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A Calculation of Higher Order Taylor Expansion Coefficients

Lorenzo Dini, Frithjof Karsch, Guido Nicotra, Christian Schmidt

UNIVERSITÄT BIELEFELD

CRC-TR 211 Strong-interaction matter under extreme conditions

1) Motivation

We are interested in the EoS of QCD at nonzero μ_B, and then we have to deal with the infamous sign problem.
The Taylor expansion around zero μ_B of the pressure is a tool that can be used for this purpose. In particular, we are interested in the higher order coefficients of the expansion.
To simplify the problem we introduce μ_B on the lattice using a linear prescription (Ref. [1]). In this way we need much less operators, and they can all constructed using the building blocks:

$$D_k = \mathrm{Tr}\left(\left[M^{-1}\frac{\partial M}{\partial \mu}\right]^k\right) \equiv \mathrm{Tr}\left(A^{-k}\right) \tag{1}$$

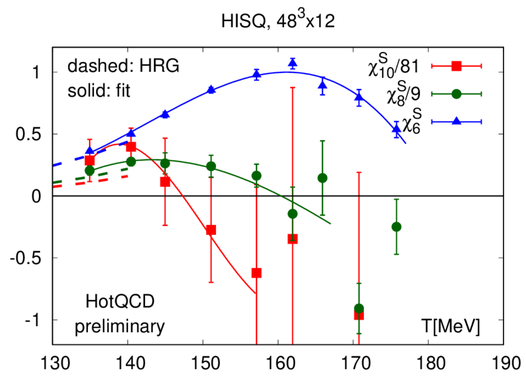

Figure 1: Preliminary higher order net strangeness susceptibilities using the traditional method (see section below) for the evaluation of traces. The higher the order, the larger are the uncertainties. We need new strategies to overcome the bottlenecks of the traditional method: we need to improve both the efficiency and the precision of our method.

2) Methodology

- **Conventional Way:**
  The usual way to evaluate such an operator as (1) is to apply iteratively the CG algorithm to invert the fermion matrix M and manually apply $M' \equiv \frac{\partial M}{\partial \mu}$ for each power that appears in (1), as it is done in Ref. [2].
  To speed up this process it is possible to apply the deflation method on the starting vector of each single inversion of the symmetric matrix $M^\dagger M$. However, deflation needs to be repeated, because each application of the M' matrix mixes the low and high modes of the fermionic matrix.

- **New Way:**
  If we are able to evaluate the N_e smallest eigenvalues λ_i of the matrix $A \equiv M\left(\partial M/\partial\mu\right)^{-1}$, then we can write (1) as:

$$D_k = \sum_{i=0}^{N_e} \lambda_i^{-k} + D_k^{(R)} \tag{2}$$

  Where $D_k^{(R)}$ is constructed using the operator A projected out of the eigenspace that we have calculated.
  In order to evaluate the eigenvalues λ_i of the non-hermitian matrix A we are implementing a non-symmetric Lanczos Algorithm (BiLanczos). An alternative method to evaluate the spectrum of A was recently proposed in Ref. [3].

The main advantages of this technique are the following: in the large k limit we can measure D_k almost exactly using the eigenvalues that we evaluated.
When the $D_k^{(R)}$ is not negligible, we can measure that part applying a BiCG alogorithm only once, using the eigenvectors to speed up the process via the deflation method.
In the linear μ framework, though, the most general coefficient of order $2N$ of the pressure expansion, i.e. C_{2N}, is a sum of elements with the following form:

$$C_{klm} = \langle (D_k)^l \rangle^m \tag{3}$$

With $k + l + m = 2N$.
Starting from D_k we can, in principle, evaluate all the other coefficients with $l, m \neq 0$ using unbiased estimator and increasing our accuracy of D_k.

3) Implementation

We are implementing a BiLanczos algorithm to find the eigentriplets (eigenvalues and right and left eigenvectors) of the matrix A.
In order to do that we implemented a routine that, starting from a gauge configuration of a $N_s^3 \times N_\tau$ lattice, creates an array of $N_\tau \times N_\tau$ matrices M', with N_s^3 number of elements, using HISQ fermions. Then, using cuBLAS library we do a batched inversion of these matrices in parallel on GPU, in order to obtain $(M')^{-1}$. The inverse remains even-odd ordered and then we can apply A to a vector. Starting from there, we are implementing a Thick Restarting version of the BiLanczos algorithm (Ref. [4]).

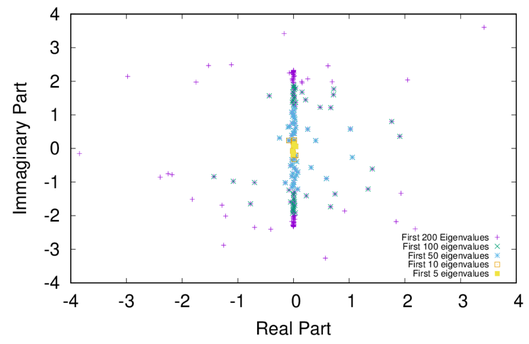

Figure 2: Preliminary results for the spectrum in the complex plane of a simpler non-hermitian matrix (here it is M), obtained using the method explained in this section. The numerical precision will be improved with a fully reBiOrthogonalization process during the BiLanczos, via a Modified Gram-Schmidt procedure.

4) Outlook

We will try to improve not only our measurement strategy as explained in the Methodology section, but also our sampling and analysis strategies:

- **At production level**:
  We need a huge amount of statistic to get a precise estimate of the coefficients C_{2N} in (3) with $l \neq 0$. That is because the tails of the distribution of the gauge configurations with respect to the operator D_k become more and more important for higher l. The idea is to improve our gauge sampling strategy, enhancing the tails contribution using Wang-Landau sampling.

- **At measurement and analysis level:**
  When we want to calculate the contribution to the coefficients with $m \neq 0$ (see Eq. (3)), it becomes crucial to measure D_k and D_k^l with very high precision, because the relative error scales with a factor m.
  There are two sources of uncertainty in these kinds of calculation: the *gauge noise* and the *statistical noise*. The latter is due to the number of random vectors that we use to estimate the traces (η). To reduce the gauge noise we can adopt the strategies mentioned above. To reduce the statistical one, we can again use deflation as a method to reducing the variance of the random variables:

$$\mathcal{O} = \eta_i^\dagger A^{-1} \eta_i \tag{4}$$

  Then, evaluating the mean value of $\mathcal{O}$ on the noisy vectors with a smaller variance we will have a more precise result. In addition, we will need less random sources and then the measurement will be more efficient (see Ref. [5]).

References

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