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The volume source technique for flavor singlets: a second look

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Abstract. We reconsider the volume source technique for the determination of flavor singlet quantities on the lattice. We point out a difficulty arising in the case of fermions in real representations of the gauge group and propose an improved version of the method (IVST) based on random gauge transformations of the background configuration. We compare the performance of IVST with the method based on stochastic estimators (SET). We consider the case of the $N = 1$ supersymmetric Yang–Mills theory, where just one fermionic flavor is present, the gluino in the adjoint representation, and only flavor singlet states are possible. This work is part of an inclusive analysis of the spectrum of the lightest particles of the theory, based on the simulation of the model on a $16^3 \cdot 32$ lattice with dynamical gluinos in the Wilson scheme.

1 Introduction

Supersymmetry (SUSY) is broken on the lattice owing to the finite lattice spacing a. We consider the $N = 1$ supersymmetric Yang–Mills theory (SYM) with gauge group SU(2) and Wilson discretization in the fermion sector. Here SUSY is also explicitly broken by the Wilson term. However, by properly tuning the (renormalized) gluino mass to zero, SUSY is expected to be recovered in the continuum limit [1] with exponentially small $O(a)$ deviations.

The manifestation of SUSY occurs at the non-perturbative level, the most interesting phenomenological implication being the expected ordering of the bound-states of the theory in supermultiplets. In the low-energy sector in particular, effective Lagrangians for SYM predict [2, 3] two Wess–Zumino supermultiplets. The spin-0 particles are represented by meson-like bound states of the gluino and by glueballs, respectively, of opposite parity (this classification is of course only valid in the absence of mixings, which are however expected). The spin-$\frac{1}{2}$ particle of the multiplet is in both cases a gluino–glue bound-state.

We focus here on the problem of determining the masses of meson-like gluino bound states. Borrowing the terminology of QCD, these represent "flavor singlet" states. Indeed, SYM resembles $N_f = 1$ QCD, with the quark in the fundamental representation replaced by the gluino in the adjoint representation. The lattice computation of flavor singlet correlators is difficult because of the presence of disconnected diagrams (see [4] for a recent review on the topic). The exact evaluation of the correlator for these diagrams is not feasible since it requires the trace over color and space-time indices of the fermion propagator in the background of the gauge configuration, which in turn involves the solution of an "all-points to all-points" inversion problem *for any given gauge configuration.* The first approach to the subject was based on a volume source [5], the so-called "volume source technique" (VST). For a given background configuration the method delivers an estimate of the correlator which, however, contains spurious terms represented by non-closed loops. In [5], where QCD was considered, it was argued that these terms disappear in the ensemble-average on the basis of gauge invariance. In this paper we reconsider this argument more generally, showing that it is not applicable to models where the fermions are in real representations of the gauge group, as is the case for any representation of SU(2) and for the adjoint representation of SU(N_c). We propose a new formulation of the method, based on random gauge transformations of the background gauge configuration, which solves the problem. Due to the randomness introduced by the gauge transformation, IVST is analogous to the well known stochastic estimator technique SET [6]. In both cases the systematic error introduced by the computational procedure is converted into a statistical one and can be controlled by increasing the number of stochastic estimates. As a consequence IVST and SET can be directly compared.

This work represents the sequel of a long-standing project having the goal of a lattice verification of the non-perturbative low-energy properties of SYM. We refer to [7] and the references therein for the scope and goals of past studies. The model is simulated by means of the dynamical-gluino two-step multi-bosonic algorithm. Details on the algorithm can be found in [8]. The present analysis is based on a sample of configurations of SU(2) SYM on a $16^3 \cdot 32$ lattice. Partial results have been reported in [9].

In the next section we shall reconsider the theory of VST and propose the improved version of it, IVST. In Sect. 3 the numerical results will be presented, comparing IVST and SET; finally Sect. 4 contains our conclusions.

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2 The volume source technique revisited

In this section we consider lattice gauge theory with gauge group $SU(N_c)$. The results of primary interest are for the gauge group SU(2) or for models with fermions in the adjoint representation of the gauge group. This includes SYM in particular. In the following, Greek letters denote Dirac indices, Latin letters color, Tr_d and Tr_c are the respective traces. With the usual bilinears $\bar{\psi}(x)\Gamma\psi(x)$ as insertion operators for the singlet mesonic states, where $\Gamma = 1$ or γ_5, the disconnected part of the mesonic correlator in the background of a gauge configuration $\{U\}$ can be written as

$$C_{\Gamma,\mathrm{disc}}[U](x_0 - y_0) = \frac{1}{V_s}\mathrm{Tr}_d\left[\Gamma S(x_0)\right]\,\mathrm{Tr}_d\left[\Gamma S(y_0)\right]\,, \quad (1)$$

where the time-slice sum $S(x_0)$ represents the trace over color and space indices of the inverse fermion-matrix, i.e. the propagator in the background of the gauge configuration $\{U\}$:

$$S_{\alpha\beta}(x_0) = \sum_{\mathbf{x}} \mathrm{Tr}_c\left[Q^{-1}_{x\alpha,x\beta}\right]\,. \quad (2)$$

VST delivers an estimate of $S_{\alpha\beta}(x_0)$ at the price of a single inversion for each value of the color and Dirac index. The inversion problem with the volume source ω_V reads

$$QZ = {\omega_V}^{[a,\alpha]}\,, \quad \left(\omega_V^{[a,\alpha]}\right)_{xb\beta} = \delta_{ab}\,\delta_{\alpha\beta}\,, \quad (3)$$

with solution

$$Z^{[a,\alpha]}_{xb\beta} = [Q^{-1}\omega_V^{[a,\alpha]}]_{xb\beta} = Q^{-1}_{xb\beta,xa\alpha} + \sum_{y\neq x} Q^{-1}_{xb\beta,ya\alpha} \quad (4)$$

When $Z^{[a,\alpha]}$ in the above equation is used to estimate the time-slice sum (2),

$$S_{\alpha\beta}(x_0) \to \tilde{S}_{\alpha\beta}(x_0) = \sum_{\mathbf{x},a} Z^{[a,\beta]}_{xa\alpha}\,, \quad (5)$$

the last term in (4) yields contributions to the disconnected part of the correlator (1) which represent non-closed loops. Such elements of the inverse fermion-matrix with $x \neq y$ are non-gauge-invariant and are canceled in the average over the gauge-ensemble (which is gauge-invariant). However, there are also contact terms in the correlator, which are potential sources of systematic errors.

In the original work [5], which introduced VST in the context of QCD, these unwanted terms were avoided by considering the correlator

$$\hat{C}_{\Gamma,\mathrm{disc}}[U](x_0 - y_0) = \frac{1}{V_s}\mathrm{Tr}_d\left[\Gamma\tilde{S}(x_0)\right]\,\mathrm{Tr}_d\left[\Gamma\tilde{S}^{\dagger}(y_0)\right] \quad (6)$$

with one of the time slices conjugated. Owing to the fact that the product $\mathbf{3}\otimes\mathbf{3}$ of fundamental representations of SU(3) does not contain the trivial representation, a gauge-invariant contact term does not appear. The argument holds more generally for the fundamental representation of $SU(N_c)$ for $N_c > 2$.

In the case of gauge group SU(2), which has real representations only, or in the case of the adjoint representation of $SU(N_c)$, this prescription, however, does not help. For SU(2) the product of two fundamental representations contains the trivial one, which leads to non-vanishing contact terms again. The same is true for the adjoint representations of $SU(N_c)$.

We now want to consider the gauge invariance of the contact terms in detail. We focus on the correlator (1); for (6) the discussion is analogous.

Consider the following average over gauge transformations $g(x)$ (*gauge-average*):

$$\left\langle \tilde{S}_{\alpha\beta}(x_0)\tilde{S}_{\gamma\delta}(y_0)\right\rangle_g = \left\langle \sum_{\mathbf{x},w,a} Q^{-1}_{xa\alpha,wa\beta}[U^g] \sum_{\mathbf{y},z,b} Q^{-1}_{yb\gamma,zb\delta}[U^g]\right\rangle_g\,. \quad (7)$$

The gauge-average induces an average over the gauge-orbit $\{U^g\}$. Using

$$Q^{-1}_{x,y}[U^g] = g^{\dagger}(x)Q^{-1}_{x,y}[U]g(y) \quad (8)$$

and the general formula

$$\left\langle g_{ab}(x)g^{-1}_{a'b'}(x')\right\rangle_g = A\,\delta_{xx'}\delta_{ab'}\delta_{a'b}\,,$$
$$A = \begin{cases} \frac{1}{N_c}, & \text{fundamental} \\ \frac{1}{N_c^2-1}, & \text{adjoint} \end{cases} \quad (9)$$

(in the adjoint representation g are real orthogonal matrices of dimension $N_c^2 - 1$), the gauge-average of (7) reads for $x_0 \neq y_0$

$$\left\langle \tilde{S}_{\alpha\beta}(x_0)\tilde{S}_{\gamma\delta}(y_0)\right\rangle_g = \sum_{\mathbf{x}}\mathrm{Tr}_c\left[Q^{-1}_{x\alpha,x\beta}\right]\sum_{\mathbf{y}}\mathrm{Tr}_c\left[Q^{-1}_{y\gamma,y\delta}\right] + A\sum_{\mathbf{x},\mathbf{y}}\mathrm{Tr}_c\left[Q^{-1}_{x\alpha,y\beta}Q^{-1}_{y\gamma,x\delta}\right]\,. \quad (10)$$

The above expression represents the *gauge-invariant part* of $\tilde{S}_{\alpha\beta}(x_0)\tilde{S}_{\gamma\delta}(y_0)$.

Let us now consider the *ensemble-average* of $\tilde{S}_{\alpha\beta}(x_0) \times \tilde{S}_{\gamma\delta}(y_0)$. In the limit of infinite statistics any given gauge-orbit is completely covered, implying that the ensemble-average delivers in particular a gauge-average. Using the result in (10) this implies

$$\left\langle \tilde{S}_{\alpha\beta}(x_0)\tilde{S}_{\gamma\delta}(y_0)\right\rangle_U \quad (11)$$
$$= \left\langle S_{\alpha\beta}(x_0)S_{\gamma\delta}(y_0)\right\rangle_U + A\left\langle \sum_{\mathbf{x},\mathbf{y}}\mathrm{Tr}_c\left[Q^{-1}_{x\alpha,y\beta}Q^{-1}_{y\gamma,x\delta}\right]\right\rangle_U\,.$$

We thus obtain that replacement (5) in (1) produces an error term for the *full* disconnected correlator

$$\tilde{C}_{\Gamma,\mathrm{disc}}(x_0 - y_0) = C_{\Gamma,\mathrm{disc}}(x_0 - y_0) + \Delta C_{\Gamma,\mathrm{disc}}(x_0 - y_0)\,, \quad (12)$$

$$\Delta C_{\Gamma,\mathrm{disc}}(x_0 - y_0) \qquad (13)$$
$$= A\,\frac{1}{V_s}\left\langle \sum_{\mathbf{x},\mathbf{y}} \mathrm{Tr}_c[\mathrm{Tr}_d\left[Q^{-1}_{x,y}\Gamma\right]\ \mathrm{Tr}_d\left[Q^{-1}_{y,x}\Gamma\right]]\right\rangle_U .$$

The conclusion is that the error term in (4) produces a systematic error in the correlator, *which does not vanish in the ensemble-average even in the limit of infinite statistics.* This error is due to gauge-invariant contact terms in the correlator, as shown above. The spurious term resembles the connected contribution

$$C_{\Gamma,\mathrm{conn}}[U](x_0 - y_0) = -f\,\frac{1}{V_s}\sum_{\mathbf{x},\mathbf{y}} \mathrm{Tr}_{cd}\left[Q^{-1}_{x,y}\Gamma\,Q^{-1}_{y,x}\Gamma\right],$$
$$f = \begin{cases} 1, & \text{fundamental} \\ 2, & \text{adjoint} \end{cases} \qquad (14)$$

the only difference being in the Dirac structure and the numerical factor. This outcome is not surprising considering that gauge invariance strongly constrains the space-time and color structure. We have checked the presence of the error term numerically for both types of correlators (1) and (6) for gauge group SU(2); see Sect. 3.

At this point we make the simple observation that the error is removed by using the gauge-average of $\tilde{S}_{\alpha\beta}(x_0)$ to determine the time-slice sums, since

$$\left\langle \tilde{S}_{\alpha\beta}(x_0)\right\rangle_g = S_{\alpha\beta}(x_0)\,. \qquad (15)$$

In practice this is obtained by averaging $\tilde{S}_{\alpha\beta}(x_0)$ over a sufficiently large number N_g of gauge configurations obtained from the original one by random gauge transformations [9][1] $g(x)$, namely with a flat probability distribution

$$\frac{\mathrm{d}p}{\mathrm{d}g} = 1\,, \qquad (16)$$

where $\mathrm{d}g$ denotes the Haar measure on the gauge group. Besides solving the problem of the error (13) in the correlator, the method brings the additional benefit of disentangling the systematic error inherent in VST from the statistical one: in the limit of an infinite number of random gauge transformations $N_g \to \infty$ the former goes to zero, only the second one surviving. In this view the improved version of VST is analogous to the techniques based on stochastic estimators, the randomness of the source being replaced by that of the gauge transformation.[2] This allows for a direct comparison of the two methods, which is carried out in the next section.

3 Numerical analysis

The simulation parameters of the gauge sample are $\beta = 2.3$ and $\kappa = 0.194$. The estimated value of the lattice spacing is, in QCD units, $a \approx 0.06\,\mathrm{fm}$ ($a^{-1} \approx 3.3\,\mathrm{GeV}$); there are indications [10] that the gluino is still relatively heavy ($m_{\tilde{g}} \gtrsim 200\,\mathrm{MeV}$ on the basis of QCD-inspired arguments). The set-up of the two-step multi-bosonic algorithm is the same as in [11], and ~ 4000 thermalized configurations were stored every 5 or 10 cycles. In order to obtain an estimate of the autocorrelation time of the disconnected part of the mesonic correlator, an analysis of the autocorrelation time of the smallest eigenvalue of the hermitian fermion-matrix was performed. The procedure is based on the expectation that the disconnected part of the mesonic correlator is strongly related to the infrared behavior of the fermion-matrix. After that, a subsample of 218 supposedly uncorrelated configurations was selected. This constitutes the sample for the numerical analysis.

3.1 Time-slice sums

For each configuration, 50 estimates of the time-slice sums (2) were performed, each obtained by applying a random gauge transformation on the original gauge configuration as explained in the previous section. The computations were performed in 64-bit arithmetic. Improved summation techniques were employed to ensure accuracy.

In the case of SYM the Majorana nature of the gluino field (invariance under charge conjugation) allows one to compute the inverse of the fermion-matrix for only half of the matrix-elements in Dirac space. This implies that, in the case of SU(2) SYM, only 6 fermion-matrix inversions must be performed for each configuration, compared to 12 inversions needed for QCD. So the total number of inversions N_{inv} required for a determination of the time-slice sum with N_{est} estimates is $N_{\mathrm{inv}} = 6N_{\mathrm{est}}$.[3]

As IVST is based on stochastic estimations, a comparison with stochastic-source methods SET suggests itself. We consider the SET variant with complex $\mathbf{Z}_2$ noise in the spin explicit variant SEM [12]. In this case each estimate of the time-slice sum is obtained by inverting the fermion-matrix with source $(\omega_S^{[\alpha]})_{xb\beta} = \delta_{\alpha\beta}\,\eta^{[\alpha]}_{xb}$, where $\eta^{[\alpha]}_{xb}$ are independent stochastic variables chosen at random among $\frac{1}{\sqrt{2}}(\pm 1 \pm \mathrm{i})$. For SET one has then $N_{\mathrm{inv}} = 2N_{\mathrm{est}}$. (Again a factor of 2 less comes from the symmetry of SYM.) We computed 165 estimates of the time-slice sums, in this case using 32-bit arithmetic.

In Fig. 1 the evolution of the estimated value of $\mathrm{Tr}[Q^{-1}\Gamma] \equiv \sum_{x_0} \mathrm{Tr}_d[S(x_0)\Gamma]$ for a chosen configuration is displayed as a function of the number of needed inversions N_{inv}. The error bounds represent the statistical uncertainty on the stochastic estimation. For both IVST and SET the value stabilizes after 150–200 inversions, with compatible results. This test on a single configuration only serves as a cross-check of the two methods, the physical information being contained in the ensemble-averages, Fig. 2. In the scalar case the two methods give compatible results after only 50 inversions. In the pseudoscalar case, fluctuations

[1] After the completion of this study we noticed that the use of random gauge transformations in VST was recently pointed out in [4].

[2] Actually on the basis of (8) IVST could be seen as a stochastic estimator method with a particular stochastic volume source.

[3] N_{est} coincides with N_g of previous section. The change of notation is for the sake of the homogeneity when comparing with SET.

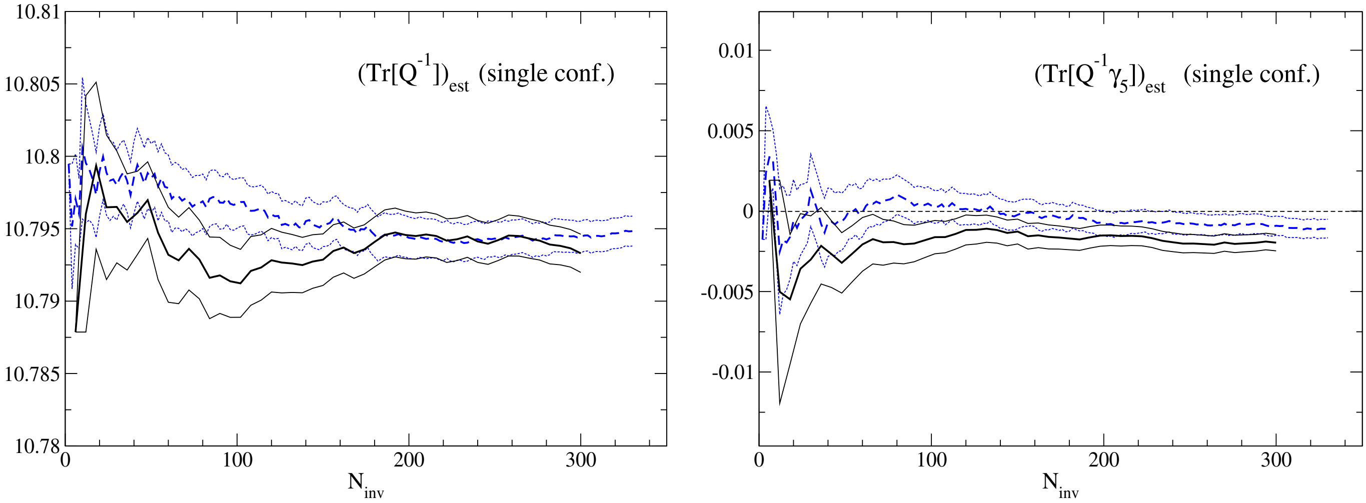

Fig. 1. Evolution of the estimated value of $\mathrm{Tr}[Q^{-1}]$ and $\mathrm{Tr}[Q^{-1}\gamma_5]$ for a chosen configuration as a function of the number of the needed inversions (with error bounds). Full lines: IVST, dashed lines: SET

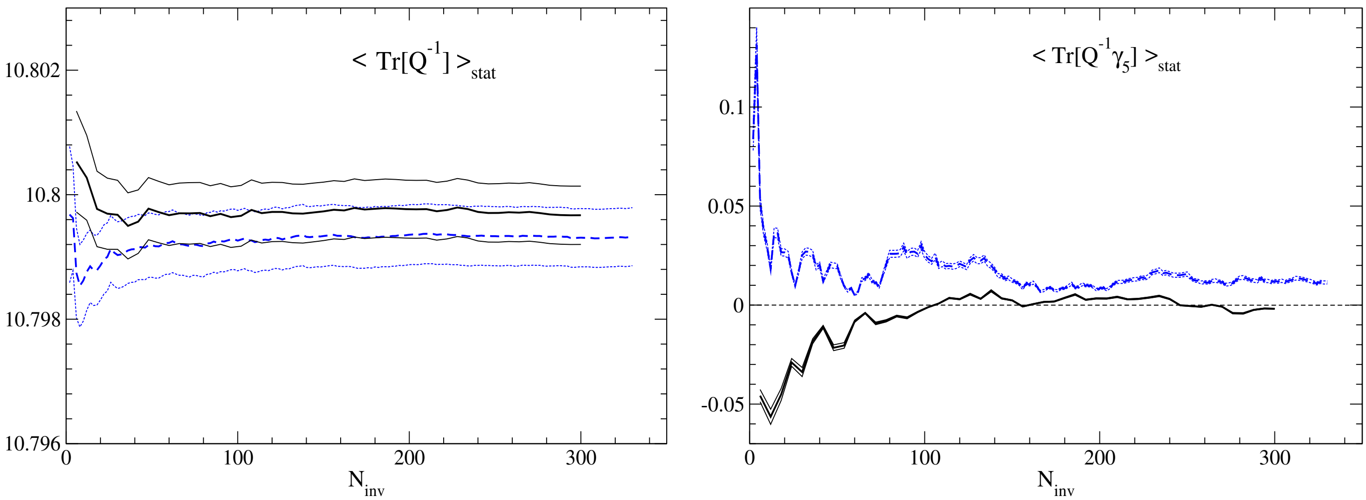

Fig. 2. Evolution of the average value of $\mathrm{Tr}[Q^{-1}]$ and $\mathrm{Tr}[Q^{-1}\gamma_5]$ over the complete sample as a function of the number of the needed inversions (with error bounds). Full lines: IVST, dashed lines: SET

much larger than the error bounds indicate additional effects. The fluctuations appear to be more relevant for SET, where 32-bit arithmetic was used. Moreover, in the latter case the estimate has an offset, while in the case of IVST the expected value (zero) is approached after ~ 100 inversions.

The evolution of the statistical error of the estimation for one configuration is displayed in Fig. 3, showing the a priori non-obvious result that the two methods introduce the same amount of stochastic uncertainty. The error in the estimation of the ensemble-average is shown in Fig. 4. We see that in both cases the error stabilizes after 100 inversions. In the pseudoscalar case, IVST seems to outperform SET, although the large instabilities prevent us from drawing firm conclusions.

3.2 Correlators and masses

In order to show the effect of the error term (13), we computed the disconnected correlator in two ways: (i) following the correct procedure according to (15) (IVST); (ii) performing the gauge-average as in (10). As one can see in Fig. 5 for the pseudoscalar meson, the error term produces a sizeable effect on the disconnected correlator. IVST and SET are in good agreement. The effective mass is shown in Fig. 6. The impact of the error on the effective mass is suppressed in the first time slices where the connected contribution (14) plays a larger role. However in the last time slices, where the disconnected contribution dominates, the effect of the error term shows-up in the form of a pronounced instability of the effective mass as a function of the time-separation (for $\Delta t = 13$ an estimate is not even possible). In the last few time-separations $\Delta t = 14, 15$, IVST delivers a better result compared to SET (no estimate is possible with SET for $\Delta t = 15$). Since the disconnected contribution to the mesonic correlator is essentially of infrared nature, the region of large time-separations is important for the determination of masses.

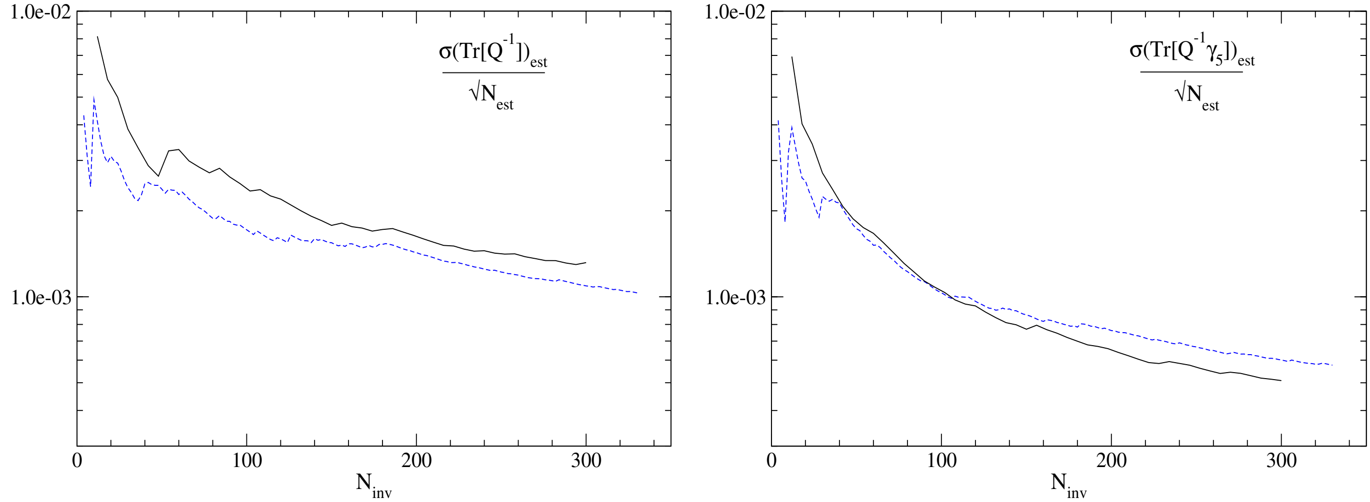

Fig. 3. Evolution of the statistical error of the estimated value of $\mathrm{Tr}[Q^{-1}]$ and $\mathrm{Tr}[Q^{-1}\gamma_5]$ for the same configuration as in Fig. 1, as a function of the number of the needed inversions. Full lines: IVST, dashed lines: SET

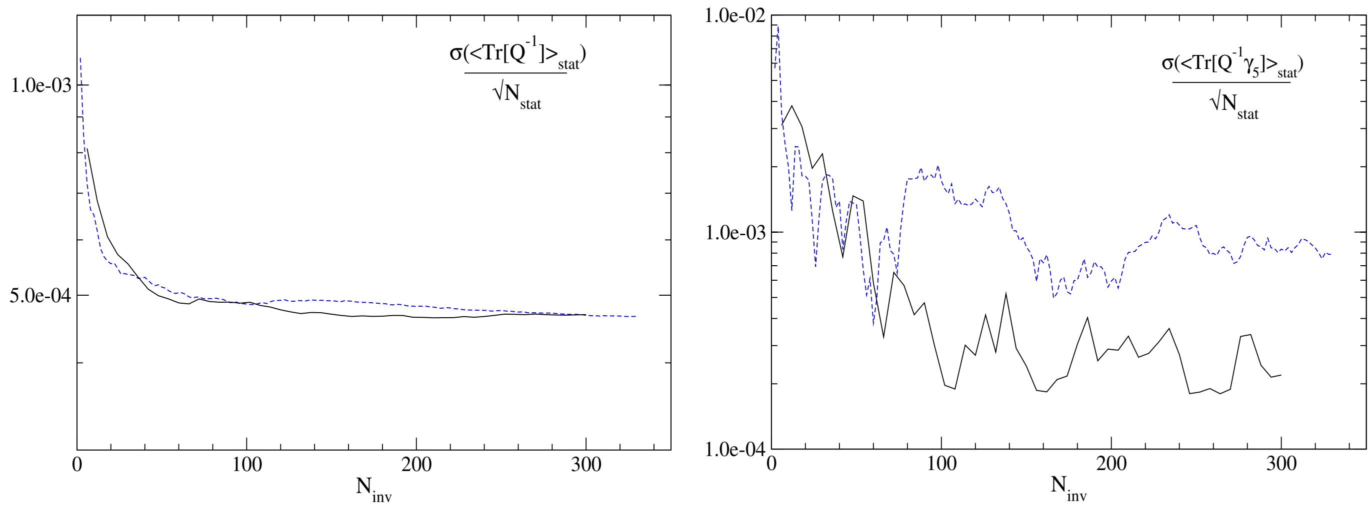

Fig. 4. Evolution of the statistical error on the average value of $\mathrm{Tr}[Q^{-1}]$ and $\mathrm{Tr}[Q^{-1}\gamma_5]$ over the complete sample as a function of the number of the needed inversions. Full lines: IVST, dashed lines: SET

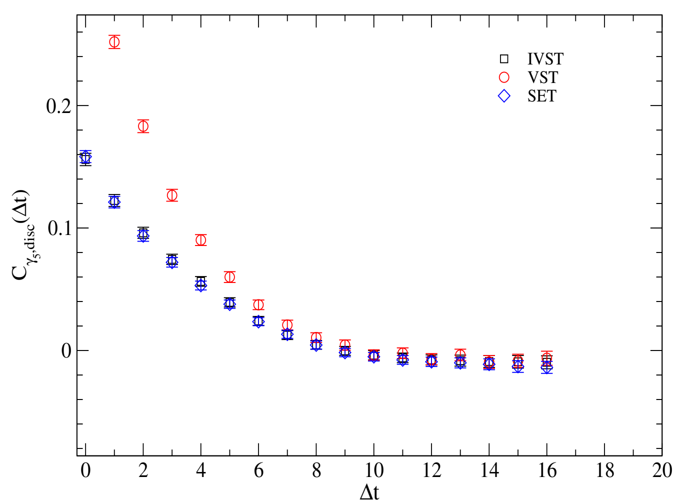

Fig. 5. The disconnected pseudoscalar correlator $C_{\Gamma,\mathrm{disc}}(\Delta t)$

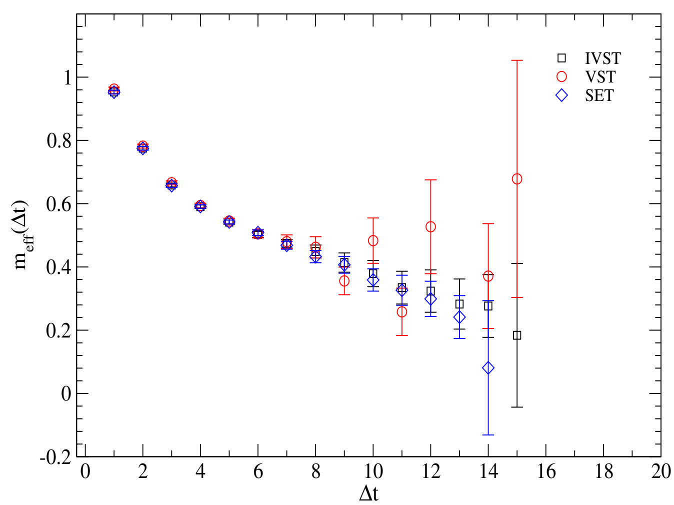

Fig. 6. The effective mass of the pseudoscalar meson

4 Conclusions

We propose an improved version of the volume source technique which eliminates erroneous contact terms in the case of fermions in real representations of the gauge group. The improved version is based on random gauge transformations and is analogous to stochastic estimator methods. Comparison between IVST and SET shows agreement and substantial equivalence. In few cases, e.g. for the determination of effective masses, IVST seems to give slightly better results. A study with higher statistical precision should put these observations on firmer ground.

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