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Interner Bericht

Giant Eigenproblems from Lattice Gauge Theory on CRAY T3E Systems

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Giant Eigenproblems from Lattice Gauge Theory on CRAY T3E Systems

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Abstract

The determination of physical properties of flavor singlet objects like the η' meson by computer simulation requires the computation of functionals of the inverse fermionic matrix M^{-1}. So far, only stochastic methods could cope with the enormous size of M. In this paper, we introduce an alternative approach which is based on the computation of a subset of low-lying eigenmodes of the fermionic matrix. The high quality of this 'truncated eigenmode approximation' (TEA) is demonstrated by comparison with the pion correlator, a flavor octet quantity, which is readily computable through a linear system of equations. We show that TEA can successfully approximate the flavor singlet η' correlator. We find that the systematic error of the method is tolerable. As the determination of the chosen subset of 300 eigenmodes requires about 3.5 Tflops-hours CPU-time per canonical ensemble and at least 15 GBytes of memory, the power of high-end supercomputers like the CRAY T3E is indispensable.

Key words: QCD; meson mass calculations

1 Introduction

A major goal of non-perturbative lattice quantum chromodynamics (LQCD) is the determination of hadronic mass states which are characterized by non-valence contributions, such as flavor singlet mesons. Their correlation functions, $C_{\eta'}(t_1 - t_2)$, contain so-called 'disconnected diagrams', i.e. correlators between closed virtual fermion loops. The reliable determination of these disconnected diagrams has been a long- standing issue ever since the early days of lattice gauge theory. It can be reduced to the numerical problem of how to achieve information about functionals of the inverse fermionic matrix M^{-1}.

The first attempts in this direction have been started only a few years ago, using the so-called stochastic estimator method (SE) [1] to compute the trace of M^{-1}. This approach requires to solve the linear system $Mx = \xi$ on some hundred source vectors ξ, with ξ being Z_2 or Gaussian noise vectors. Meanwhile, substantial progress could be achieved for the determination of the η' by application of refined smearing methods [2], where for the first time a proper signal-to-noise-ratio could be established. However, SE introduces stochastic noise, in addition to the stochastics already inherited from the Monte Carlo process.

In the following, we describe the determination of the η' mass based on the computation of a set of low-lying eigenmodes of $Q = \gamma_5 M$, the hermitian form of M. We use the implicitly restarted Arnoldi method, a generalization of the standard Lanczos procedure. A crucial ingredient is the Chebyshev acceleration technique to achieve a transformation of the spectrum to a form suitable for the Arnoldi eigenvalue determination. The low-lying modes given, it is possible to estimate the entire matrix Q^{-1} and those matrix functionals or functions of Q and M which are sensitive to long-range physics.

In section 1, we introduce the meson correlators and in section 2, we shortly review their computation by conventional means. Section 3 is devoted to TEA and the organization of the computation on the CRAY T3E by use of the parallel Arnoldi package (PARPACK). In section 4, we assess the viability of TEA by comparing the correlator of the π meson as computed from TEA with the result from the conventional approach. As the π is a flavor octet quantity it can easily be computed through the solution of a linear system of equations by iterative Krylov subspace algorithms [3]. Finally, we apply TEA to the computation of the η' meson correlator and compare with results from SE computations.

2 Meson Correlators

In LQCD, hadronic masses are extracted from the large-time behavior of correlation functions. The correlator of the flavor octet π meson is defined as

$$C_\pi(t \equiv t_1 - t_2) = \left\langle \sum_{n,m} \mathrm{Tr}\Big[Q^{-1}(n,t_1;m,t_2)Q^{-1}(m,t_2;n,t_1)\Big] \right\rangle_U , \qquad (1)$$

while the flavor singlet η' meson correlator is composed of two terms, one being connected and equivalent to the pion correlator, the second being the disconnected contribution from the correlation of virtual quark loops:

$$C_{\eta'}(t) = C_\pi(t) - 2\left\langle \sum_{n,m} \mathrm{Tr}\Big[Q^{-1}(n,t_1;n,t_1)\Big]\mathrm{Tr}\Big[Q^{-1}(m,t_2;m,t_2)\Big] \right\rangle_U . \qquad (2)$$

$\langle \ldots \rangle_U$ indicates the average over a canonical ensemble of gauge field configurations. Q is the hermitian Wilson-Dirac matrix [3], i.e. $Q = \gamma_5 M$; n and

m denote spatial lattice sites, t_1 and t_2 determine the time separation t. The color and Dirac indices are suppressed. For large times t, the respective correlation functions become proportional to $\exp(-m_0 t)$, where m_0 is the mass of the particle described by the correlation function. Since our lattice has anti-periodic boundary conditions in time direction, the correlation functions actually consist of a sum over two contributions, $\exp(-m_0 t)$ and $\exp(+m_0 t)$, i.e. they will exhibit a *cosh*-like behaviour ($C \sim cosh(m_0 t)$).

3 Conventional Computation of Correlators

In the conventional computation of the π-correlator (1) the source point is held fixed (e.g. at index tupel $(1,1) \equiv (\vec{1},1)$), where the first index symbolizes the spatial vector $(1,1,1)$ and the second one denotes the time component:

$$C_\pi(t_1) = \left\langle \sum_n \mathrm{Tr}\Big[Q^{-1}(n,t_1;1,1)Q^{-1}(1,1;n,t_1)\Big] \right\rangle_U . \tag{3}$$

Using $\gamma_5 M \gamma_5 = M^\dagger$, we obtain:

$$C_\pi(t_1) = \left\langle \sum_n \mathrm{Tr}\Big[M^{-1}(n,t_1;1,1)M^{-1^\dagger}(1,1;n,t_1)\Big] \right\rangle_U . \tag{4}$$

Thus it suffices to determine 12 columns (3×4 for the color and Dirac indices) of M^{-1} in order to compute (4). The columns $c(n,t)$ of M^{-1} are obtained by solving the linear system

$$M(n,t_1;m,t_2)c(m,t_2) = \delta(1,1;n,t_1); \tag{5}$$

where δ is the Kronecker delta function. Of course, the statistics could be improved by averaging over many or even all source points. However this would be prohibitively expensive as the effort increases with the number of sources.

For $C_{\eta'}$, however, the second term,

$$\sum_{n,m} \mathrm{Tr}\Big[Q^{-1}(n,t_1;n,t_1)\Big]\mathrm{Tr}\Big[Q^{-1}(m,t_2;m,t_2)\Big], \tag{6}$$

depends on the diagonal elements of Q^{-1} which cannot be determined from one source point alone. Instead of going through all sites the method of choice is the *stochastic estimator* technique (SE). One creates series of complex numbers $(c_i)_j$ such that they converge to the diagonal elements $Q^{-1}(i,i)$. The series are constructed through noise vectors η_k,

$$(c_i)_j = \sum_{k=1}^{j} \eta_k(i) Q^{-1} \eta_k(i)/j \tag{7}$$

$Q^{-1}\eta_k$ is determined by solving the corresponding linear system $Qx = \eta$. In order to achieve a satisfying approximation, 400 noise vectors η_k are required [2]. Therefore the flavor singlet calculations are about 30 times more expensive than the octet ones.

4 TEA

We start from the following equation:

$$Q^{-1}(n,t_1;m,t_2) = \sum_i \frac{1}{\lambda_i} \frac{|\psi_i(n,t_1)\rangle\langle\psi_i(m,t_2)|}{\langle\psi_i|\psi_i\rangle} \ , \tag{8}$$

where λ_i and ψ_i are the eigenvalues and the eigenvectors of Q respectively. Note that Q is hermitian indefinite [1]. We approximate the sum on the right hand side by restriction to the 300 lowest-lying eigenvalues and their corresponding eigenvectors. Due to the factor $1/\lambda_i$ one can hope that the low-lying eigenmodes will dominate the sum [2]. We emphasize that we have an approximation for the entire matrix $Q^{-1}(i,j)$. Therefore, we can retrieve the diagonal elements of the disconnected diagrams as well as the π correlator on all source points.

To compute the eigenvalues and their corresponding eigenvectors we employ the Implicitly Restarted Arnoldi Method (IRAM). The huge size of Q requires parallel supercomputers. We work on two CRAY T3E systems with 512 nodes each, located at Forschungszentrum Jülich, Germany and at NERSC, Berkeley, USA. A comfortable parallel implementation of IRAM is provided by the PARPACK package [5]. In order to overcome the problem of slow convergence for the low-lying eigenvalues we apply the Chebyshev polynomial acceleration technique, where the eigenvalue spectrum is transformed such that the 300 smallest eigenvalues become much larger than the rest of the spectrum, a situation favorable for eigenvalue calculations by IRAM.

We work on a $16^3 \times 32$ lattice i.e. 16 lattice sites in space and 32 lattice sites in time direction. Taking into account the Dirac and color indices, we see that the Dirac matrix acts on a $12 \times 16^3 \times 32 = 1.572.864$ dimensional vector space. This explains why we cannot invert the entire Dirac matrix, since this would need about 40 TByte memory space, whereas the determination of 300 low-lying eigenvectors leads to about 15 GByte memory space only. Our computations are based on canonical ensembles of 200 field configurations with $n_f = 2$ flavors of dynamical sea quarks, generated at 4 different quark masses, in the framework of the SESAM project [2]. Fast and automated access to an archive space of approximately 6 TBytes is required to store all eigenvectors from the SESAM ensembles. Thus, computations of this kind are not feasible without the facilities available at supercomputer centers. It takes about 3.5 Tflops-hours to solve for 300 low-lying modes on each ensemble. In the eigenmode

[1] The hermitian matrix Q leads to an orthogonal eigenbase. If we compute the eigenmodes from the non-normal matrix M instead, the resulting eigenbase is non-orthogonal. In our investigations, we found no convergence of the low modes from the non-orthogonal eigenbase.

[2] In the result section, we will come back to the question of cancellation effects due to positive and negative eigenvalues.

approach the CPU-time is decreasing with lighter quark masses, as in that case the eigenvalues become smaller and one can expect that they will dominate the sum earlier. This is a substantial advantage of TEA compared to the SE approach, where smaller eigenvalues lead to a slower convergence of the linear system solvers. With 400 stochastic estimates it takes about 1.5 Tflops-hours to treat an ensemble of 200 gauge configurations. However, in future simulations (i.e. for lighter quark masses) TEA will soon become superior to SE.

5 Results

The correlator C_π can serve as simple test for the quality of TEA. Fig. 1 compares C_π as determined by eq. (5) with the result from TEA. The low modes are expected to describe long range physics. Accordingly, TEA underestimates the true C_π for small time separations ($t < 8$). On the other hand, the large time behavior is represented quite well. Since the π correlator can be determined extremely accurately by the conventional method, a tiny truncation effect is still visible in the large time range of the propagator. This deviation decreases for smaller quark masses, as well as for a larger number of eigenmodes. Nevertheless, the deviation for large t still are surprisingly small: Let us sum (1) over t_1 and t_2,

$$\sum_{t_1,t_2} C_\pi(t_1 - t_2) = \sum_i \frac{1}{\lambda_i^2}. \tag{9}$$

Here all contributions are positive and no cancellation occurs as in the case for $C_{\eta'}$.

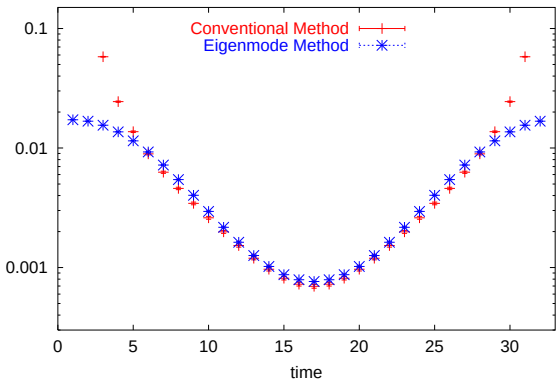

Fig. 1. Comparison of C_π from TEA and from the conventional computation.

The situation is even more favorable for the disconnected part of η'. Let us again consider the sum over t_1 and t_2:

$$\sum_{n,t_1,m,t_2} \mathrm{Tr}\Big[Q^{-1}(n,t_1;n,t_1)\Big]\mathrm{Tr}\Big[Q^{-1}(m,t_2;m,t_2)\Big] = \left(\sum_i \frac{1}{\lambda_i}\right)^2. \tag{10}$$

Obviously, the positive and negative eigenvalues can cancel each other here. We find that convergence is achieved from about 150 eigenvalues on! TEA and SE agree well within the error bars that are due to the gauge field fluctuations.

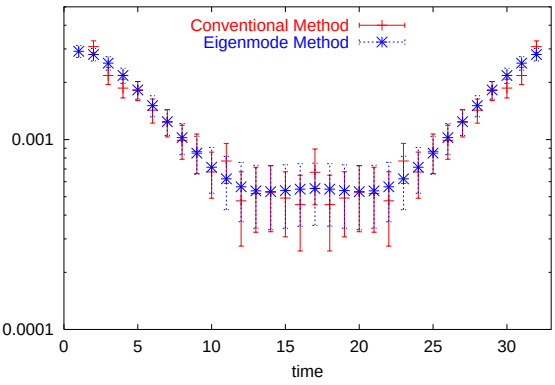

Fig. 2. Comparison of the disconnected correlator from SE and TEA. The large errors in both cases are solely due to gauge field noise.

In conclusion our results show that TEA is comparable to SE for the computation disconnected diagrams [4]. The costs are similar to SE computations at present. Going to realistic light masses, TEA will become superior to SE since low modes tend to dominate more and more.

Acknowledgments

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