The existence of positive representations for complex weights

2007 J. Phys. A: Math. Theor. 40 9399

(http://iopscience.iop.org/1751-8121/40/31/016)

J. Phys. A: Math. Theor. **40** (2007) 9399–9412 doi:10.1088/1751-8113/40/31/016

The existence of positive representations for complex weights

L L Salcedo

Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, E-18071 Granada, Spain

Received 22 February 2007, in final form 19 June 2007
Published 19 July 2007
Online at stacks.iop.org/JPhysA/40/9399

Abstract
The necessity of computing integrals with complex weights over manifolds with a large number of dimensions, e.g., in some field theoretical settings, poses a problem for the use of Monte Carlo techniques. Here it is shown that very general complex weight functions $P(x)$ on $\mathbb{R}^d$ can be represented by real and positive weights $p(z)$ on $\mathbb{C}^d$, in the sense that for any observable f, $\langle f(x)\rangle_P = \langle f(z)\rangle_p$, $f(z)$ being the analytical extension of $f(x)$. The construction is extended to arbitrary compact Lie groups.

PACS numbers: 02.70.−c, 11.15.Ha, 02.30.Cj, 02.50.Ng

1. Introduction

The computation of expectation values in statistical mechanics and in quantum field theory in its functional integral formulation requires taking averages of functions with a large number of variables. In the continuous case this means integration over manifolds with large dimensions. In such cases standard numerical integration techniques are no longer efficient and one has to resort to Monte Carlo methods. Unfortunately, in some applications of great practical interest such as lattice quantum chromodynamics in the presence of a baryonic chemical potential [1, 2], the Boltzmann weight to be used in the averages is not positive or even real. This fact prevents a straightforward application of the Monte Carlo method in these cases.

For a (real and positive) probability density function (PDF) $P(x)$, expectation values can be estimated by a pure Monte Carlo method in which the points are independently sampled from $P(x)$. The dispersion in the estimate of $\langle f\rangle_P$ in the pure Monte Carlo method is $\sigma_P(f)/\sqrt{N}$, where $\sigma_P^2(f)$ is the variance of f and N is the number of independent sampling points [3, 4]. If sampling $P(x)$ is very costly it may be more convenient to use the so-called reweighting method, in which an auxiliary PDF $P_0(x)$ is sampled instead, making use of the identity

$$\langle f\rangle_P = \frac{\langle f P P_0^{-1}\rangle_{P_0}}{\langle P P_0^{-1}\rangle_{P_0}}. \tag{1.1}$$

For a generic observable $f(x)$ this method is less efficient as it suffers from the importance sampling problem: less points fall in the relevant region (i.e., where $P(x)$, rather than $P_0(x)$, is large), and the dispersion $\sigma_P(f)/\sqrt{N_{\text{eff}}}$ increases. A typical signal of this problem is the presence of large fluctuations in both the numerator and the denominator in (1.1) when $P_0(x)$ and $P(x)$ are too different.

Nevertheless, the reweighting method can be translated immediately to the cases in which the weight function $P(x)$ is complex. (With some abuse of language such complex density functions are still referred to as PDFs.) A positive $P_0(x)$ is chosen (a standard choice being[1] $P_0(x) = \lambda|P(x)|$) and used to generate the samples. Although the importance sampling problem is not well defined here in general (being $P(x)$ complex sampling it is meaningless), the same large fluctuation problem which appeared in the case of the positive $P(x)$ is present here as a sign (or rather phase) problem, since often the average of the phase, $\langle P/|P|\rangle_{|P|}$, is very small but not its variance[2].

There are cases, however, where a sampling of a complex $P(x)$ can be given a meaning. A clear instance of this is a PDF defined on $\mathbb{R}$ such that $P(x) = P_0(x - \mathrm{i}a)$, where $P_0(x)$ is positive (for real x) and analytic on a region containing $\mathbb{R}$ and $\mathbb{R} - \mathrm{i}a$. Then for $f(z)$ analytic on a region containing $\mathbb{R}$ and $\mathbb{R} + \mathrm{i}a$, $\langle f(x)\rangle_P = \langle f(x + \mathrm{i}a)\rangle_{P_0}$. In this case the Monte Carlo method can be applied using as sampling points $z_k = x_k + \mathrm{i}a, k = 1, \ldots, N$, where the x_k are generated from $P_0(x)$, and taking as observable $f(z)$ (the analytic extension of $f(x)$). This example suggests a technique consisting of sampling the complex plane, or more generally a suitable complexified version of the original manifold where the complex $P(x)$ is defined, using an appropriate real and positive $p(z)$, and trade the computation of $\langle f(x)\rangle_P$ by that of $\langle f(z)\rangle_p$. In practice this program has been applied by means of the so-called complex Langevin method [12, 13]. For positive $P(x)$ this approach produces a random walk which asymptotically samples the probability density function. This property is easily shown from the associated Fokker–Planck equation of which $P(x)$ is the stable stationary solution. The stochastic differential equation can be applied to the complex case using $P(z)$, the analytical extension of $P(x)$. For some $P(x)$, it can be shown that the random walk will reach a stable equilibrium which samples a certain $p(z)$ with the correct expectation values [14]. In those cases the method is very useful since then essentially the same local algorithms used in the real case apply. Unfortunately, for many relevant complex $P(x)$ there is no steady solution or, if there is, it does not display the correct expectation values [15–31]. As shown in [27] the latter problem arises from the fact that the Fokker–Planck equation admits more solutions in the space of distributions than in the space of ordinary functions. However, the complex Langevin method guarantees at most that the PDF obtained from projection of $p(z)$ on the real axis is a distributional solution of the Fokker–Planck equation, not that it should coincide with the original $P(x)$. In essence the problem is: in that approach everything depends on $P(z)$ and this function does not favor integration along the real axis from integration along many other curves on the complex plane (which can be viewed as a real axis after an analytic change of variables). Regrettably, unlike the real Langevin case, no practical criterion is known to decide *a priori* whether a given $P(x)$ will produce a steady random walk (rather than a state that looks stationary on a finite time computer simulation) and if so, whether such steady solution is really sampling the input PDF $P(x)$. (See however [32, 33].)

Given the limited success of the complex Langevin method, a natural question is to what extent a given complex weight can be represented at all by means of any suitable ordinary (i.e., positive) PDF on the complexified manifold. A partial answer was given in [34] where it was

[1] Taking $P_0(x)$ to be proportional to $|P(x)|$ needs not be the optimal choice in practice, see e.g. [5].

[2] See [1, 2] for alternative techniques, such as Taylor expansion, in the context of lattice QCD and [6–11] for other approaches to the complex action problem.

shown that one-dimensional complex PDFs admit such representation. In [35] it was shown that all complex weights on $\mathbb{R}^d$ of the form Gaussian times polynomial of any degree and in any number of dimensions are also representable by positive PDFs on $\mathbb{C}^d$. Since this set is dense in $L^2(\mathbb{R}^d)$, this suggests that representability is a quite general property. In the present work we extend those results by proving representability for smooth complex PDFs on $\mathbb{R}^d$, which are either rapidly decreasing at infinity or periodic. The latter case is then generalized to smooth PDFs defined on any compact matrix Lie group manifold.

2. Representation for PDFs of the form charge-dipole pair

Let $P(\boldsymbol{x})$ be the complex 'probability' density function for which we want to compute expectation values of 'observables' $f(\boldsymbol{x})$,

$$\langle f\rangle_P := \frac{\int \mathrm{d}\mu(\boldsymbol{x})P(\boldsymbol{x})f(\boldsymbol{x})}{\int \mathrm{d}\mu(\boldsymbol{x})P(\boldsymbol{x})}. \tag{2.1}$$

P and f are complex in general, $\mathrm{d}\mu(\boldsymbol{x})$ is a positive measure and the normalization $\int \mathrm{d}\mu(\boldsymbol{x})P(\boldsymbol{x})$ is different from zero. A positive representation of $P(\boldsymbol{x})$ is a real non-negative probability density function $p(\boldsymbol{z})$ defined on the complex extension of the original real manifold, with some positive measure $\mathrm{d}\mu(\boldsymbol{z})$, in such a way that

$$\langle f\rangle_P = \langle f\rangle_p := \frac{\int \mathrm{d}\mu(\boldsymbol{z})p(\boldsymbol{z})f(\boldsymbol{z})}{\int \mathrm{d}\mu(\boldsymbol{z})p(\boldsymbol{z})}, \tag{2.2}$$

where $f(\boldsymbol{z})$ stands for the analytical extension of $f(\boldsymbol{x})$. Of course, a precise definition requires to specify the space of allowed test functions f. For a real manifold such as $\mathbb{R}^d$, a usual choice is that of the set of polynomials. For complex probabilities which are periodic (real manifold equivalent to a torus), the natural test functions are of the form $\mathrm{e}^{\mathrm{i}n\cdot x}$. In general, the larger the set of test functions the smaller the number of representable complex probabilities. Hereafter we will assume that $P(\boldsymbol{x})$ and $p(\boldsymbol{z})$ are normalized, i.e., the denominators in (2.1) and (2.2) are unity.

The key idea of the construction is to decompose $P(\boldsymbol{x})$ as a sum of simpler PDFs

$$P(\boldsymbol{x}) = \sum_n P_n(\boldsymbol{x}) \tag{2.3}$$

all of them with positive normalization, or, equivalently,

$$P(\boldsymbol{x}) = \sum_n w_n P_n(\boldsymbol{x}), \tag{2.4}$$

with normalized P_n and $w_n \geqslant 0$, and then find positive and normalized representations $p_n(\boldsymbol{z})$ for the $P_n(\boldsymbol{x})$ so that

$$p(\boldsymbol{z}) = \sum_n w_n p_n(\boldsymbol{z}) \tag{2.5}$$

provides the desired positive representation of $P(\boldsymbol{x})$.

A suitable choice is to take the P_n of the form Dirac delta distribution plus a derivative of a Dirac delta. If P is viewed as a hypothetical (complex) charge distribution with positive total charge, it can be decomposed as a sum of simpler distributions of the form positive charge (delta distribution) plus a dipole (derivative of delta) at the same point, with complex dipolar moment. In $\mathbb{R}^d$ this is

$$Q(\boldsymbol{x};\boldsymbol{h}) = \delta(\boldsymbol{x}) + \boldsymbol{h}\cdot\nabla\delta(\boldsymbol{x}), \qquad \boldsymbol{x}\in\mathbb{R}^d, \qquad \boldsymbol{h}\in\mathbb{C}^d. \tag{2.6}$$

As shown constructively in [35] such distribution admits a positive representation of the form Gaussian times polynomial. A similar but simpler solution is considered here.

Let us start by considering the one-dimensional PDF:

$$Q_1(x) = \delta(x) + \delta'(x), \qquad x \in \mathbb{R}. \tag{2.7}$$

It can be represented on the complex plane by the positive and normalized PDF

$$q_1(z) = \frac{1}{8\pi}\left|1 - \frac{z}{2}\right|^2 \mathrm{e}^{-|z/2|^2}, \qquad z \in \mathbb{C}, \tag{2.8}$$

that is

$$\begin{aligned}\int_{\mathbb{C}} \mathrm{d}^2 z q_1(z) z^n &= \int_{\mathbb{R}} \mathrm{d}x\, Q_1(x) x^n \\ &= \delta_{n,0} - \delta_{n,1}, \qquad n = 0, 1, 2, \ldots,\end{aligned} \tag{2.9}$$

where $\mathrm{d}^2 z = \mathrm{d}\,\mathrm{Re}\, z \mathrm{d}\,\mathrm{Im} z$ is the Lebesgue measure on $\mathbb{R}^2$. This can be checked by direct computation using polar coordinates, or alternatively, writing q_1 as

$$\begin{aligned} q_1(z) &= \left(1 + \frac{\partial}{\partial z} + \frac{\partial}{\partial z^*} + 2\frac{\partial}{\partial z}\frac{\partial}{\partial z^*}\right) g(z), \\ g(z) &:= \frac{1}{4\pi}\mathrm{e}^{-|z/2|^2}, \end{aligned} \tag{2.10}$$

integrating by parts and noting that $\langle z^n \rangle_g = \delta_{n,0}$.

Now a positive representation of $Q(\boldsymbol{x}; \boldsymbol{h})$ is easily obtained as follows:

$$q(\boldsymbol{z}; \boldsymbol{h}) = \int_{\mathbb{C}} \mathrm{d}^2 z_1\, q_1(z_1) \delta(\boldsymbol{z} - z_1 \boldsymbol{h}). \tag{2.11}$$

($\delta(\boldsymbol{z} - \boldsymbol{z}_0)$ being the Dirac delta distribution at $\boldsymbol{z}_0$ of the measure $\mathrm{d}^{2d} z$.) Indeed,

$$\begin{aligned}\langle f(\boldsymbol{z})\rangle_{q_h} &= \int_{\mathbb{C}^d} \mathrm{d}^{2d} z\, f(\boldsymbol{z}) q(\boldsymbol{z}; \boldsymbol{h}) \\ &= \int_{\mathbb{C}^d} \mathrm{d}^{2d} z\, f(\boldsymbol{z}) \int_{\mathbb{C}} \mathrm{d}^2 z_1\, q_1(z_1) \delta(\boldsymbol{z} - z_1 \boldsymbol{h}) \\ &= \int_{\mathbb{C}} \mathrm{d}^2 z_1\, f(z_1 \boldsymbol{h}) q_1(z_1) \\ &= \int_{\mathbb{R}} \mathrm{d}x_1\, f(x_1 \boldsymbol{h})(\delta(x_1) + \delta'(x_1)) \\ &= f(\boldsymbol{0}) - \boldsymbol{h} \cdot \boldsymbol{\nabla} f(\boldsymbol{0}) \\ &= \int_{\mathbb{R}^d} \mathrm{d}^d x\, f(\boldsymbol{x}) Q(\boldsymbol{x}; \boldsymbol{h}) \\ &= \langle f(\boldsymbol{x})\rangle_{Q_h}. \end{aligned} \tag{2.12}$$

In the fourth equality we have used that $f(z_1 \boldsymbol{h})$ depends analytically on z_1 and $q_1(z)$ is a representation of $Q_1(x)$.

The support of the distribution $q(\boldsymbol{z}; \boldsymbol{h})$ is at most a plane, and Gaussian-like on that plane. From the Monte Carlo point of view this is considerably more efficient than the solutions presented in [35] which had a larger size (Gaussian-like with non-vanishing width in all $2d$ directions).

3. Periodic PDFs

Next let us apply this technique to find positive representations for periodic PDFs functions on $\mathbb{R}^d$. The advantage of the periodic case is that the manifold is effectively compact, topologically a d-dimensional torus. Specifically, we take $P(\boldsymbol{x})$ with period 1 in each direction,

$$P(\boldsymbol{x}+\boldsymbol{n}) = P(\boldsymbol{x}), \qquad \boldsymbol{x} \in \mathbb{R}^d, \qquad \boldsymbol{n} \in \mathbb{Z}^d, \tag{3.1}$$

and normalized to unity with measure $\mathrm{d}\mu(\boldsymbol{x}) = \mathrm{d}^d x$ on the d-dimensional torus $T^d = [0,1]^d$ (suitably compactified). In addition, we assume $P(\boldsymbol{x})$ to be a smooth (i.e. C^∞) function on the torus[3]. A positive representation of $P(\boldsymbol{x})$ is a smooth non-negative function $p(\boldsymbol{z})$ on $\mathbb{C}^d$ which is periodic (in the real directions)

$$p(\boldsymbol{z}+\boldsymbol{n}) = p(\boldsymbol{z}), \qquad \boldsymbol{z} \in \mathbb{C}^d, \qquad \boldsymbol{n} \in \mathbb{Z}^d, \tag{3.2}$$

and such that $\langle \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{n}\cdot\boldsymbol{x}} \rangle_P = \langle \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{n}\cdot\boldsymbol{z}} \rangle_p$ for all $\boldsymbol{n} \in \mathbb{Z}^d$, that is

$$\int_{T^d} \mathrm{d}^d x \; P(\boldsymbol{x})\, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{n}\cdot\boldsymbol{x}} = \int_{\tilde{T}^d} \mathrm{d}^{2d} z \; p(\boldsymbol{z})\, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{n}\cdot\boldsymbol{z}}, \qquad \boldsymbol{n} \in \mathbb{Z}^d, \tag{3.3}$$

where the integration manifold of $\boldsymbol{z}$ is the complexified torus $\tilde{T}^d = [0,1]^d \times \mathbb{R}^d$. This manifold is non-compact in the imaginary direction. For subsequent use, we note that the periodic version of $Q(\boldsymbol{x};\boldsymbol{h})$,

$$Q^p(\boldsymbol{x};\boldsymbol{h}) = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} Q(\boldsymbol{x}+\boldsymbol{n};\boldsymbol{h}), \tag{3.4}$$

admits the positive representation

$$q^p(\boldsymbol{z};\boldsymbol{h}) = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} q(\boldsymbol{z}+\boldsymbol{n};\boldsymbol{h}), \tag{3.5}$$

the sum being convergent (as a distribution). All the functions considered, being periodic, are well defined (single-valued) on T^d or $\tilde{T}^d$.

We can decompose $P(\boldsymbol{x})$ in the form

$$P(\boldsymbol{x}) = P_0(\boldsymbol{x}) + \nabla \cdot \boldsymbol{F}(\boldsymbol{x}), \tag{3.6}$$

where $P_0(\boldsymbol{x})$ is chosen to be everywhere strictly positive, smooth (on the torus) and normalized to unity. A sensible choice is $P_0(\boldsymbol{x}) = 1$; however, we will keep the possibility of a more general choice to maintain the analogy with the non-compact case, below. By Hodge's decomposition theorem [36], there is a complex vector field $\boldsymbol{F}(\boldsymbol{x})$ which is also smooth on the torus (smooth and periodic on $\mathbb{R}^d$). Such $\boldsymbol{F}(\boldsymbol{x})$ is non-unique. A natural solution is just the electric field-like solution: let

$$\rho(\boldsymbol{x}) := P(\boldsymbol{x}) - P_0(\boldsymbol{x}), \tag{3.7}$$

then (3.6) becomes

$$\nabla \cdot \boldsymbol{F}(\boldsymbol{x}) = \rho(\boldsymbol{x}). \tag{3.8}$$

The electric field-like solution is

$$\boldsymbol{F}(\boldsymbol{x}) = \nabla \Phi(\boldsymbol{x}), \tag{3.9}$$

where $\Phi(\boldsymbol{x})$ is a smooth periodic solution of

$$\nabla^2 \Phi(\boldsymbol{x}) = \rho(\boldsymbol{x}). \tag{3.10}$$

[3] Smoothness is invoked to simplify the treatment. Likely the constructions presented here can be extended to suitable spaces of distributions.

More explicitly,

$$\begin{aligned}\rho(\boldsymbol{x}) &= \sum_{\boldsymbol{n}\in\mathbb{Z}^d,\boldsymbol{n}\neq\boldsymbol{0}} \rho_{\boldsymbol{n}}\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}},\\ \Phi(\boldsymbol{x}) &= \sum_{\boldsymbol{n}\in\mathbb{Z}^d,\boldsymbol{n}\neq\boldsymbol{0}} \frac{1}{(2\pi\mathrm{i})^2}\frac{\rho_{\boldsymbol{n}}}{\boldsymbol{n}^2}\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}},\\ \boldsymbol{F}(\boldsymbol{x}) &= \sum_{\boldsymbol{n}\in\mathbb{Z}^d,\boldsymbol{n}\neq\boldsymbol{0}} \frac{\boldsymbol{n}}{2\pi\mathrm{i}}\frac{\rho_{\boldsymbol{n}}}{\boldsymbol{n}^2}\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}}.\end{aligned} \tag{3.11}$$

Note that $\boldsymbol{F}(\boldsymbol{x})$ is smooth because $\rho(\boldsymbol{x})$ is smooth (i.e., $|\rho_{\boldsymbol{n}}|$ decreases for large $\boldsymbol{n}$ faster that any inverse power). $\rho_{\boldsymbol{0}}$ vanishes due to $\int \mathrm{d}^d x\, \rho(\boldsymbol{x}) = 0$, since $P(\boldsymbol{x})$ and $P_0(\boldsymbol{x})$ are both normalized to unity.

Having a valid $\boldsymbol{F}(\boldsymbol{x})$, (3.6) can be rewritten as

$$P(\boldsymbol{x}) = \int_{\mathbb{R}^d} \mathrm{d}^d y\, P_0(\boldsymbol{y})(\delta(\boldsymbol{x}-\boldsymbol{y}) + \boldsymbol{H}(\boldsymbol{y})\cdot\boldsymbol{\nabla}\delta(\boldsymbol{x}-\boldsymbol{y})) \tag{3.12}$$

with

$$\boldsymbol{H}(\boldsymbol{y}) = \frac{\boldsymbol{F}(\boldsymbol{y})}{P_0(\boldsymbol{y})}. \tag{3.13}$$

The vector field $\boldsymbol{H}(\boldsymbol{x})$ is also smooth on T^d. In turn this can be rewritten as

$$\begin{aligned}P(\boldsymbol{x}) &= \int_{\mathbb{R}^d} \mathrm{d}^d y\, P_0(\boldsymbol{y})\, Q(\boldsymbol{x}-\boldsymbol{y};\boldsymbol{H}(\boldsymbol{y}))\\ &= \int_{T^d} \mathrm{d}^d y\, P_0(\boldsymbol{y})\, Q^p(\boldsymbol{x}-\boldsymbol{y};\boldsymbol{H}(\boldsymbol{y})),\end{aligned} \tag{3.14}$$

where $Q^p(\boldsymbol{x};\boldsymbol{H}(\boldsymbol{y}))$ is just $Q^p(\boldsymbol{x};\boldsymbol{h})$ of (3.4) with $\boldsymbol{h} = \boldsymbol{H}(\boldsymbol{y})$. Therefore, $P(\boldsymbol{x})$ has been written as a sum of charge-dipole distributions of the form (2.6). A positive representation of $P(\boldsymbol{x})$ is thus readily found:

$$\begin{aligned}p(\boldsymbol{z}) &= \int_{T^d} \mathrm{d}^d y\, P_0(\boldsymbol{y}) q^p(\boldsymbol{z}-\boldsymbol{y};\boldsymbol{H}(\boldsymbol{y}))\\ &= \int_{\mathbb{R}^d} \mathrm{d}^d y\, P_0(\boldsymbol{y}) q(\boldsymbol{z}-\boldsymbol{y};\boldsymbol{H}(\boldsymbol{y})),\end{aligned} \tag{3.15}$$

where $q^p(\boldsymbol{z};\boldsymbol{H}(\boldsymbol{y}))$ or $q(\boldsymbol{z};\boldsymbol{H}(\boldsymbol{y}))$ are just $q^p(\boldsymbol{z};\boldsymbol{h})$ or $q(\boldsymbol{z};\boldsymbol{h})$ with $\boldsymbol{h} = \boldsymbol{H}(\boldsymbol{y})$. The positive representation $p(\boldsymbol{z})$ is also smooth and periodic on $\mathbb{C}^d$ and so smooth on $\tilde{T}^d$.

4. Positive representations for PDFs on compact Lie groups

Let us now consider the extension of the previous construction to Lie group manifolds. Such manifolds appear often in applications such as lattice gauge theories. Specifically, as real manifold we take a connected and compact Lie group G of dimension d, which for convenience will be taken as a matrix group. Hence all elements are of the form $g = \exp(\boldsymbol{x}\cdot\boldsymbol{T})$, where $\boldsymbol{x}\in\mathbb{R}^d$ and the d matrices $\boldsymbol{T}$ define a basis of the d-dimensional Lie algebra. The complexified manifold is the connected but non-compact Lie group $\tilde{G} = \{\tilde{g} = \exp(\boldsymbol{z}\cdot\boldsymbol{T}), \boldsymbol{z}\in\mathbb{C}^d\}$. A compact Lie group G admits a two-sided invariant metric $\mathrm{g}_{\mu\nu}$ which endows G with a Riemannian manifold structure [37]. The metric can be normalized so that the corresponding volume element, $\mathrm{d}^d x\sqrt{\mathrm{g}}$, is the Haar measure of G normalized to unity [38][4]. This measure

[4] $\mathrm{g} = \det \mathrm{g}_{\mu\nu}$ and x^μ are just any local coordinates, not necessarily the normal coordinates appearing in $\mathrm{e}^{\boldsymbol{x}\cdot\boldsymbol{T}}$.

is used in the evaluation of expectation values. For expectation values on $\tilde{G}$ we also take its Haar measure.

A natural set of test functions is that of arbitrary polynomials of the matrix elements of $g \in G$, $f(g) = f(\{g_{ij}\})$. The analytical extension of these polynomials corresponds just to replace g with $\tilde{g}$, i.e., $f(\{\tilde{g}_{ij}\})$.

The construction of a positive representation $p(\tilde{g})$ of a smooth normalized complex PDF $P(g)$ on G is as follows. Let $P_0(g)$ be strictly positive, smooth and normalized (for instance $P_0 = 1$), then the difference $P - P_0$ integrates to zero on G and, by Hodge decomposition in a compact manifold, we can write (using differential geometry notation [36])

$$P(g) = P_0(g) - d^\dagger F(g), \tag{4.1}$$

where $F(g) = F_\mu(g)\,\mathrm{d}x^\mu$ is a 1-form on G. Equivalently,

$$P(g) = P_0(g) + \nabla_\mu F^\mu(g), \tag{4.2}$$

where ∇_μ is the covariant derivative on G as a Riemannian manifold, with the usual Levi-Civita connection, and $F^\mu(g) = \mathrm{g}^{\mu\nu}(g)F_\nu(g)$. The smooth vector field $F^\mu(g)$ is not unique and the electric field-like solution can be adopted, for instance, [36]:

$$F^\mu(g) = \nabla^\mu(\nabla^2)^{-1}(P(g) - P_0(g)). \tag{4.3}$$

Using (4.2) and upon integration by parts,

$$\begin{aligned}\langle f(g)\rangle_P &= \int \mathrm{d}\mu(g) P(g) f(g) \\ &= \int \mathrm{d}\mu(g) P_0(g)(1 - H^\mu(g)\partial_\mu) f(g),\end{aligned} \tag{4.4}$$

with

$$H^\mu(g) = P_0(g)^{-1} F^\mu(g). \tag{4.5}$$

Clearly, $H^\mu(g)\partial_\mu f(g)$ describes an infinitesimal point transformation, and this can be implemented as an infinitesimal left translation by means of a smooth field $\mathcal{H}(g)$ taking values on the Lie algebra

$$H^\mu(g)\partial_\mu f(g) = \frac{\mathrm{d}}{\mathrm{d}x_1} f(\mathrm{e}^{x_1\mathcal{H}(g)}g)\bigg|_{x_1=0}. \tag{4.6}$$

With the help of the distribution $Q_1(x_1)$ in (2.7), the expression in (4.4) can then be rewritten as

$$\langle f(g)\rangle_P = \int \mathrm{d}\mu(g) P_0(g) \int_{\mathbb{R}} \mathrm{d}x_1\, Q_1(x_1) f(\mathrm{e}^{x_1\mathcal{H}(g)}g). \tag{4.7}$$

Since the dependence on x_1 in f is analytic, we can use the positive representation of $Q_1(x_1)$ on $\mathbb{C}$, $q_1(z_1)$, to write

$$\langle f(g)\rangle_P = \int \mathrm{d}\mu(g) P_0(g) \int_{\mathbb{C}} \mathrm{d}^2 z_1\, q_1(z_1) f(\mathrm{e}^{z_1\mathcal{H}(g)}g). \tag{4.8}$$

This allows us to express the expectation value using a positive representation on $\tilde{G}$,

$$\langle f(g)\rangle_P = \langle f(\tilde{g})\rangle_p := \int \mathrm{d}\mu(\tilde{g}) p(\tilde{g}) f(\tilde{g}), \tag{4.9}$$

with

$$p(\tilde{g}) = \int \mathrm{d}\mu(g) P_0(g) q(\tilde{g}, g; \mathcal{H}(g)) \tag{4.10}$$

and

$$q(\tilde{g}, g; \mathcal{H}(g)) = \int_{\mathbb{C}} \mathrm{d}^2 z_1 \, q_1(z_1) \delta(\mathrm{e}^{z_1 \mathcal{H}(g)} g, \tilde{g}). \tag{4.11}$$

Here $\delta(\tilde{g}_0, \tilde{g})$ denotes the Dirac delta distribution at $\tilde{g}_0$ for the Haar measure $\mathrm{d}\mu(\tilde{g})$ on $\tilde{G}$. The extension to non-connected G is obvious.

5. Positive representations for PDFs on $\mathbb{R}^d$

For PDFs on $\mathbb{R}^d$ the previous construction based on a superposition of charge-dipole pairs can also be carried out, but it is technically more involved due to the lack of compactness of the real manifold. We will assume the normalized complex PDF $P(\boldsymbol{x})$ to be in Schwartz space, i.e. smooth (infinitely differentiable) and rapidly decreasing at infinity ($P(\boldsymbol{x})$ and all its derivatives go to zero faster than any inverse power of $|\boldsymbol{x}|$). The space of test functions can then be chosen as the set of polynomials of $\boldsymbol{x}$.

We choose a suitable positive and normalized $P_0(\boldsymbol{x})$ and write $P(\boldsymbol{x})$ as

$$P(\boldsymbol{x}) = P_0(\boldsymbol{x}) + \boldsymbol{\nabla} \cdot \boldsymbol{F}(\boldsymbol{x}). \tag{5.1}$$

Proceeding formally we then obtain a positive representation with

$$p(\boldsymbol{z}) = \int_{\mathbb{R}^d} \mathrm{d}^d x \, P_0(\boldsymbol{x}) \int_{\mathbb{C}} \mathrm{d}^2 z_1 \, q_1(z_1) \delta(\boldsymbol{z} - \boldsymbol{x} - z_1 \boldsymbol{H}(\boldsymbol{x})), \tag{5.2}$$

with $\boldsymbol{H}(\boldsymbol{x}) = \boldsymbol{F}(\boldsymbol{x})/P_0(\boldsymbol{x})$.

There is a number of issues to be considered in this construction, such as the existence of a suitable $P_0(\boldsymbol{x})$ and of the vector field $\boldsymbol{F}(\boldsymbol{x})$, the convergence of $p(\boldsymbol{z})$ as defined in (5.2), since the integral is on a non-compact manifold, and finally, the convergence of the moments $|\boldsymbol{z}|^n$ of $p(\boldsymbol{z})$ for all non-negative n.

Assuming for the moment that suitable $P_0(\boldsymbol{x})$ and $\boldsymbol{F}(\boldsymbol{x})$ exist, the two latter points will be fulfilled *a fortiori* provided the set of integrals

$$I_{\boldsymbol{n}} = \int_{\mathbb{C}^d} \mathrm{d}^{2d} z \, p(\boldsymbol{z}) |\boldsymbol{z}^{\boldsymbol{n}}| \tag{5.3}$$

exists, where $\boldsymbol{z}^{\boldsymbol{n}} := \prod_{\mu=1}^{d} z_\mu^{n_\mu}$ and n_μ are non-negative integers. Equivalently, the integrals

$$I_{\boldsymbol{n}} = \int_{\mathbb{R}^d} \mathrm{d}^d x \, P_0(\boldsymbol{x}) \int_{\mathbb{C}} \mathrm{d}^2 z_1 \, q_1(z_1) |(\boldsymbol{x} + z_1 \boldsymbol{H}(\boldsymbol{x}))^{\boldsymbol{n}}| \tag{5.4}$$

should be convergent. We will take $P_0(\boldsymbol{x})$ also in Schwartz space and momentarily assume that $\boldsymbol{H}(\boldsymbol{x})$ is smooth. In this case the only problem of convergence may come from the large $|\boldsymbol{x}|$ or large $|z_1|$ sectors of the integral. Since $P_0(\boldsymbol{x})$ and $q_1(z_1)$ are rapidly decreasing, *convergence is ensured provided $\boldsymbol{H}(\boldsymbol{x})$ is bounded by a polynomial*. This condition turns out to be rather restrictive since it implies that $\boldsymbol{F}(\boldsymbol{x})$ should be rapidly decreasing and moreover it should go to zero at a rate not much slower than $P_0(\boldsymbol{x})$ itself.

Since both $P(\boldsymbol{x})$ and $P_0(\boldsymbol{x})$ are smooth and rapidly decreasing, so is their difference, ρ:

$$\rho(\boldsymbol{x}) := P(\boldsymbol{x}) - P_0(\boldsymbol{x}), \tag{5.5}$$

and the equation on $\boldsymbol{F}(\boldsymbol{x})$ is

$$\boldsymbol{\nabla} \cdot \boldsymbol{F}(\boldsymbol{x}) = \rho(\boldsymbol{x}). \tag{5.6}$$

The electric field-like solution, (3.9), exists and is smooth, but unfortunately it will not be rapidly decreasing at infinity, in general. Because $\rho(\boldsymbol{x})$ is in Schwartz space so is its Fourier transform, $\tilde{\rho}(\boldsymbol{k})$. Then, $(\boldsymbol{k}/|\boldsymbol{k}|^2)\tilde{\rho}(\boldsymbol{k})$ is rapidly decreasing but not necessarily smooth at

$\boldsymbol{k} = 0$; correspondingly, its Fourier transform is smooth but not rapidly decreasing, in general. Indeed, unless $\rho(\boldsymbol{x})$ has radial symmetry, the electric field will have the (in three dimensions) well-known multipolar contributions which fall as an inverse power for large $\boldsymbol{x}$ [39]. To find a suitable $\boldsymbol{F}(\boldsymbol{x})$ it is better to view this quantity as (minus) a dipolar density so that its divergence is the charge density $\rho(\boldsymbol{x})$. Because the total charge carried by $\rho(\boldsymbol{x})$ is zero, it should be possible to build it as a superposition of dipoles with complex dipolar moment. Moreover, if $\rho(\boldsymbol{x})$ is smooth or rapidly decreasing or of compact support, it should be possible to choose $\boldsymbol{F}(\boldsymbol{x})$ with the same properties (the support of $\boldsymbol{F}(\boldsymbol{x})$ being larger than that of $\rho(\boldsymbol{x})$ in general). A suitable solution is as follows:

$$\boldsymbol{F}_{\boldsymbol{a}}(\boldsymbol{x}) = -(\boldsymbol{x}-\boldsymbol{a})\int_1^\infty \mathrm{d}\lambda\, \lambda^{d-1}\rho(\lambda(\boldsymbol{x}-\boldsymbol{a})+\boldsymbol{a}), \qquad \boldsymbol{x} \neq \boldsymbol{a}, \tag{5.7}$$

where the basepoint $\boldsymbol{a}$ is an arbitrary point in $\mathbb{R}^d$. Intuitively this solution corresponds to an arrangement of linear chains of dipoles, all chains starting at $\boldsymbol{a}$ and ending at each of the points in the support of ρ, in which each 'positive' charge of one dipole is canceled by the 'negative' one of the next dipole in the chain. The total charge at $\boldsymbol{a}$ equals that in $\rho(\boldsymbol{x})$ which is zero.

It is immediate to verify that $\nabla \cdot \boldsymbol{F}_{\boldsymbol{a}}(\boldsymbol{x}) = \rho(\boldsymbol{x})$ for all $\boldsymbol{x} \neq \boldsymbol{a}$. Also it is clear that $\boldsymbol{F}_{\boldsymbol{a}}(\boldsymbol{x})$ is rapidly decreasing at infinity (or of compact support if $\rho(\boldsymbol{x})$ is) and smooth at all points except the basepoint. At $\boldsymbol{x} = \boldsymbol{a}$, the solution $\boldsymbol{F}_{\boldsymbol{a}}(\boldsymbol{x})$ will not be smooth in general, however this problem is easily fixed by taking a smooth average over $\boldsymbol{a}$,

$$\boldsymbol{F}(\boldsymbol{x}) = -\int_1^\infty \mathrm{d}\lambda\, \lambda^{d-1}\int_{\mathbb{R}^d} \mathrm{d}^d a\, C(\boldsymbol{a})(\boldsymbol{x}-\boldsymbol{a})\rho(\lambda(\boldsymbol{x}-\boldsymbol{a})+\boldsymbol{a}), \tag{5.8}$$

where we choose the weighting function $C(\boldsymbol{a})$ to be smooth, of compact support, positive and normalized to unity. Upon taking the average over $\boldsymbol{a}$, the Fourier transform $\tilde{\boldsymbol{F}}(\boldsymbol{k})$ can be shown to be rapidly decreasing, in addition to smooth, so $\boldsymbol{F}(\boldsymbol{x})$ belongs to Schwartz space[5].

The remaining issue is whether $P_0(\boldsymbol{x})$ can be chosen so that $\boldsymbol{H}(\boldsymbol{x}) = \boldsymbol{F}(\boldsymbol{x})/P_0(\boldsymbol{x})$ is polynomially bounded. Since the discussion is rather technical, this is shown in the appendix. Here we only note that $P_0(\boldsymbol{x})$ should not go to zero too quickly for large $|\boldsymbol{x}|$, as compared to $P(\boldsymbol{x})$. Otherwise the falloff of $\rho(\boldsymbol{x})$ and $\boldsymbol{F}(\boldsymbol{x})$ would be dominated by that of $P(\boldsymbol{x})$ and the ratio $\boldsymbol{F}(\boldsymbol{x})/P_0(\boldsymbol{x})$ could fail to be bounded by a polynomial.

6. Alternative constructions

The positive representation of a given complex PDF is by no means unique [35]. For periodic density functions we present here alternative positive representations to those studied in section 3. They have the virtue of being quite localized on $\mathbb{C}^d$ or $\tilde{T}^d$. This is convenient for their use in Monte Carlo integration since the localization decreases the fluctuations in the average over samples.

The construction is based on decomposing the periodic and smooth $P(\boldsymbol{x})$ as a weighted sum (with positive weight) of simpler PDFs of the form

$$P_{\boldsymbol{n}}(\boldsymbol{x}) = 1 + A_{\boldsymbol{n}}\, \mathrm{e}^{2\pi \mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}}, \qquad \boldsymbol{n} \in \mathbb{Z}^d, \qquad \boldsymbol{n} \neq \boldsymbol{0}. \tag{6.1}$$

[5] Of course, here we are addressing the generic case. In many practical cases this complicated construction is not needed. For instance, if $\rho(\boldsymbol{x})$ is of the form Gaussian times polynomial, it is immediate, by going to Fourier space, to find a valid $\boldsymbol{F}(\boldsymbol{x})$ which is also of the form Gaussian times polynomial.

If the normalization of $P(\boldsymbol{x})$ is positive such decomposition is clearly always possible after a discrete Fourier decomposition. $P_{\boldsymbol{n}}(\boldsymbol{x})$ has expectation values

$$\langle \mathrm{e}^{-2\pi \mathrm{i}\boldsymbol{m}\cdot\boldsymbol{x}}\rangle_{P_{\boldsymbol{n}}} = \begin{cases} 1 & \text{for} \quad \boldsymbol{m} = \boldsymbol{0} \\ A_{\boldsymbol{n}} & \text{for} \quad \boldsymbol{m} = \boldsymbol{n}, \\ 0 & \text{otherwise.} \end{cases} \qquad \boldsymbol{m} \in \mathbb{Z}^d \tag{6.2}$$

Actually the parameter $A_{\boldsymbol{n}}$ is redundant. Indeed, the expectation values of two PDFs $p(\boldsymbol{z})$ and $p'(\boldsymbol{z}) = p(\boldsymbol{z} + \boldsymbol{a})$ are related by

$$\langle \mathrm{e}^{-2\pi \mathrm{i}\boldsymbol{m}\cdot\boldsymbol{z}}\rangle_{p'} = \mathrm{e}^{2\pi \mathrm{i}\boldsymbol{m}\cdot\boldsymbol{a}} \langle \mathrm{e}^{-2\pi \mathrm{i}\boldsymbol{m}\cdot\boldsymbol{z}}\rangle_{p}, \qquad \boldsymbol{a} \in \mathbb{C}^d. \tag{6.3}$$

Therefore, it is sufficient to find positive representations for $A_{\boldsymbol{n}} = 1$, since other values are generated by a translation (barring the trivial case $A_{\boldsymbol{n}} = 0$):

$$P_{\boldsymbol{n}}(\boldsymbol{x}) = 1 + \mathrm{e}^{2\pi \mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}}, \qquad \boldsymbol{n} \neq \boldsymbol{0}. \tag{6.4}$$

Let $p_{\boldsymbol{n}}(\boldsymbol{z})$, with $\boldsymbol{z} = \boldsymbol{x} + \mathrm{i}\boldsymbol{y}$, be a positive representation of $P_{\boldsymbol{n}}(\boldsymbol{x})$. Because $p_{\boldsymbol{n}}(\boldsymbol{z})$ is also periodic with respect to $\boldsymbol{x}$, it can be decomposed in discrete Fourier modes, $\mathrm{e}^{2\pi \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}$. The expectation values of $\mathrm{e}^{-2\pi \mathrm{i}\boldsymbol{m}\cdot\boldsymbol{z}}$ indicate that the Fourier modes $\boldsymbol{k} = \boldsymbol{0}$ and $\boldsymbol{k} = \boldsymbol{n}$ should be present. The mode $\boldsymbol{k} = -\boldsymbol{n}$ must also be present for $p_{\boldsymbol{n}}(\boldsymbol{z})$ to be real. The minimum required is thus

$$p_{\boldsymbol{n}}(\boldsymbol{z}) = h_0(\boldsymbol{y}) + h(\boldsymbol{y})\, \mathrm{e}^{2\pi \mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}} + h^*(\boldsymbol{y})\, \mathrm{e}^{-2\pi \mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}}, \qquad \boldsymbol{z} = \boldsymbol{x} + \mathrm{i}\boldsymbol{y}, \tag{6.5}$$

and $h_0(\boldsymbol{y})$ real. Furthermore,

$$h_0(\boldsymbol{y}) \geqslant 2|h(\boldsymbol{y})| \tag{6.6}$$

ensures the positivity of $p_{\boldsymbol{n}}(\boldsymbol{z})$.

A solution is easily found using the ansatz

$$h(\boldsymbol{y}) = a_1 \delta(\boldsymbol{y} - \boldsymbol{y}_1) - a_2 \delta(\boldsymbol{y} - \boldsymbol{y}_2), \qquad a_1, a_2 \geqslant 0. \tag{6.7}$$

At least two delta distributions with weights of opposite sign are required to satisfy $\langle \mathrm{e}^{2\pi \mathrm{i}\boldsymbol{n}\cdot\boldsymbol{z}}\rangle_{p_{\boldsymbol{n}}} = 0$. Saturation of the bound provides $h_0(\boldsymbol{y}) = 2|h(\boldsymbol{y})|$. The remaining conditions $\langle 1\rangle_{p_{\boldsymbol{n}}} = \langle \mathrm{e}^{-2\pi \mathrm{i}\boldsymbol{n}\cdot\boldsymbol{z}}\rangle_{p_{\boldsymbol{n}}} = 1$ give the solution

$$p_{\boldsymbol{n}}(\boldsymbol{z}) = \frac{2\mathrm{e}^{2\pi \boldsymbol{n}\cdot\boldsymbol{y}_1} \cos^2(\pi \boldsymbol{n}\cdot\boldsymbol{x})\delta(\boldsymbol{y} - \boldsymbol{y}_1) + 2\mathrm{e}^{2\pi \boldsymbol{n}\cdot\boldsymbol{y}_2} \sin^2(\pi \boldsymbol{n}\cdot\boldsymbol{x})\delta(\boldsymbol{y} - \boldsymbol{y}_2)}{\mathrm{e}^{2\pi \boldsymbol{n}\cdot\boldsymbol{y}_1} + \mathrm{e}^{2\pi \boldsymbol{n}\cdot\boldsymbol{y}_2}}, \quad \boldsymbol{n} \neq \boldsymbol{0}, \tag{6.8}$$

where $\boldsymbol{y}_1, \boldsymbol{y}_2 \in \mathbb{R}^d$ are only constrained to satisfy

$$2 = \mathrm{e}^{2\pi \boldsymbol{n}\cdot\boldsymbol{y}_1} - \mathrm{e}^{2\pi \boldsymbol{n}\cdot\boldsymbol{y}_2}. \tag{6.9}$$

The support of $p_{\boldsymbol{n}}(\boldsymbol{z})$ is $\mathbb{R}^d + \mathbb{R}^d$ (or rather $T^d + T^d$). This is quite localized as compared to $\mathbb{C}^d$ or $\tilde{T}^d$. The localization within this family of PDFs increases (meaning lower Shannon entropy relative to $T^d + T^d$ [6]) by taking $\boldsymbol{n}\cdot\boldsymbol{y}_2 \to -\infty$ so that the branch $\boldsymbol{y} = \boldsymbol{y}_1$ dominates the density function. The limit does not exist, even in the weak sense, since the test functions $\mathrm{e}^{-\mathrm{i}\boldsymbol{m}\cdot\boldsymbol{z}}$ are of rapid growth on $\mathbb{C}^d$ away from the real axis.

[6] The Shannon entropy of a probability density function P relative to another PDF P_0 is defined as $\langle -\log(P/P_0)\rangle_P$. The larger the entropy the less localized is the probability.

7. Concluding remarks

We have shown that very general complex PDFs can be represented by positive representations upon analytical extension of the original manifold. This allows us to sample them as required in the Monte Carlo method. The existence of these positive representations was not granted given the repeated failure of algorithms such as the complex Langevin approach when applied to general complex weight functions. A virtue of our construction is that it does not depend on the analytical extension of $P(\boldsymbol{x})$ itself. In general one cannot expect $P(\boldsymbol{z})$ to be well behaved on the complex manifold. This problem affects severely the complex Langevin approach. Nevertheless, it should be clear that our construction, as it stands, is more of formal interest than of practical use. First, the normalization of $P(\boldsymbol{x})$ is generally not known; the normalization is needed to choose $P_0(\boldsymbol{x})$ and so to obtain the difference $\rho(\boldsymbol{x})$. Second, given $\rho(\boldsymbol{x})$, $F(\boldsymbol{x})$ is not easy to construct. In fact, in practical cases, such as large lattices, only algorithms that are local (i.e., not much more than nearest neighbors) have a chance to be viable. This does not seem to be the case of, say, (5.8).

Another limitation is related to importance sampling which was one of the main problems appearing in the reweighting method, (1.1). Strictly speaking this problem does not exist if a pure Monte Carlo method is applied to $p(\boldsymbol{z})$. However, a lack of importance sampling manifests itself as an enhancement in the fluctuations of averages over samples. Because the positive representation $p(\boldsymbol{z})$ is not unique, there are different representations of a given $P(\boldsymbol{x})$, all of them with the same expectation values on analytic functions (but of course with different expectation values for arbitrary, non-analytic, test functions). For instance, the convolution of a given representation $p(\boldsymbol{z})$ with a positive function $C(\boldsymbol{z})$ with radial symmetry and rapidly decreasing at infinity yields a new representation $p'(\boldsymbol{z})$ (this is because analytic functions are invariant under such convolution) [35]. The new representation will be wider, i.e., less localized, than the original one. As a consequence, although the expectation values of (analytic) observables will be equal, $\langle f\rangle_p = \langle f\rangle_{p'}$, the dispersion will be different, being larger for $p'(\boldsymbol{z})$. Therefore, it becomes crucial in the representation approach to find representations as localized, with entropy as small, as possible.

This can be seen in another way. Equation (5.2) indicates that the Monte Carlo method can be applied in the following manner. First, a sample of $\boldsymbol{x}$ is generated from $P_0(\boldsymbol{x})$, and then, for each $\boldsymbol{x}$ the field $\boldsymbol{H}(\boldsymbol{x})$ is computed and a sample of z_1 is generated from $q_1(z_1)$ to compute $\langle f(\boldsymbol{x} + z_1\boldsymbol{H}(\boldsymbol{x}))\rangle_{q_1}$. This $\boldsymbol{x}$-dependent average is then itself averaged over the sample of $P_0(\boldsymbol{x})$ to finally yield $\langle f(\boldsymbol{z})\rangle_p$. However, in most, if not all, cases it will be more sensible to compute the average over q_1 exactly,

$$\langle f(\boldsymbol{x} + z_1\boldsymbol{H}(\boldsymbol{x}))\rangle_{q_1} = f(\boldsymbol{x}) - \boldsymbol{H}(\boldsymbol{x})\cdot\nabla f(\boldsymbol{x}), \tag{7.1}$$

rather than using Monte Carlo. So a better approach is to directly compute

$$\langle f\rangle_P = \langle f - \boldsymbol{H}\cdot\nabla f\rangle_{P_0}. \tag{7.2}$$

(Interestingly, this formula does not require the analytical extension of $f(\boldsymbol{x})$.) Such an approach is to be compared with the standard one, (1.1),

$$\langle f\rangle_P = \left\langle f + P_0^{-1}(P - P_0)f\right\rangle_{P_0}, \tag{7.3}$$

where, as in (7.2), we have assumed P and P_0 to be normalized (not the case in practice). The two constructions are rather similar (formally $\boldsymbol{H} = P_0^{-1}\nabla^{-1}(P - P_0)$) so *a priori* there is no compelling reason to expect that the importance sampling problem gets better in (7.2) than in (7.3). (An exception would be perhaps the cases in which f is particularly flat, since then this good property is enhanced by the derivative in (7.2).)

Despite these critical remarks, it remains the fact that, as shown here, the representation problem admits a solution for very general complex PDFs $P(\boldsymbol{x})$. Clearly, representability is a necessary condition for the success of any other approach based on analytical extension, whatever the method used in the construction of the positive representation.

From the mathematical point of view, several interesting problems pose themselves. One is finding more general construction methods, in addition to the one presented here based on the charge-dipole decomposition. Another is carrying out the construction for more general manifolds and more general complex PDFs. Also challenging is the problem of finding positive representations of minimal entropy for a given $P(\boldsymbol{x})$: as mentioned before, by convolution it is always possible to increase the entropy, but there is no general mechanism to decrease it, so a minimum value is to be expected. (A similar entropy minimization problem has been found in a different context in [40].) If the positivity condition on $p(\boldsymbol{z})$ is relaxed, a quite localized representation is $p(\boldsymbol{z}) = P(\boldsymbol{x})\delta(\boldsymbol{y})$. Quite likely, this is the optimum solution if $P(\boldsymbol{x})$ is positive. In the general case of complex $P(\boldsymbol{x})$, imposing $p(\boldsymbol{z})$ to be positive will probably imply a greater delocalization on the complex manifold. Finally, one can try to extend the representativity problem. In fact in our discussion we have made use of a map K from the space of test functions $f(\boldsymbol{x})$ to that of functions $\tilde{f}(\boldsymbol{z})$ by means of analytical extension, as well as the adjoint map $K^\dagger$ which is a projection from the set of PDFs $p(\boldsymbol{z})$ on the complex manifold to that of complex density $P(\boldsymbol{x})$: $K|f\rangle = |\tilde{f}\rangle$, $\langle K^\dagger p| = \langle P|$ (note that the map $p \mapsto P$ is single-valued although $P \mapsto p$ is not). That is

$$\langle f\rangle_P = \langle P|f\rangle = \langle K^\dagger p|f\rangle = \langle p|Kf\rangle = \langle p|\tilde{f}\rangle = \langle \tilde{f}\rangle_p. \tag{7.4}$$

From this point of view, more general representations K could be sought which could be of practical interest.

Acknowledgments

This work is supported in part by funds provided by the Spanish DGI and FEDER funds with grant FIS2005-00810, Junta de Andalucía grants FQM225-05, FQM481 and P06-FQM-01735 and EU Integrated Infrastructure Initiative Hadron Physics Project contract RII3-CT-2004-506078.

Appendix. Polynomial growth of $\boldsymbol{H}(\boldsymbol{x})$

Here we want to show that $P_0(\boldsymbol{x})$ can be chosen in such a way that $\boldsymbol{H}(\boldsymbol{x})$ is bounded by a polynomial. We take it as evident that for any complex Schwartz function P' on $\mathbb{R}^d$ there is a positive function P_0' such that (i) P_0' is in Schwartz space, (ii) $P_0'(\boldsymbol{x}) \geqslant |P'(\boldsymbol{x})|$ for all $\boldsymbol{x} \in \mathbb{R}^d$, and (iii) P_0' is a decreasing function, i.e., $P_0'(\boldsymbol{x}_1) \leqslant P_0'(\boldsymbol{x}_2)$ if $|\boldsymbol{x}_1| \geqslant |\boldsymbol{x}_2|$.[7] We apply this property to the function $P'(\boldsymbol{x}) := |\boldsymbol{x}|^{2d}P(\boldsymbol{x})$ and take $P_0(\boldsymbol{x}) := |\boldsymbol{x}|^{-2d}P_0'(\boldsymbol{x})$ for $|\boldsymbol{x}| \geqslant R$, for a sufficiently large R. The definition of $P_0(\boldsymbol{x})$ is completed in the region $|\boldsymbol{x}| < R$ so that it is smooth and normalized. Therefore, for $|\boldsymbol{x}| \geqslant R$, $|P(\boldsymbol{x})| \leqslant P_0(\boldsymbol{x})$ and

$$|\rho(\boldsymbol{x})| \leqslant 2P_0(\boldsymbol{x}), \qquad P_0(\boldsymbol{y}) \leqslant \frac{|\boldsymbol{x}|^{2d}}{|\boldsymbol{y}|^{2d}}P_0(\boldsymbol{x}), \qquad |\boldsymbol{y}| \geqslant |\boldsymbol{x}|. \tag{A.1}$$

[7] To obtain P_0' consider the auxiliary function

$$P_0''(\boldsymbol{x}) = \sup\{|P'(\boldsymbol{y})|, |\boldsymbol{y}| \geqslant |\boldsymbol{x}|\}.$$

By construction P_0'' satisfies all conditions (i-iii), except perhaps the property of being smooth. It seems obvious that P_0'' can be suitable smoothed out to obtain a valid P_0'.

(As in section 5, $\rho = P - P_0$.) In order to use these inequalities we recall that in (5.8) the support of the positive function $C(\boldsymbol{a})$ is compact, so $\boldsymbol{a}$ lies inside a ball of some size R_C, and moreover $\lambda \geqslant 1$. Thus the inequalities (A.1) apply at the point $\lambda(\boldsymbol{x} - \boldsymbol{a}) + \boldsymbol{a}$ provided $R > R_C$. This allows us to write

$$|\boldsymbol{F}(\boldsymbol{x})| \leqslant \int_1^\infty \mathrm{d}\lambda\, \lambda^{d-1} \int_{\mathbb{R}^d} \mathrm{d}^d a\, C(\boldsymbol{a}) \frac{2|\boldsymbol{x} - \boldsymbol{a}||\boldsymbol{x}|^{2d}}{|\lambda(\boldsymbol{x} - \boldsymbol{a}) + \boldsymbol{a}|^{2d}} P_0(\boldsymbol{x}), \qquad |\boldsymbol{x}| \geqslant R. \tag{A.2}$$

On the other hand $|\lambda(\boldsymbol{x} - \boldsymbol{a}) + \boldsymbol{a}| \geqslant \lambda(|\boldsymbol{x}| - |\boldsymbol{a}|)$, hence

$$\begin{aligned} |\boldsymbol{F}(\boldsymbol{x})| &\leqslant 2 \int_1^\infty \mathrm{d}\lambda\, \lambda^{-d-1} \int_{\mathbb{R}^d} \mathrm{d}^d a\, C(\boldsymbol{a}) \frac{|\boldsymbol{x} - \boldsymbol{a}||\boldsymbol{x}|^{2d}}{(|\boldsymbol{x}| - |\boldsymbol{a}|)^{2d}} P_0(\boldsymbol{x}) \\ &\leqslant \frac{2}{d} \frac{(|\boldsymbol{x}| + R_C)|\boldsymbol{x}|^{2d}}{(|\boldsymbol{x}| - R_C)^{2d}} P_0(\boldsymbol{x}), \qquad |\boldsymbol{x}| \geqslant R. \end{aligned} \tag{A.3}$$

As a consequence,

$$\begin{aligned} &|\boldsymbol{F}(\boldsymbol{x})| \leqslant k|\boldsymbol{x}| P_0(\boldsymbol{x}), \qquad \text{for} \quad |\boldsymbol{x}| \geqslant R, \\ &k = \frac{2}{d} \frac{1 + R_C/R}{(1 - R_C/R)^{2d}}, \end{aligned} \tag{A.4}$$

and $\boldsymbol{H}(\boldsymbol{x})$ is bounded by $k|\boldsymbol{x}|$.

References

[1] Muroya S, Nakamura A, Nonaka C and Takaishi T 2003 *Prog. Theor. Phys.* **110** 615 (*Preprint* hep-lat/0306031)
[2] Lombardo M P 2004 *Prog. Theor. Phys. Suppl.* **153** 26 (*Preprint* hep-lat/0401021)
[3] Negele J W and Orland H 1988 *Quantum Many Particle Systems (Frontiers in Physics* vol 68) (Reading, MA: Addison-Wesley)
[4] Madras N 2002 *Lectures on Monte Carlo Methods (Fields Institute Monographs* vol 16) (Providence, RI: American Mathematical Society)
[5] Fodor Z and Katz S D 2002 *J. High Energy Phys.* JHEP03(2002)014 (*Preprint* hep-lat/0106002)
[6] Anagnostopoulos K N and Nishimura J 2002 *Phys. Rev.* D **66** 106008 (*Preprint* hep-th/0108041)
[7] Azcoiti V, Di Carlo G, Galante A and Laliena V 2002 *Phys. Rev. Lett.* **89** 141601 (*Preprint* hep-lat/0203017)
[8] Ambjorn J, Anagnostopoulos K N, Nishimura J and Verbaarschot J J M *J. High Energy Phys.* JHEP10(2002)062 (*Preprint* hep-lat/0208025)
[9] Moreira S, Baeurle A G and Fredrickson G 2003 *Phys. Rev. Lett.* **91** 150201 (*Preprint* physics/0304086)
[10] Markham J F and Kieu T D 1998 *Nucl. Phys.* B **516** 729 (*Preprint* hep-lat/9610006)
[11] Baaquie B E and Seng Y S 2002 *Int. J. Mod. Phys.* C **13** 587 (*Preprint* hep-lat/0009028)
[12] Parisi G 1983 *Phys. Lett.* B **131** 393
[13] Klauder J R 1984 *Phys. Rev.* A **29** 2036
[14] Haymaker R W and Peng Y-c 1990 *Phys. Rev.* D **41** 1269
[15] Ambjorn J and Yang S K 1985 *Phys. Lett.* B **165** 140
[16] Ambjorn J, Flensburg M and Peterson C 1986 *Nucl. Phys.* B **275** 375
[17] Ambjorn J and Yang S-K 1986 *Nucl. Phys.* B **275** 18
[18] Hamber H W and Ren H-c 1985 *Phys. Lett.* B **159** 330
[19] Flower J, Otto S W and Callahan S 1986 *Phys. Rev.* D **34** 598
[20] Schoenmaker W J 1987 *Phys. Rev.* D **36** 1859
[21] Bilic N, Gausterer H and Sanielevici S 1988 *Phys. Rev.* D **37** 3684
[22] Soderberg B 1988 *Nucl. Phys.* B **295** 396
[23] Haymaker R W and Wosiek J 1988 *Phys. Rev.* D **37** 969
[24] Okamoto H, Okano K, Schulke L and Tanaka S 1989 *Nucl. Phys.* B **324** 684
[25] Okano K, Schulke L and Zheng B 1991 *Phys. Lett.* B **258** 421
[26] Gausterer H and Lee S 1992 *Preprint* hep-lat/9211050
[27] Salcedo L L 1993 *Phys. Lett.* B **305** 125
[28] Fujimura K, Okano K, Schulke L, Yamagishi K and Zheng B 1994 *Nucl. Phys.* B **424** 675 (*Preprint* hep-th/9311174)
[29] Gausterer H 1998 *Nucl. Phys.* A **642** 239

[30] Berges J and Stamatescu I O 2005 *Phys. Rev. Lett.* **95** 202003 (*Preprint* hep-lat/0508030)
[31] Berges J, Borsanyi S, Sexty D and Stamatescu I O 2007 *Phys. Rev.* D **75** 045007 (*Preprint* hep-lat/0609058)
[32] Lee S 1994 *Nucl. Phys.* B **413** 827
[33] Adami C and Koonin S E 2001 *Phys. Rev.* C **63** 034319 (*Preprint* nucl-th/0009021)
[34] Weingarten D 2002 *Phys. Rev. Lett.* **89** 240201 (*Preprint* quant-ph/0210195)
[35] Salcedo L L 1997 *J. Math. Phys.* **38** 1710 (*Preprint* hep-lat/9607044)
[36] Nakahara M 1990 *Geometry, Topology and Physics (Graduate student series in physics)* (Bristol: Institute of Physics Publishing)
[37] Barut A O and Raczka R 1986 *Theory of Group Representations and Applications* (Singapore: World Scientific)
[38] Choquet-Bruhat Y, Dewitt-Morette C and Dillard-Bleick M 1982 *Analysis, Manifolds and Physics: part I. Basics* (Amsterdam: North-Holland)
[39] Jackson J D 1975 *Classical Electrodynamics* (New York: Wiley)
[40] Salcedo L L 1998 *Lett. Math. Phys.* **43** 233 (*Preprint* quant-ph/9706015)