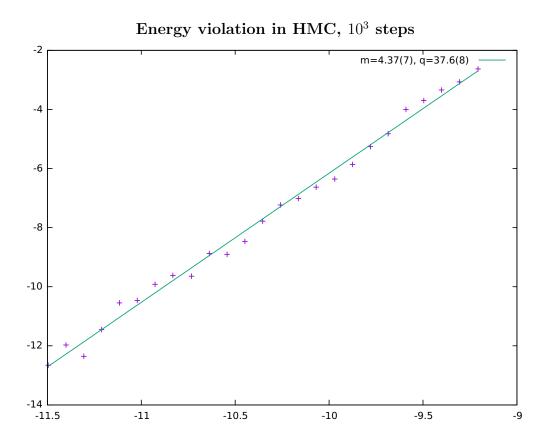


Figure 2:  $\log \Delta H$  vs  $\log \tau$  (purple):  $(p,q)=(2,0);\ n=10;\ g=-2.2431;$   $L=10^3;$  Linear fit (green):  $m=4.37\pm0.07,\ q=37.6\pm0.8$ 

### Energy violation in HMC, 10<sup>4</sup> steps 0.5 m=1.95(5), q=18.1(5) 0 -0.5 -1 -1.5 -2 -2.5 -3 -3.5 -4 -4.5 -5 L -11.5 -11 -9.5 -10.5 -10

Figure 3:  $\log \Delta H$  vs  $\log \tau$  (purple):  $(p,q)=(2,0);\ n=10;\ g=-2.2431;$   $L=10^4;$  Linear fit (green):  $m=1.95\pm0.05,\ q=18.1\pm0.1$ 

### Energy violation in HMC, $10^5$ steps m=1.74(4), q=17.5(4) 1.5 1 0.5 0 -0.5 -1 -1.5 -2 -2.5 -3 L -11.5 -11 -10.5 -9.5 -10 -9

Figure 4:  $\log \Delta H$  vs  $\log \tau$  (purple):  $(p,q)=(2,0);\ n=10;\ g=-2.2431;$   $L=10^5;$  Linear fit (green):  $m=1.74\pm0.04,\ q=17.5\pm0.4$ 

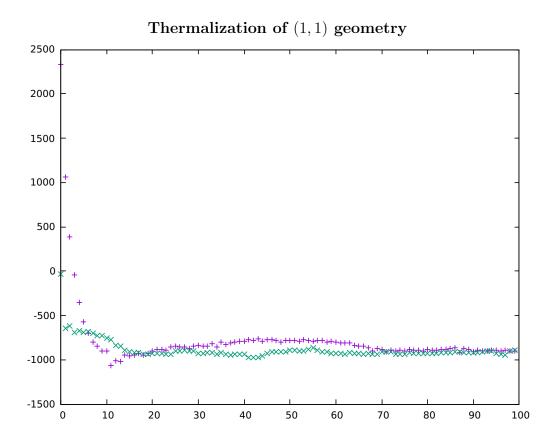


Figure 5: Action Tr  $D^4+g$  Tr  $D^2$  vs Monte Carlo time; (p,q)=(1,1); n=20;  $g=-2.5; L=100; \tau_{\rm cold10}=0.0001; \tau_{\rm cold90}=0.0005; \tau_{\rm hot}=0.001;$  time: 5s.

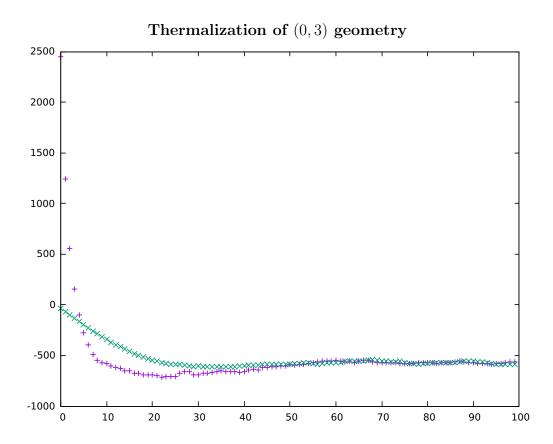


Figure 6: Action Tr  $D^4+g$  Tr  $D^2$  vs Monte Carlo time; (p,q)=(0,3); n=20; g=-2.5; L=100;  $\tau=0.0001;$  time: 36s.

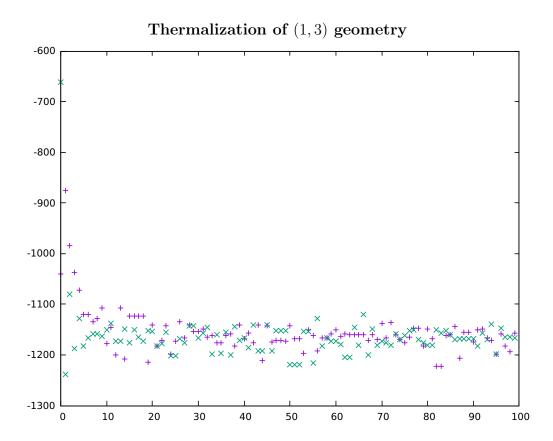


Figure 7: Action Tr  $D^4+g$  Tr  $D^2$  vs Monte Carlo time; (p,q)=(1,3); n=20;  $g=-2.5; L=100; \tau_{\rm cold10}=0.001; \tau_{\rm cold90}=0.0005; \tau_{\rm hot}=0.0005;$  time: 5m 40s.

## Action (2,0): comparison Metropolis/HMC 0 HMC Metropolis + -500 -1000 -1500 -2000 -2500 -3000 -3.5 -2.5 -3 -2 -4 -1.5

Figure 8: Action Tr  $D^4+g$  Tr  $D^2$  vs g; Metropolis (Green) and HMC (purple);  $(p,q)=(2,0);\ n=20;\ L=100;\ \tau=0.0001;$  time 13m 20s

# Order parameter (2,0): comparison Metropolis/HMC O.7 HMC + Metropolis O.4 O.3 O.2 O.1

Figure 9: Order parameter vs g; Metropolis (Green) and HMC (purple);  $(p,q)=(2,0);~n=20;~L=100;~\tau=0.0001;$  time 13m 20s

-2.5

-2

-1.5

-3

-3.5

-4