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MICROCANONICAL AND HYBRID SIMULATIONS OF LATTICE QUANTUM CHROMODYNAMICS WITH DYNAMICAL FERMIONS

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ABSTRACT

Lattice QCD is simulated using Microcanonical and Hybrid (Microcanonical/Langevin) methods to facilitate the inclusion of dynamical fermions (quarks). We report on simulations with 4 flavours of light dynamical quarks on a $10^3 \times 6$ lattice to study the finite temperature deconfinement/chiral transition which should be observable in relativistic heavy ion collisions, as a function of quark mass. A first order transition is observed at large mass, weakens at intermediate mass and strengthens for very small quark mass.

INTRODUCTION

The grassman nature of fermion fields precludes their direct simulation by Monte Carlo methods. All methods which are practical except on the smallest lattices are based on the observation that one can replace the fermi fields by bose fields if we replace the Dirac operator by its inverse. The main problem then is calculating this inverse as efficiently as possible, and avoiding having to calculate it more than once per sweep of the lattice. This second restriction requires that the changes in the fields during each sweep be small. The most promising methods to date appear to be the Microcanonical and Langevin schemes and more recently a hybrid of the two which preserves the

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best features of each. The principal advantage of these schemes is that the calculation of the inversion of the Dirac operator is replaced by the solution of a set of linear equations which is faster to implement. The small change requirement is met by the fact that the fields evolve continuously, described by a differential equation. The microcanonical and hybrid algorithms have been used extensively by the Argonne/University of Illinois group to study Lattice QCD.

I will only report on recent and ongoing work studying thermodynamics on a $10^3 \times 6$ lattice to study the finite temperature deconfinement and chiral transitions which could be observed in relativistic heavy ion collisions (e.g. at RHIC). These simulations were done in collaboration with E.V.E. Kovacs (Argonne) and J. B. Kogut (University of Illinois).

Section 2 gives a brief description of the microcanonical method. Section 3 describes the hybrid scheme. In section 4 the simulations on the $10^3 \times 6$ lattice are described. Finally section 5 contains the summary and conclusions.

MICROCANONICAL METHOD

In the microcanonical approach [1] of Callaway-Rahman, adapted to include dynamical fermions by Polonyi-Wyld, one notes that the classical Lagrangian

$$L = \frac{1}{2} \sum_{\substack{\mu \\ \text{links } \ell}} \dot{U}_\mu^\dagger(\ell) \hat{P} \dot{U}_\mu(\ell) + \sum_{\substack{\text{even} \\ \text{sites } mn}} \psi_m^\dagger [(-\not{D} + m)(\not{D} + m)]_{mn} \psi_n \\ - \omega^2 \sum_{\substack{\text{even} \\ \text{sites } n}} \psi_n^\dagger \psi_n - \beta \sum_{\square} \text{tr}[UUUU + \text{h.c.}],$$

where $\hat{P} = \text{diag}(1,1,0)$ in colour space and “.” indicates derivative with respect to a new, fictitious time, has canonical partition function

$$Z = \int_{\text{phase space}} e^{-H},$$

where the fields have been rescaled to make the classical temperature $kT = 1$. Integrating out the (pseudo) fermion fields and both gauge and fermi momenta yields

$$Z = \text{constant} \int dU \det(\not{D} + m) e^{-\beta \sum_{\square} \text{tr}[UUUU + \text{h.c.}]}$$

Hence we obtain the physics of 4-flavour (staggered fermions) Lattice QCD.

One now uses the known equivalence between canonical and microcanonical statistical mechanics to transform to the microcanonical formulation. Here the same physics is obtained from solving the classical equations of motion derived from L or H , and calculating QCD observables as long time averages, assuming ergodicity.

Simulations in this approach involve the numerical integration (Verlet) of these equations of motion (molecular dynamics). This in turn requires the numerical solution of linear equations of the form

$$(-\not{D} + m)(\not{D} + m)\psi = \phi.$$

We currently use the conjugate gradient algorithm to perform this inversion.

HYBRID ALGORITHM

The hybrid algorithm of Duane [2] involves periodic replacement of the “momenta” in the microcanonical Hamiltonian with random “momenta” having a Maxwell-Boltzmann distribution at a fixed “temperature” (usually taken to be 1), during the simulation. Clearly, once equilibrium obtains, such a replacement does not disturb this equilibrium, since all that is required for different parts of the system to be in thermodynamic equilibrium is that they have the same temperature. One can consider that the “momenta” have been allowed to thermalize with a heat bath at the chosen temperature.

This guarantees ergodicity, and tuning the “refreshment” frequency gives more rapid coverage of phase space than either the microcanonical (no refreshment) or Langevin (refresh every sweep) methods. Because of its stochastic nature it is not quite as sensitive to metastability as the microcanonical scheme.

THERMODYNAMICS ON A $10^3 \times 6$ LATTICE

We have used both methods (microcanonical and hybrid) to study the mass dependence of the finite temperature deconfinement/chiral transition on a $10^3 \times 6$ lattice. This augments previous simulations on $8^3 \times 4$ lattices [3] where the transition occurs on the strong coupling side of the cross over region (Here it occurs in the cross over region, nearer the continuum physics.) We use staggered fermions, yielding 4 light flavours of quarks. Studies at fermion masses of .05 to .25 (lattice units) have already been completed [4]. Extension down to mass of .025 is nearing completion [5] and we include preliminary data here.

Fig. 1. Wilson Line vs. sweep ($dt = .02$) for $\beta = 5.509$, $m = .25$ from an ordered start.

Fig. 2. Wilson Line and $\langle \bar{\psi} \psi \rangle$ as functions of β a) for $m = .05$, b) for $m = .025$.

So far these simulations have involved over 4500 ST-100 hours (equivalent to 3000 CRAY X-MP hours) and over 500 CRAY X-MP hours of computer time.

At $m = .25$ we still observe the first order deconfinement transition of the pure gauge theory [6], which drives the chiral transition for the quenched fermion case [7]. This is indicated by the metastability in the Wilson Line close to the transition (Fig.1).

For $m = .05$ to $.1$, although there is a rapid crossover, we have not observed any clear signs of metastability or any other clear signals of a phase transition [4].

Preliminary data at $m = .025$ show a much more rapid crossover than at intermediate masses as shown in fig. 2 where the wilson line and $\langle \bar{\psi}\psi \rangle$ are plotted as functions of β for $m = .05$ and $m = .025$. (Note, the absence of error bars on the graph at $m = .025$ indicates the preliminary nature of the data).

In fig. 3 we show the time evolution of the Wilson Line at $\beta = 5.1$ for 50,000 sweeps, starting from an ordered start. Fig. 4a shows an expanded version of the first 10,000 sweeps showing the rapid crossover between the 4000th and 7000th sweep. Fig. 4b is a histogram of these 10,000 sweeps. This clearly shows a bimodal distribution as might be expected if the transition were first order. We have not, as yet seen any sign of the metastability normally associated with such a first order transition.

Calculation of the time correlation lengths from this preliminary data is summarized in the following table. Since the time autocorrelation function is not a simple exponential and the data is very noisy these should only be taken as a rough guide. (In fact, a further 40,000 sweeps at $\beta = 5.1$ performed since this presentation showed correlation times ~ 1 , an indication that the long time correlations seen at this beta are probably the system "ringing" after the sudden transition. Such "ringing" is also an indication of long time modes in the system, which is why we include this result here.) Clearly more analysis is needed to determine whether we are seeing critical slowing down, or the return to a first order transition.

WILSON LINE TIME EVOLUTION: BETA=5.1, M=.025

Fig. 3. Wilson Line time evolution ($dt = .01$), $m = .025$ 50,000 sweeps.

WILSON LINE TIME EVOLUTION: BETA=5.1, M=.025

(a)

WILSON LINE TIME EVOLUTION: BETA=5.1, M=.025

(b)

Fig. 4. a) Enlargement of first 10,000 sweeps of fig. 3,
b) Distribution of values of the Wilson Line for these 10,000 sweeps.

TABLE: Time correlation lengths at $m = .025$

β	$\tau_{\langle\bar{\psi}\psi\rangle}$	$\tau[\text{Wilson Line}]$
5.4	0.7	2.1
5.3	0.9	1.2
5.2	1.5	1.7
5.15	5.1	2.4
5.12	7.2	4.7
5.1	19.*	13.*
5.0	1.0	0.3

*—see note in text

CONCLUSIONS

The behaviour of the deconfinement/chiral transition in lattice QCD as a function of the fermion mass, as observed on a $10^3 \times 6$ lattice with 4 degenerate fermion flavours can be divided into 3 regions.

1. **LARGE FERMION MASS:** In this range of fermion mass ($> .1 - .25$) we observe the first order deconfinement transition of the pure gauge theory.
2. **INTERMEDIATE FERMION MASS:** Here the transition softens and possibly disappears.
3. **FERMION MASS $\rightarrow 0$ (THE CHIRAL LIMIT)** The chiral symmetry restoration transition appears and drives the phase transition. It is not clear whether this phase transition appears for small but finite mass or only in the chiral limit. The order of this transition has yet to be resolved. Further simulations at this mass are in progress.

The critical value of beta at $m = 0$ is determined to be $5.01 \pm .03$ by linear extrapolation, yielding a chiral transition temperature

$$T_c = (2.14 \pm .10) \Lambda_{\overline{MS}}$$

Clearly we need to go to larger lattices in order to determine the continuum behaviour of the finite temperature phase transition. Algorithm improvements are needed to reduce the CPU time needed for such simulations, and those to determine other hadron properties such as masses and matrix elements.

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