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THE ITERATIVE HOPPING EXPANSION ALGORITHM FOR MONTE CARLO CALCULATIONS WITH VERY LIGHT FERMIONS

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Abstract: The number of numerical operations necessary for a Monte Carlo simulation with very light fermions (like u- and d-quarks in quantum chromodynamics) is estimated within the iterative hopping expansion method.

The main difficulty for a fully realistic Monte Carlo simulation of a quantum gauge field theory with light fermions is the inclusion of the effects of virtual quark loops into the updating procedure. The reason of the difficulty is, that the effective interaction induced by the light fermion loops is inherently non-local on the gauge field configuration.

Approaching very small dynamical fermion masses, like the physical u- and d-quark masses in QCD, the non-locality of the effective action on the gauge field sets in rather suddenly. In QCD, the unambiguous sign of a light quark mass is the smallness of the pion- to ϱ-meson mass ratio $r_{\pi\varrho} \equiv m_\pi / m_\varrho$. (Something like $r_{\pi\varrho}$ has to be preferred for the characterization of light quark masses, because it is rather difficult to give a renormalization group invariant meaning directly to the quark mass parameters used in the numerical calculations.) The physical value of $r_{\pi\varrho}$ is about 0.18. In the only existing calculation of QCD spectrum with light dynamical quarks on a reasonably large (actually 8^4) lattice [1], the value of $r_{\pi\varrho}$ is in the range of 0.8 - 0.5, i.e. still rather far away from the desirable region. The calculations in Ref. [1] took already a rather large amount of computer time: about 300 CPU hours on a CYBER 205 supercomputer. Therefore, one has to ask, whether it is at present conceivable at all that a reliable QCD spectrum calculation with the required very light dynamical quarks can be done in the near futute, using existing or foreseeable computing possibilities. I want to stress that, in my opinion, the main difficulty is presumably not the lattice size (8^4 seems enough for the first studies), but the smallness of the physical quark mass. For very light quarks, the non-locality of the effective action causes severe convergence problems for all known algorithms.

The Monte Carlo simulation in Ref. [1] is based on the iterative hopping expansion (IHE) algorithm [2]. In the present letter the computational requirements of a QCD spectrum calculation with very light (i. e. physical) dynamical quarks will be estimated within the IHE framework. For similar estimates and discussions of other presently available algorithms see a recent paper by D. Weingarten [3]. First the IHE algorithm will be shortly recapitulated. Then the number of numerical operations necessary for a Monte Carlo simulation will be given for a range of lattice sizes and maximum orders in the hopping parameter expansion. Finally, the results of some studies on the existing 8^4 configurations from Ref. [1] will be summarized, and possible future improvements of the algorithm will be discussed.

In the present paper always Wilson lattice-fermions [4] will be considered. In this case the hopping parameter (K) expansion of the change of the effective action ΔS^q_{eff} can be written like [2]

$$\Delta S^q_{eff} = \sum_{j=1}^{\infty} \frac{K^j}{j} \mathrm{Tr} D^j \quad . \tag{1}$$

The 2 x 2 block-matrix $D = (D_{ij})$ $(i,j = 1, 2)$ itself is a series in hopping parameter:

$$\begin{aligned}
D_{11} &= \sum_{l=3,5,\ldots} K^l M(U)^l_{x,x+\hat{\mu}} \, (1+\gamma_\mu) \, \Delta U(x,\mu) \quad , \\
D_{12} &= \sum_{l=4,6,\ldots} K^l M(U)^l_{x,x} \, (1-\gamma_\mu) \, \Delta U(x,\mu)^+ \quad , \\
D_{21} &= \sum_{l=4,6,\ldots} K^l M(U)^l_{x+\hat{\mu},x+\hat{\mu}} \, (1+\gamma_\mu) \, \Delta U(x,\mu) \quad , \\
D_{22} &= \sum_{l=3,5,\ldots} K^l M(U)^l_{x+\hat{\mu},x} \, (1-\gamma_\mu) \, \Delta U(x,\mu)^+ \quad .
\end{aligned} \tag{2}$$

Here γ_μ denotes the Dirac-matrix, $\Delta U(x,\mu)$ is the change of the gauge link-variable in the Metropolis updating procedure (x = point index, μ = direction index, $\hat{\mu}$ = unit vector in direction μ) and M(U) is the "hopping matrix"

$$M(U)_{x_2 x_1} = \sum_{x,\mu} (1+\gamma_\mu) U(x,\mu) \, \delta_{x_2, x+\hat{\mu}} \, \delta_{x,x_1} \quad . \tag{3}$$

The summation over μ goes over positive and negative directions.

The basic ingredients in the expansion (2) are matrix elements of the powers of the hopping matrix $\langle f|M(U)^l|i\rangle$ with some initial ($|i\rangle$) and final ($\langle f|$) vectors. These can be calculated on a given gauge field configuration by a point-by-point iteration [5]. (For more details on different aspects of the hopping parameter expansion method see also [6].) Denoting initial and final colour indices, respectively, by c_i and c_f, the corresponding Dirac spin indices by s_i and s_f and the final point index by x_f, the iterative equation can be written like

$$\begin{aligned}
&\varphi_{l+1}(c_f, s_f, c_i, s_i, x_f) = \\
&= \sum_{\mu} \sum_{c_1 s} (1-\gamma_\mu)_{s_f s} \, U(x,\mu)^+_{c_f c} \, \varphi_l(c, s, c_i, s_i, x_f+\hat{\mu}) \, .
\end{aligned} \tag{4}$$

It is important that, due to the nearest neighbour structure of the hopping matrix, the number of points where the iteration (4) has to be performed is limited by the fixed initial and final points and by the maximum order of the hopping expansion. This is illustrated by Fig. 1 in the generic case, where the initial point is i and the final point is f.

For light quark masses the hopping expansion (1 - 2) has to be evaluated up to high orders at every link updating. As a consequence, the main computational task is to evaluate the hopping expansion coefficients of ΔS^q_{eff}. Everything else is negligible, typically only at most at the 10^{-4} level of the whole computation. Therefore, the number of numerical operations necessary for one updating sweep is, to a good approximation, given by

$$N_{op} = N_{link} \; N_{point} \; N_1 \quad . \tag{5}$$

Here N_{link} is the number of links on the lattice (note that the iteration has to be performed only once, even if more Metropolis hits are done on a single link), N_{point} is the total number of lattice points (x_f) where Eq. (4) has to be evaluated and N_1 is the number of operations necessary to calculate φ_{l+1} once from φ_l in Eq. (4). Counting a triadic operation (a+b·c) as a single one, we have $N_1 = 144 \cdot 112 \cong 1.6 \cdot 10^4$ real operations. Here the first factor stands for the 12 initial spin-colour indices times the 12 final spin-colour indices. The number of iterated points N_{point} depends both on the maximum order of the hopping expansion and on the lattice size. A careful counting gives the numbers in Table I for some interesting range of orders and lattice sizes. Note that for a fixed maximum order and for large lattices N_{point} tends to a constant independent from the lattice size. Therefore, the number of operations N_{op} is growing, in this case, only linearly with the number of lattice points. If, however, the increase of the lattice volume is accompanied by a change of bare parameters in such a way that the lattice size is constant in physical units, then the required order in the hopping expansion grows and the number of iterated points N_{point} is roughly proportional to the volume. In this limit N_{op} grows quadratically with the number of lattice points in accordance with the arguments in Ref. [3]. The resulting numbers of required operations for one sweep are shown in Table II.

The comparison of the IHE to the algorithm of Weingarten and Petcher [7,3] seems favourable (for a comparison to other algorithms see [3]). Taking 8^4 lattice and $n_f = 3$ light quark flavours with $N_{GS} = 50$ Gauss-Seidel iterations, the

number of operations for one sweep given in Ref. [3] is $\sim 5 \cdot 10^{13}$. This is an order of magnitude more than the corresponding number in Table II for 24^{th} order hopping expansion. This comparison refers strictly to the updating. The Weingarten-Petcher algorithm may have some advantage in the subsequent calculation of the quark propagator matrix elements necessary for a spectrum calculation. In the case of IHE a complete determination of the quark propagator matrix (from every point to every other point) is roughly equivalent to a full sweep. In Ref. [3] more emphasis was given to a calculation on 6^4 lattice with $n_f = 2$ light flavours. In this case the comparison is somewhat less favourable for IHE, but in my opinion at least 8^4 is required if light quarks (and light pions) are aimed at. Taking $n_f = 2$ flavours is unacceptable, since the hopping parameter for the s-quark is only slightly less than for u- and d-quarks.

The comparison of different algorithms making different approximations is, of course, not entirely straightforward. Even a direct confrontation on small lattices is not necessarily conclusive, since the convergence properties can sensitively depend on the lattice size. In our case, for instance, it is not completely clear whether the 24^{th} order hopping expansion or the 50 Gauss-Seidel iterations are more suitable for reaching a convergent result in the case of very light quarks. I believe that the chances of 24^{th} order IHE are certainly not worse. This is suggested by the comparison of the smallest quark mass values, where e. g. meson propagators can be reliably extracted in a quenched calculation from a 24^{th} order hopping series and from quark propagators calculated by Gauss-Seidel iteration (see, for instance, Refs. [5,1]). In addition, as detailed studies show (see Refs. [2,1] and below), the quark propagator combinations appearing in the expansion of ΔS^q_{eff} in Eq. (1) are better convergent than e. g. the meson propagators or the individual quark matrix elements themselves. It is an advantage of the IHE algorithm that it can be directly applied to the more convergent combinations.

In order to see, what is the best way to obtain the value of ΔS^q_{eff}, once the hopping expansion coefficients are known, I studied the hopping series on the 8^4 gauge configurations produced in Ref. [1] for $N_f = 3$ degenerate quark flavours at the gauge coupling $\beta \equiv 6/g^2 = 5.3$ and hopping parameter $K_q = 0.168$. On these configurations $\tau_{\pi\rho}$ is about 0.5, therefore the dynamical quarks are light (even if still not light enough). The hopping expansion coefficients of ΔS^q_{eff} were determined on 200 randomly chosen links during a Metropolis updating with 10 hits per link and acceptance rate of the proposed changes of about 50 % (per hit). Since

the lowest non-vanishing order is 4 and only even orders occur, the values of ΔS^q_{eff} were calculated from a 10^{th} order Padé-table. The stability of ΔS^q_{eff} obtained from the highest (actually 8^{th} to 10^{th} order) Padé-approximants was investigated. It turned out that the Padé-tables are in most cases rather stable and hence suitable for the calculation of ΔS^q_{eff}. The errors of ΔS^q_{eff} were estimated from the standard deviations of the 10 "best" Padé's, which are closest to each other among the 30 highest order ones considered. This way of determining the values from the Padé-table was successfully applied to the meson and baryon propagator time-slices in the quenched calculation of Ref. [1]. There the obtained hadron masses agreed well with the result of the standard procedure based on the pole position. As already mentioned, in the present case the situation is even better, since ΔS^q_{eff} is more convergent than the hadron propagators. It turned out that in about 80 % of all hits the estimated relative error of ΔS^q_{eff} was less or equal to 1 %. In 14 % of the cases errors up to 5 % occured, in 4 % of the hits errors up to 15 % and in 2 % of the hits up to 50 %. The deviation between the average value extracted from the Padé-table and the value given by the hopping series itself was, in the first group of hits (with $\lesssim 1$ % error) only a few percent, in the second group up to 20 % and in the last two groups up to $\sim$100 %. Since about 95 % of the total change in the action comes from the pure gauge action, the estimated errors of ΔS^q_{eff} correspond typically to errors of the action-change below the 1 permill level. The effect of these, relatively small, errors on the hadron masses is unclear at present. This question can be investigated in the future e. g. by artificially adding a similarly distributed noise to the pure gauge action difference in a quenched calculation.

The investigation of the Padé-tables also showed that in a substantial subset of Metropolis hits the high orders are not necessary for a $\sim$1 % accuracy of ΔS^q_{eff} If this average accuracy turns out, in the future, to be enough for a good hadron mass determination, then the updating can be optimized by monitoring the degree of convergence. In case of good convergence the iteration can be broken down below 24^{th} order, but in a few critical instances the iteration can be continued up to substantially higher orders than the average maximum order.

In summary, it seems plausible that the required very light quark mass range can be reached by the IHE algorithm, provided that the amount of numerical operations given by Table II can be performed. Taking 1000 sweeps on 8^4 lattice in 24^{th} order of the hopping expansion requires $\sim 5 \cdot 10^{15}$ operations. This is quite a lot, but it is possible to do by computers performing at the GFLOP rate.

Acknowledgement

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Table I The total number of points N_{point} for different orders and lattices in the iteration for ΔS^{qq}_{eff} on a single link

order	6^4	8^4	10^4	12^4
12	1625	1989	2081	2093
14	2666	3668	4032	4124
16	3879	6039	7059	7423
18	5168	9056	11354	12374
20	6464	12581	16997	19313
22	7760	16438	23926	28480
24	9056	20467	31955	39971

Table II The number of operations N_{op} according to Eq. (5) for one sweep, at different orders and on different lattices

order	6^4	8^4	10^4	12^4
12	$1.4 \cdot 10^{11}$	$5.3 \cdot 10^{11}$	$1.3 \cdot 10^{12}$	$2.8 \cdot 10^{12}$
14	$2.2 \cdot 10^{11}$	$9.7 \cdot 10^{11}$	$2.6 \cdot 10^{12}$	$5.5 \cdot 10^{12}$
16	$3.2 \cdot 10^{11}$	$1.6 \cdot 10^{12}$	$4.6 \cdot 10^{12}$	$9.9 \cdot 10^{12}$
18	$4.3 \cdot 10^{11}$	$2.4 \cdot 10^{12}$	$7.3 \cdot 10^{12}$	$1.7 \cdot 10^{13}$
20	$5.4 \cdot 10^{11}$	$3.3 \cdot 10^{12}$	$1.1 \cdot 10^{13}$	$2.6 \cdot 10^{13}$
22	$6.5 \cdot 10^{11}$	$4.3 \cdot 10^{12}$	$1.5 \cdot 10^{13}$	$3.8 \cdot 10^{13}$
24	$7.6 \cdot 10^{11}$	$5.4 \cdot 10^{12}$	$2.1 \cdot 10^{13}$	$5.3 \quad 10^{13}$

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Figure Caption

Fig. 1 Illustration of the iteration for the calculation of the hopping expansion coefficient $\langle f|M^n|i\rangle$. In every step the open points are calculated from the full ones.

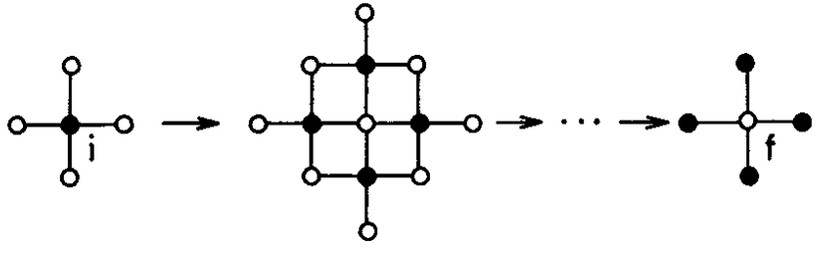

Fig.1