

New polynomially exact integration rules on $U(N)$ and $SU(N)$

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In lattice Quantum Field Theory, we are often presented with integrals over polynomials of coefficients of matrices in $U(N)$ or $SU(N)$ with respect to the Haar measure. In some physical situations, e.g., in presence of a chemical potential, these integrals are numerically very difficult since their integrands are highly oscillatory which manifests itself in form of the sign problem. In these cases, Monte Carlo methods often fail to be adequate, rendering such computations practically impossible.

We propose a new class of integration rules on $U(N)$ and $SU(N)$ which are derived from polynomially exact rules on spheres. We will examine these quadrature rules and their efficiency at the example of a 0+1 dimensional QCD for a non-zero quark mass and chemical potential. In particular, we will demonstrate the failure of Monte Carlo methods in such applications and that we can obtain polynomially exact, arbitrary precision results using the new integration rules.

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1. Introduction

One of the greatest computational challenges in models of statistical and high energy physics is the sign problem [1]. Hence, a myriad of techniques have been developed to address this problem, yet no general solution has been found to date [2]. In high energy physics, for instance, the sign problem prevents a full understanding of the early universe and heavy ion collisions. Such questions require computations using lattice QCD with a non-zero chemical potential which are impossible using current techniques due to the appearance of large cancelation errors (cf., [3, 4] for recent reviews).

Hence, alternative methods need to be developed. For instance, we have proposed and tested Quasi Monte Carlo and iterated numerical integration techniques [5, 6]. Similarly, polynomially exact integration techniques [7] and approaches using symmetrization [8, 9] have been studied. In particular, the symmetrization approach achieved stable results combining Monte Carlo with fairly small symmetry groups. The method to be proposed in the present work is based on *complete symmetrization* and results in an arbitrarily precise evaluation of the integrals considered.

We will construct completely symmetric integration rules for $U(N)$ and $SU(N)$ (section 2) which lead to polynomial exactness and test them using the 1-dimensional QCD with chemical potential (cf., e.g., [10]) as an example (sections 3 and 4). Though the 1-dimensional QCD is interesting in its own right as the strong coupling limit of QCD [11], we will use it as a benchmark only; especially since observables can be computed analytically allowing us to check the numerical results directly. In particular, we will compute the chiral condensate over a broad range of action parameters including values that are impossible (for all practical purposes) to address with standard Monte Carlo techniques.

2. Construction of polynomially exact rules derived from spheres

The construction of polynomially exact rules on $SU(N)$ and $U(N)$ is based on Theorem 2.1.

Theorem 2.1. *Let G_1 and G_2 be topological groups, $\mathcal{B}(G_1)$ and $\mathcal{B}(G_2)$ their Borel σ -algebras, $\Phi : G_1 \rightarrow G_2$ an isomorphism (i.e., a group isomorphism that is also a homeomorphism), γ_1 a (normalized) Haar measure on G_1 , and γ_2 defined by $\forall A \in \mathcal{B}(G_2) : \gamma_2(A) := \gamma_1([A]\Phi)$ where $[A]\Phi$ denotes the pre-set of A under Φ .*

Then, γ_2 is a (normalized) Haar measure.

Since $U(N) = SU(N) \rtimes U(1)$ holds where \rtimes denotes the (outer) semi-direct product, $SU(2) \cong S^3$, and $SU(N)$ is a principal $SU(N-1)$ -bundle over S^{2N-1} [12, equation (22.18)], we can write $U(N)$ and $SU(N)$ as products of spheres (up to a set of measure zero); more precisely, $U(N) \simeq \times_{j=1}^N S^{2j-1}$ and $SU(N) \simeq \times_{j=2}^N S^{2j-1}$. Thus, given a homeomorphism $\Phi : \times_j S^{2j-1} \rightarrow G$, we can push the group structure of $G \in \{U(N), SU(N)\}$ to the product of spheres turning Φ into an isomorphism as in Theorem 2.1. In other words,

$$\int_G f dh_G = \int_{\times_j S^{2j-1}} f \circ \Phi d\text{vol}_{\times_j S^{2j-1}} \quad (2.1)$$

where h_G is the normalized Haar measure on G and $\text{vol}_{\times_j S^{2j-1}} = \times_j \frac{\text{vol}_{S^{2j-1}}}{\text{vol}_{S^{2j-1}}(S^{2j-1})}$ is the product of the normalized volume measures on the spheres defined on the product σ -algebra $\otimes_j \mathcal{B}(S^{2j-1})$.

The map Φ can be constructed inductively. Let $\Phi_2 : \partial B_{\mathbb{C}^2} \cong S^3 \rightarrow SU(2); \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \mapsto \begin{pmatrix} \alpha & -\beta^* \\ \beta & \alpha^* \end{pmatrix}$ where ∂B_X is the boundary of the unit ball in X and $j_N : SU(N-1) \rightarrow SU(N); U \mapsto \begin{pmatrix} U & 0 \\ 0 & 1 \end{pmatrix}$.

Furthermore, let

$$r_{j,N} := \begin{cases} e^{i\alpha_j} \sin \varphi_j \prod_{k=1}^{j-1} \cos \varphi_k & , j < N \\ e^{i\alpha_N} \prod_{k=1}^{N-1} \cos \varphi_k & , j = N \end{cases} \quad (2.2)$$

$$r_{j,k} := \begin{cases} 0 & , j < k < N-1 \\ e^{i\alpha_k} \cos \varphi_k & , j = k < N-1 \\ -e^{i\alpha_j} \sin \varphi_k \sin \varphi_j \prod_{l=k+1}^{j-1} \cos \varphi_l & , k < j \leq N-1 \\ -e^{i\alpha_N} \sin \varphi_k \prod_{l=k+1}^{N-1} \cos \varphi_l & , k < N-1 \wedge j = N \end{cases} \quad (2.3)$$

$$r_{j,N-1} := \begin{cases} 0 & , j < N-1 \\ e^{-i\alpha_{N-1}} \cos \varphi_{N-1} & , j = N-1 \\ -e^{-i\alpha_N} \sin \varphi_{N-1} & , j = N \end{cases} \quad (2.4)$$

where $\neg_j := \sum_{k=1}^{j-1} \alpha_k + \sum_{k=j+1}^N \alpha_k$. Then, the vectors $R_{N,k} := (r_{1,k}, r_{2,k}, \dots, r_{N,k})^T$ are orthonormal and $s \in \{0, 1\}$ can be chosen such that $R_N := \left((-1)^s R_{N,1} \ R_{N,2} \ R_{N,3} \ \dots \ R_{N,N} \right) \in SU(N)$. The parameters $\alpha_j \in [0, 2\pi)$ and $\varphi_j \in [0, \frac{\pi}{2}]$ in the definition of R_N are uniquely defined by $R_{N,N} \in \partial B_{\mathbb{C}^N} \cong S^{2N-1}$ up to a set of measure zero ($r_{j,N} = 0 \Leftrightarrow \alpha_j$ non-unique). Hence, we can define

$$\Phi_N : \partial B_{\mathbb{C}^N} \times \times_{j=2}^{N-1} \partial B_{\mathbb{C}^j} \rightarrow SU(N); (R_{N,N}, r) \mapsto R_N j_N(\Phi_{N-1}(r)) \quad (2.5)$$

everywhere up to a set of measure zero.

Given suitable quadrature rules Q_j in $\partial B_{\mathbb{C}^j}$ such that none of the points in $\times_{j=2}^N Q_j$ is in the null set that Φ_N is not defined on, we obtain a quadrature rule

$$Q_{SU(N)} := \Phi_N \left[\times_{j=2}^N Q_j \right] \quad (2.6)$$

in $SU(N)$. Furthermore, the Haar measure of $U(N)$ decomposes into $h_{U(N)} = h_{SU(N)} \times h_{U(1)}$ (cf., e.g., [13, Exercise 2.1.7]), i.e., choosing a quadrature rule $Q_{U(1)}$ yields a quadrature rule $Q_{U(N)} := Q_{SU(N)} \times Q_{U(1)}$ on $U(N)$.

As we are interested in polynomially exact quadrature rules, we choose

$$Q_{U(1)} := \left\{ e^{\frac{2\pi i k}{t+1}}; k \in \mathbb{N}_{\leq t+1} \right\} \quad (2.7)$$

on $U(1)$ with equal weights $\frac{1}{t+1}$ which integrates all polynomials up to degree t exactly [14, Example 5.14]. Furthermore, since the pull-back of polynomials in $SU(N)$ have similar symmetry properties to “standard” polynomials on spheres, we consider (randomized) fully symmetric quadrature rules as described in [15] for the quadrature rules Q_j on S^{2j-1} .

Remark It should be noted that presently we do not have a complete proof of polynomial exactness for the groups $U(N)$ and $SU(N)$ with general N . However, the application below provides numerical evidence for the tested groups and polynomial degrees.

3. One dimensional lattice QCD

Let us consider the Dirac operator for a quark of mass m at chemical potential μ [10]

$$\mathfrak{D}(U) = \begin{pmatrix} m & \frac{e^\mu}{2}U_1 & & & \frac{e^{-\mu}}{2}U_n^* \\ -\frac{e^{-\mu}}{2}U_1^* & m & \frac{e^\mu}{2}U_2 & & \\ & -\frac{e^{-\mu}}{2}U_2^* & m & \frac{e^\mu}{2}U_3 & \\ & & \ddots & \ddots & \ddots \\ & & & -\frac{e^{-\mu}}{2}U_{n-2}^* & m & \frac{e^{-\mu}}{2}U_{n-1} \\ -\frac{e^\mu}{2}U_n & & & & -\frac{e^{-\mu}}{2}U_{n-1}^* & m \end{pmatrix} \quad (3.1)$$

where all empty entries are zero and the corresponding one flavor partition function

$$Z(m, \mu, G, n) = \int_{G^n} \det \mathfrak{D}(U) dh_G^n(U) \quad (3.2)$$

where $G \in \{U(N), SU(N)\}$, $N \in \mathbb{N}$, and h_G is the corresponding (normalized) Haar measure on G . (Note that the integrals $Z(m, \mu, G, n)$ can be evaluated analytically; [16, Theorem 2.2] or [17] if $n \in 2\mathbb{N}$.)

As an observable for the model, we will consider the chiral condensate

$$\chi(m, \mu, G, n) = \partial_m \ln Z(m, \mu, G, n) = \frac{\partial_m Z(m, \mu, G, n)}{Z(m, \mu, G, n)} = \frac{\int_{G^n} \partial_m \det \mathfrak{D}(U) dh_G^n(U)}{\int_{G^n} \det \mathfrak{D}(U) dh_G^n(U)}. \quad (3.3)$$

We will furthermore choose the gauge $U_j = 1$ except $U_n = U$ which yields

$$\det \mathfrak{D} = \det \left(\prod_{j=1}^n \tilde{m}_j + 2^{-n} e^{-n\mu} U^* + (-1)^n 2^{-n} e^{n\mu} U \right) \quad (3.4)$$

where $\tilde{m}_1 := m$, $\forall j \in [2, n-1] \cap \mathbb{N} : \tilde{m}_j := m + \frac{1}{4\tilde{m}_{j-1}}$, and $\tilde{m}_n := m + \frac{1}{4\tilde{m}_{n-1}} + \sum_{j=1}^{n-1} \frac{(-1)^{j+1} 2^{-2j}}{\tilde{m}_j \prod_{k=1}^{j-1} \tilde{m}_k^2}$. In particular, this reduces the integration over G^n to an integral over G .

4. Numerical Results

In this section, we will compare the quadrature rules described in section 2 to Markov Chain Monte Carlo (MC-MC) using the same number of integration points. As a prelude to these comparisons, Figure 1 shows the values of $Z(m, \mu = 1., G, n = 20)$ with $G \in \{SU(3), U(3)\}$ over a range of m values and compares them to $2^{-3n} e^{3n\mu}$ which is the order of magnitude of the non-constant term in $\det \mathfrak{D}$. We can identify three regions (I, II, and III).

For large values of m (region III) the value of Z is significantly larger than the order of magnitude of the critical terms in the point evaluation. Thus, in region III, we expect both methods (MC-MC and polynomially exact) to yield very small relative errors.

For small values of m (region I), on the other hand, $Z(m, \mu, U(3), n)$ is significantly lower than $2^{-3n} e^{3n\mu}$. The initial error will, therefore, be very large and MC-MC will produce very large relative errors. The polynomially exact quadrature should still produce machine error results, but since the point evaluation error is of the same order of magnitude as the MC-MC error (which is larger than $O(1)$), machine precision results still lose some precision. Since $Z(m, \mu, SU(3), n) - Z(m, \mu, U(3), n) \approx 2^{-3n} e^{3n\mu}$ we expect a regularizing effect on the relative error for $SU(3)$ in region I, i.e., the relative error in the MC-MC case will not be as bad as it is in the $U(3)$ case.

In the transition region (region II) of intermediate m values, we expect the MC-MC error in the $U(3)$ case to smoothly transition from machine error (region III) to some very large relative error (region I). The polynomially exact results should stay on machine error until the MC-MC error grows above 1 and then smoothly transition to the machine precision results of region I. The $SU(3)$ case, however, could show a more interesting behavior since the constant term $Z(m, \mu, SU(3), n) - Z(m, \mu, U(3), n) \approx 2^{-3n} e^{3n\mu}$ and the critical term in the point evaluation are of the same order of magnitude. This can lead to cancellation effects (particularly for MC-MC) and, thus, a relative error that is larger than the relative error in both regions I and III.

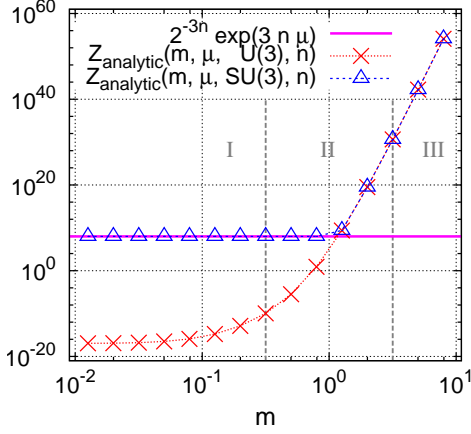


Figure 1: Order of magnitude $2^{-3n} e^{3n\mu}$ of the point evaluation of the integrand compared to the value of Z for $G \in \{U(3), SU(3)\}$.

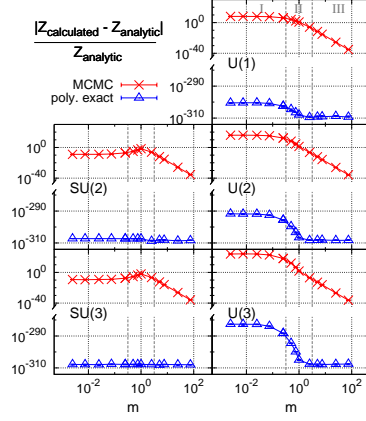


Figure 2: Comparison of the relative error of Z using MC-MC and polynomially exact quadrature. Computations were performed with 1024bit extended floats (≈ 307 digits precision).

In Figure 2, we have plotted the relative error of $Z(m, \mu = 1., G, n = 20)$ over a range of m values and for all $G \in \{U(1), U(2), SU(2), U(3), SU(3)\}$. We have performed the computations with 1024bit extended floating point arithmetic since the values of $Z(m \ll 1., \mu = 1., U(N), n = 20)$ are too low for double precision (as can be seen in Figure 1). In particular, we observe that the polynomially exact method proposed above operates on machine precision throughout the entire range of m values while MC-MC yields the expected results in each of the regions I, II, and III.

Considering the chiral condensate

$$\chi(m, \mu, G, n) = \frac{\partial_m Z(m, \mu, G, n)}{Z(m, \mu, G, n)}, \quad (4.1)$$

Figure 3 shows the values of $Z(m, \mu = 1., G, n = 8)$ and $\partial_m Z(m, \mu = 1., G, n = 8)$ over a large range of m values and with $G \in \{U(2), SU(2)\}$, as well as, the order of magnitude $2^{-2n} e^{2n\mu}$ of

the point evaluation. Adding to the complications of computing the denominator Z for small m , the numerator $\partial_m Z$ is difficult to compute, as well. Thus, we expect MC-MC results similar to the MC-MC results computing partition function $Z(m, \mu, U(N), n)$; this is precisely what we observe in Figure 4. In particular, we note that the MC-MC relative error is $O(1)$ for small m , i.e., no statistically significant results for the chiral condensate can be obtained using standard MC-MC methods. In contrast, the polynomially exact results are on machine precision as expected.

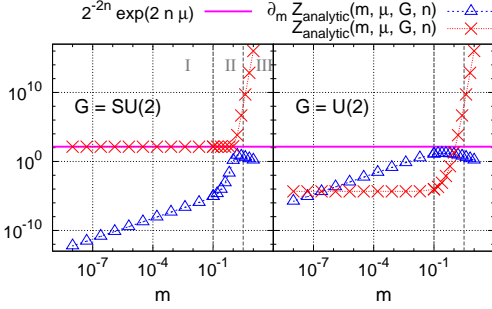


Figure 3: Order of magnitude $2^{-2n} e^{2n\mu}$ of the point evaluation of the integrand compared to the values of Z and $\partial_m Z$ for $G \in \{U(2), SU(2)\}$.

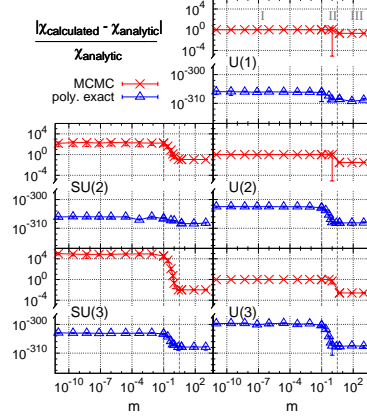


Figure 4: Comparison of the relative error of χ using MC-MC and polynomially exact quadrature. Computations were performed with 1024bit extended floats (≈ 307 digits precision).

5. Conclusion

We have developed new integration rules for the groups $U(N)$ and $SU(N)$, provided numerical verification that these rules are polynomially exact for $N \leq 3$, and compared them to Markov Chain Monte Carlo using the example of 1-dimensional QCD with a chemical potential in which a sign problem appears with Monte Carlo for certain parameter values (region I; $\prod_{j=1}^n \tilde{m}_j < 2^{-Nn} e^{Nn\mu}$). These computations have shown that, even in parameter ranges with the most severe sign problem, the chiral condensate can be computed to arbitrary precision using the newly proposed method. Standard Markov Chain Monte Carlo methods, on the other hand, exhibit large $O(1)$ relative errors, i.e., not giving any statistically significant results. We even used 1024bit extended precision for these comparisons and obtained machine precision results with the new method. Furthermore, the newly constructed quadrature rules yield an error reduction by many orders of magnitude compared to Monte Carlo in regions without the sign problem, as well. Hence, we conclude that our polynomially exact method completely avoids the sign problem.

The fact that these new integration rules overcome the sign problem and reduce the error by orders of magnitude in the 1-dimensional QCD is very promising and a notable result in its own right. However, this benchmark should be regarded as a toy model as it is necessary to demonstrate applicability of the method to higher dimensions. We are, thus, presently considering the Schwinger model as a 2-dimensional quantum field theory.

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