

1 Hamiltonian Monte Carlo, code tests

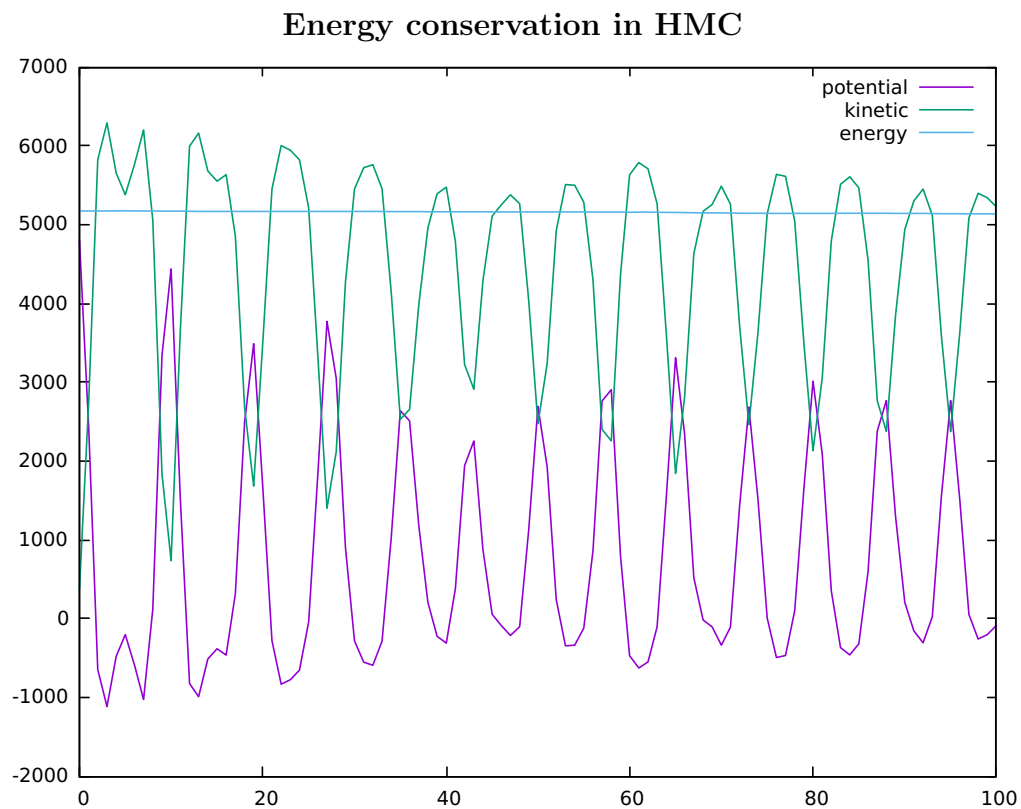


Figure 1: Action, kinetic term and Hamiltonian vs integration step; $(p, q) = (1, 1)$; $n = 20$; $g = -2.5$; $L = 100$; $\tau = 0.0001$; time: 5s.

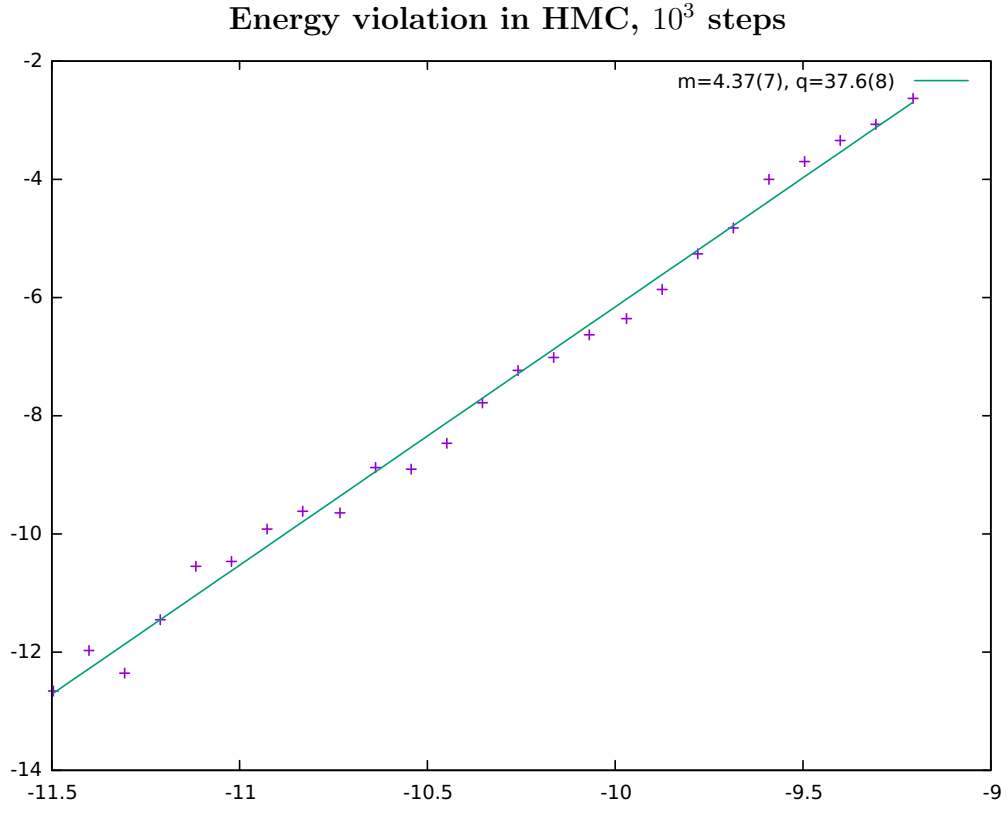


Figure 2: $\log \Delta H$ vs $\log \tau$ (purple): $(p, q) = (2, 0)$; $n = 10$; $g = -2.2431$; $L = 10^3$; Linear fit (green): $m = 4.37 \pm 0.07$, $q = 37.6 \pm 0.8$

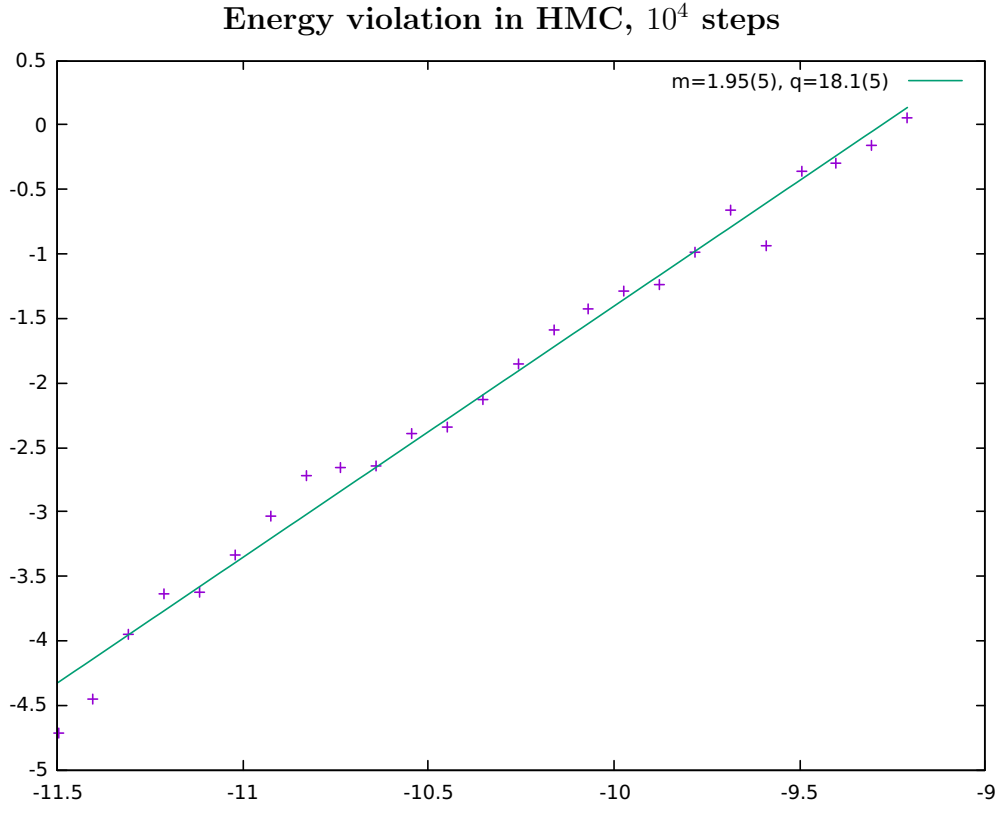


Figure 3: $\log \Delta H$ vs $\log \tau$ (purple): $(p, q) = (2, 0)$; $n = 10$; $g = -2.2431$; $L = 10^4$; Linear fit (green): $m = 1.95 \pm 0.05$, $q = 18.1 \pm 0.1$

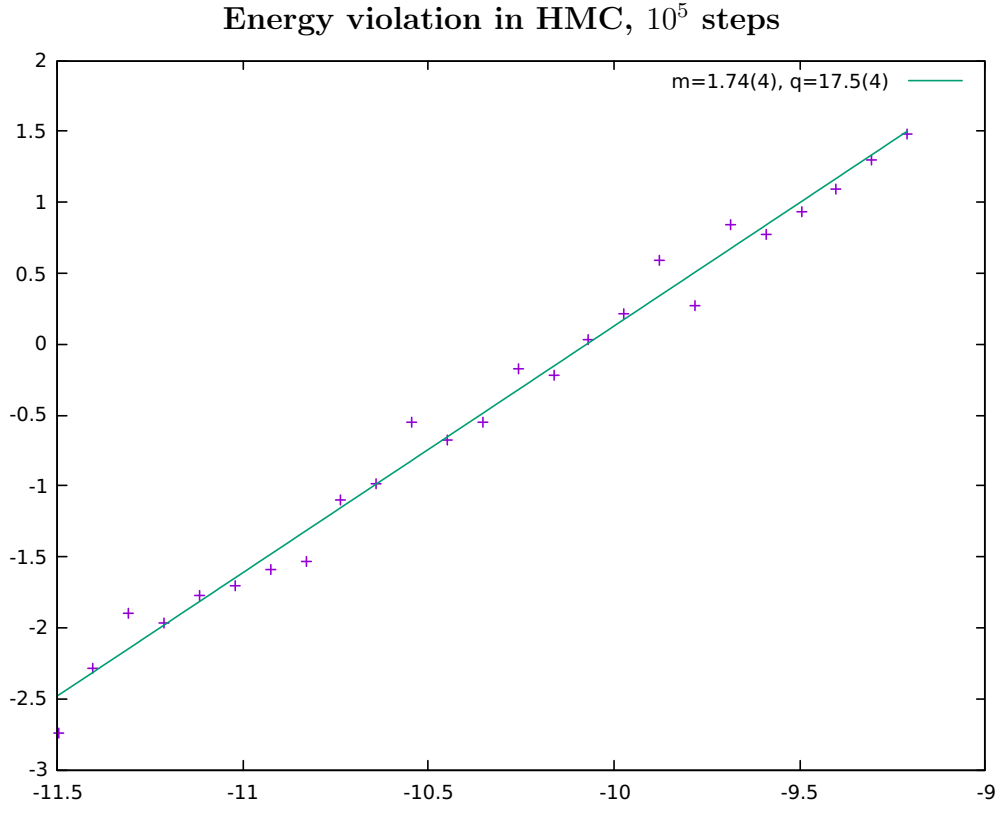


Figure 4: $\log \Delta H$ vs $\log \tau$ (purple): $(p, q) = (2, 0)$; $n = 10$; $g = -2.2431$; $L = 10^5$; Linear fit (green): $m = 1.74 \pm 0.04$, $q = 17.5 \pm 0.4$

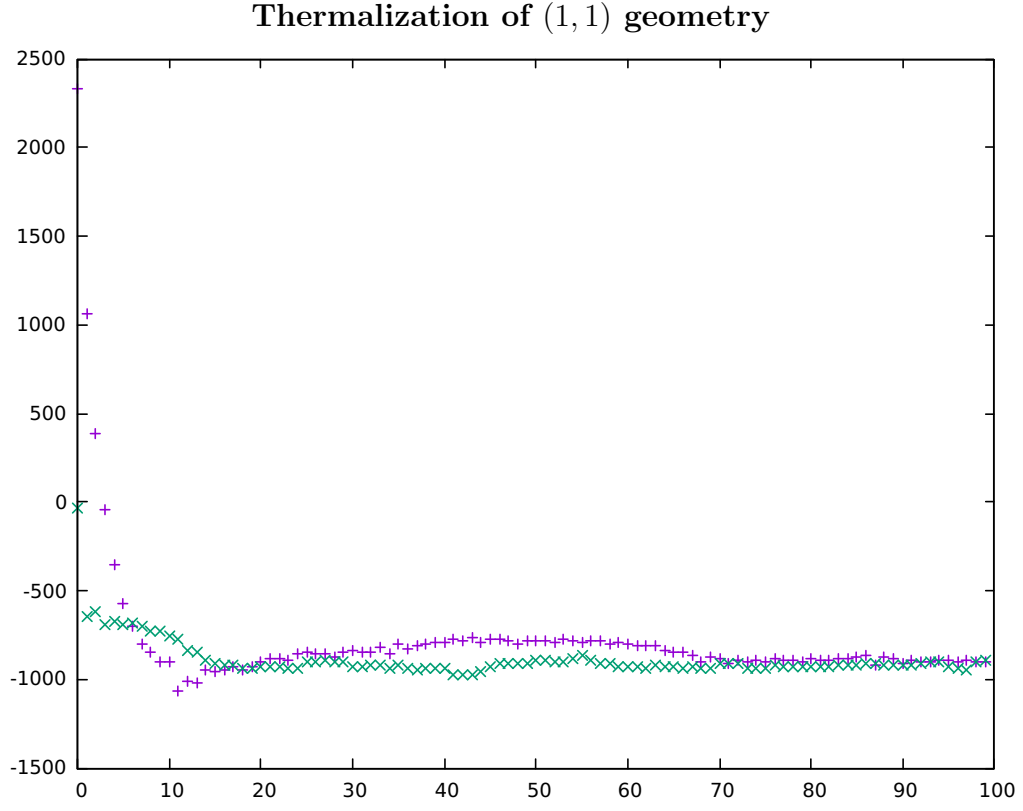


Figure 5: Action $\text{Tr } D^4 + g \text{Tr } D^2$ vs Monte Carlo time; $(p, q) = (1, 1)$; $n = 20$; $g = -2.5$; $L = 100$; $\tau_{\text{cold}10} = 0.0001$; $\tau_{\text{cold}90} = 0.0005$; $\tau_{\text{hot}} = 0.001$; time: 5s.

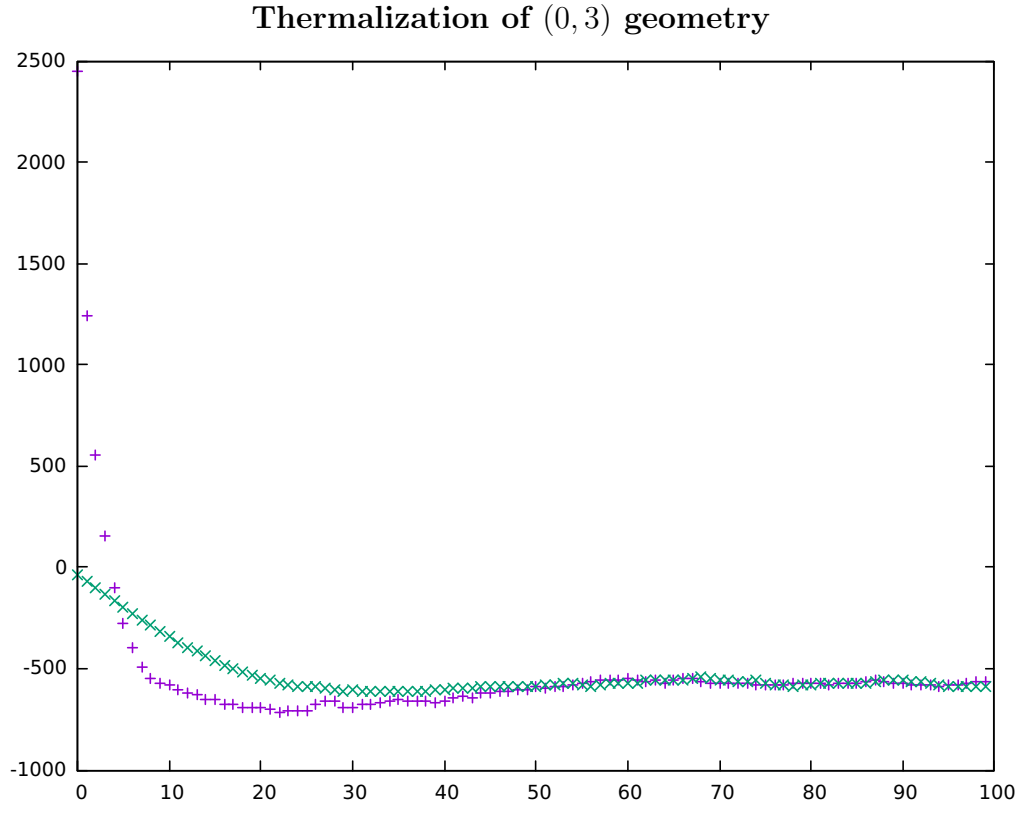


Figure 6: Action $\text{Tr } D^4 + g \text{Tr } D^2$ vs Monte Carlo time; $(p, q) = (0, 3)$; $n = 20$; $g = -2.5$; $L = 100$; $\tau = 0.0001$; time: 36s.

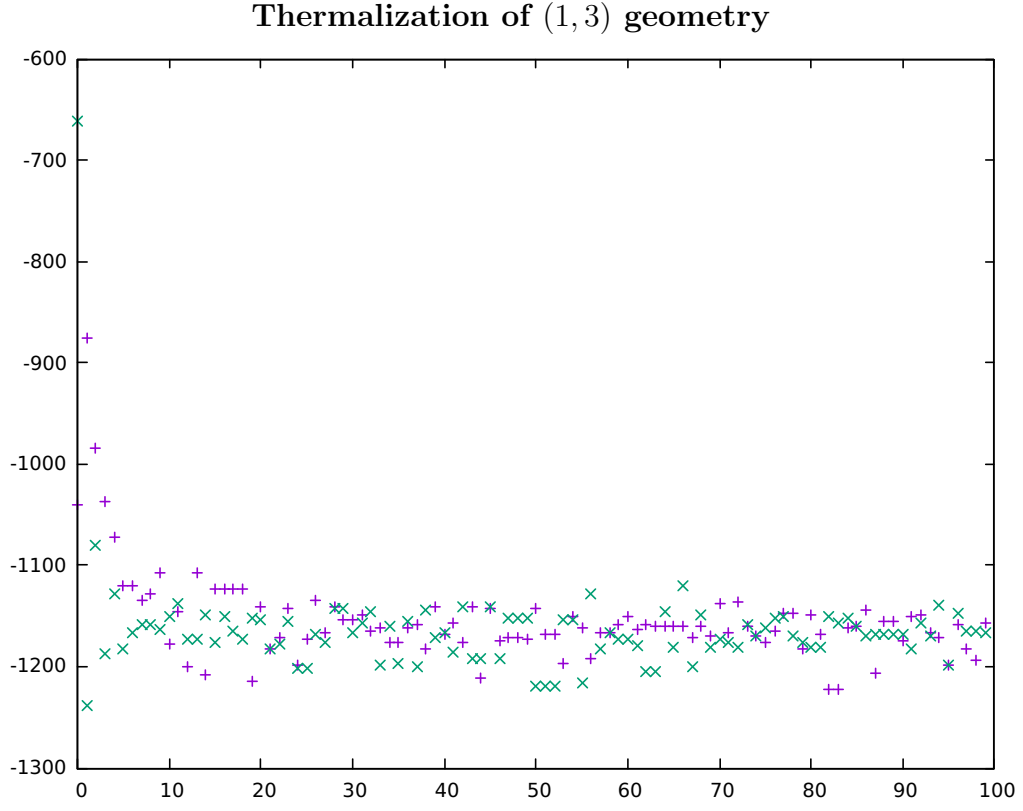


Figure 7: Action $\text{Tr } D^4 + g \text{Tr } D^2$ vs Monte Carlo time; $(p, q) = (1, 3)$; $n = 20$; $g = -2.5$; $L = 100$; $\tau_{\text{cold}10} = 0.001$; $\tau_{\text{cold}90} = 0.0005$; $\tau_{\text{hot}} = 0.0005$; time: 5m 40s.

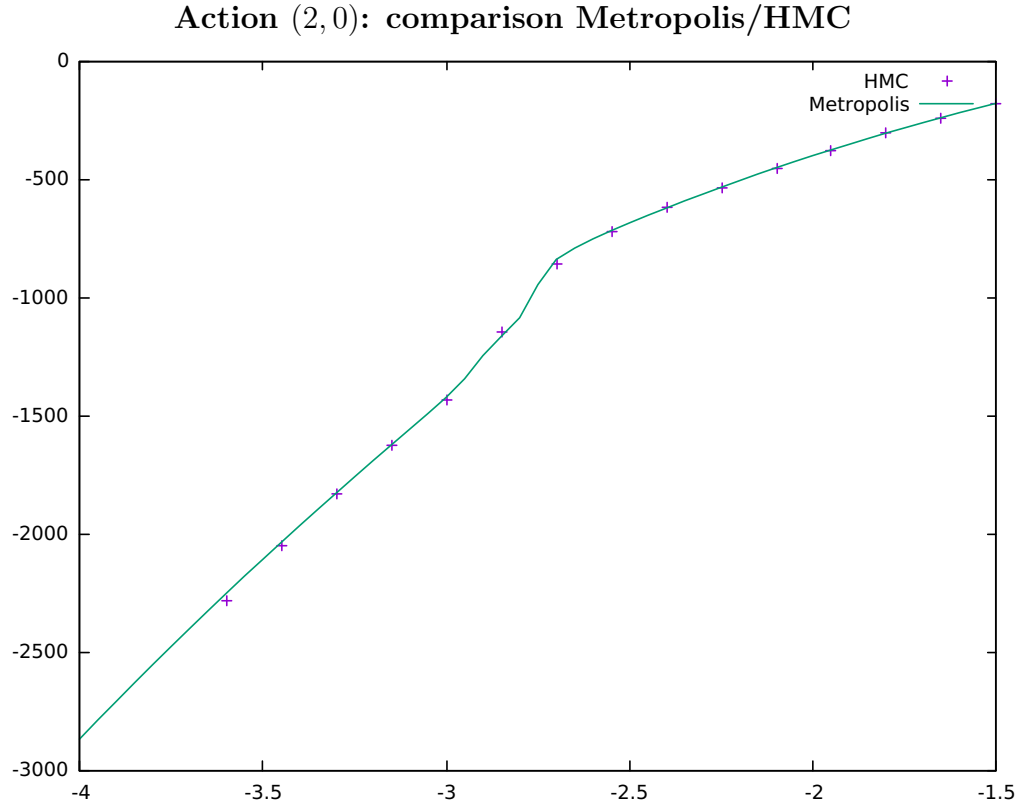


Figure 8: Action $\text{Tr } D^4 + g \text{Tr } D^2$ vs g ; Metropolis (Green) and HMC (purple); $(p, q) = (2, 0)$; $n = 20$; $L = 100$; $\tau = 0.0001$; time 13m 20s

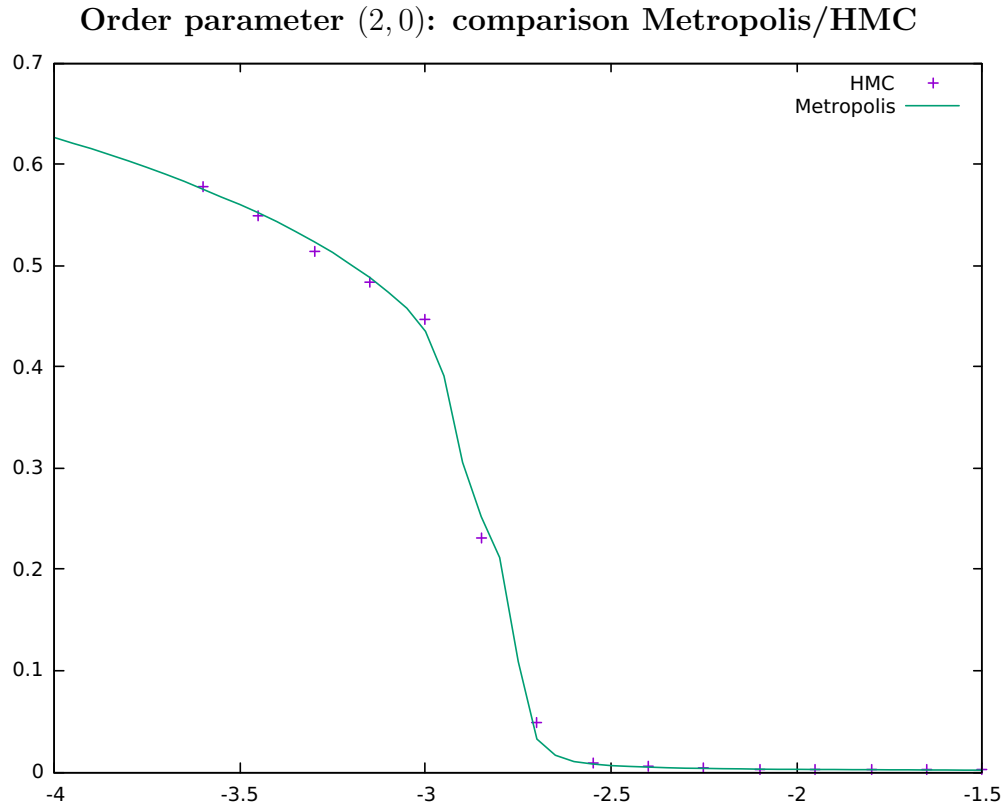


Figure 9: Order parameter vs g ; Metropolis (Green) and HMC (purple); $(p, q) = (2, 0)$; $n = 20$; $L = 100$; $\tau = 0.0001$; time 13m 20s

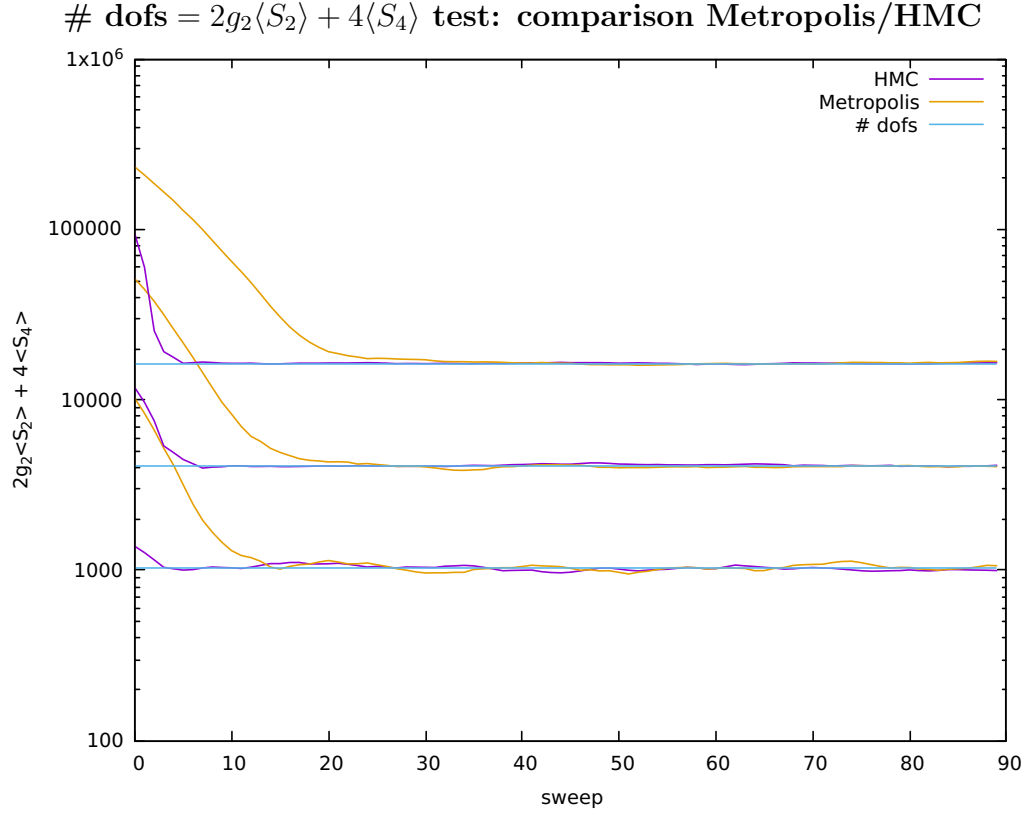


Figure 10: Convergence of the expectation value of the observable $2g_2 \text{Tr } D^2 + 4 \text{Tr } D^4$ to the number of degrees of freedom of the Dirac operator for geometry $(0,3)$. The three sets correspond to matrix size $n = 16 \times 16$, 32×32 and 64×64 .

Matrix dimension	time HMC (sec)	time Metropolis (sec)
16	23	17
32	100	428
64	1612	21218

Table 1: Time for 100 sweeps of HMC and Metropolis for geometry $(0, 3)$. Fitting of the data gives a computational cost of $O(n^{4.6})$ and $O(n^{2.6})$ for Metropolis and HMC respectively.

Autocorrelation of order parameter $(2,0)$ test: comparison Metropolis/HMC

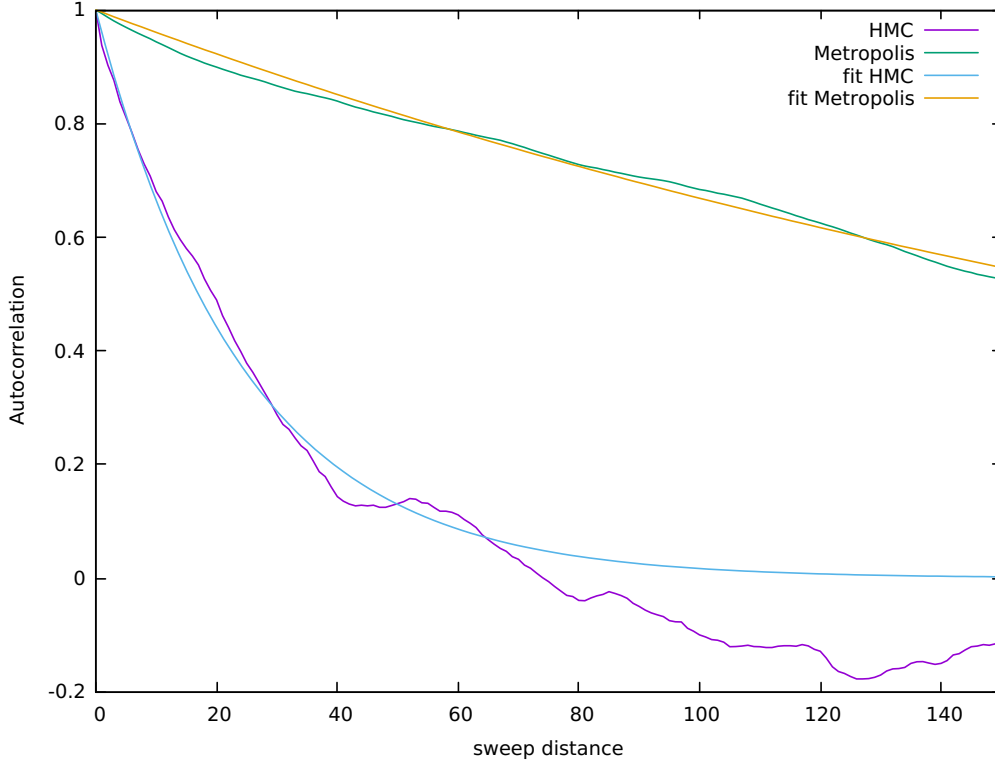


Figure 11: Autocorrelation $\chi(a) = \langle F(t)F(t+a) \rangle - \langle F(t) \rangle \langle F(t+a) \rangle$ normalized by $\chi(0)$, where $F(t)$ is the order parameter for the $(2,0)$ phase transition at Monte Carlo time t . The coupling constant $g_2 = 2.725$ was chosen to be at the phase transition. The exponential fit gives an autocorrelation time of ~ 250 sweeps for Metropolis and ~ 25 sweeps for HMC.