New symplectic integrators for Hybrid Monte Carlo algorithm in lattice QCD

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The Hybrid Monte Carlo (HMC) algorithm[1] consists of molecular dynamics (MD) trajectories, each followed by a Metropolis test. During the MD trajectory, one integrates Hamilton's equations of motion, using an integrator with a discrete stepsize Δt which must satisfy two conditions in order to maintain detailed balance: (i) simplecticity and (ii) time reversibility. The simplest and most widely used integrator wih these properties is the 2nd order leap frog (2LF) integrator with $O(\Delta t^2)$ errors. These errors are eliminated at the Metropolis accept/reject step, which makes the algorithm exact.

The acceptance at the Metropolis step depends on the magnitude of the error in the total energy. In order to reduce the error and thus increase the acceptance one could use higher order integrators. Early attempts, however, did not appear to be practical [2, 3]. This is because the efficiency of higher order integrators depends largely on the system size and these early attempts were made on rather small lattices. As the lattice size increases above a certain value V_c, the higher order integrators should perform better than the low order integrator. For Lattice QCD, it turned out that V_c becomes very large at small quark masses, so that on currently accessible computers the 2LF integrator is the best choice[4] for simulations at zero temperature.

Recently Omelyan *et al.* [5] found a new 2nd order integrator which is expected to be better than the 2LF integrator although it has twice the computational cost. We examine this new 2nd order integrator, which we call 2MN integrator, for the HMC algorithm in lattice QCD and measure its efficiency.

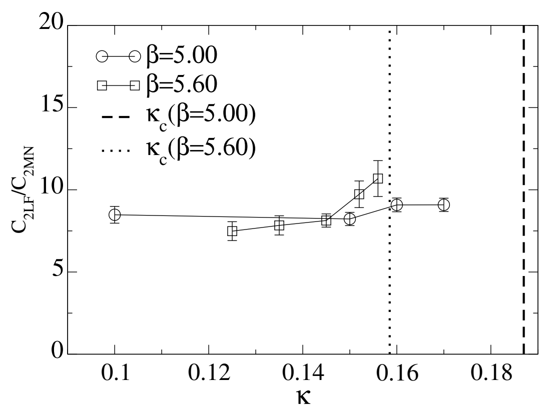

Figure 1: C_{2LF}/C_{2MN} as a function of κ. Simulations at $\beta = 5.00(5.60)$ are performed on $4^4(8^4)$ lattices.

Figure 1 shows the ratio C_{2LF}/C_{2MN} as a function of κ. C_{2LF} and C_{2MN} are coefficients of the error function of total energy. As seen in the figure, C_{2LF}/C_{2MN} is about 10, which means that the error of the 2MN integrator is about 10 times smaller than that of the 2LF integrator. If we take $C_{2LF}/C_{2MN} \approx 10$, this means that the step size of the 2MN integrator can be increased by a factor 3 ($\approx \sqrt{10}$) over that of the 2LF integrator. Since the 2MN integrator has two force calculations per elementary step, the efficiency should be measured by $\sqrt{C_{2LF}/C_{2MN}}/2$, which is about 1.5. Thus it is concluded that the 2MN integrator is about 50% faster than the 2LF integrator.

References

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