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On marginalization of phase-space distribution functions

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Abstract

We discuss marginalization procedures based on integration of quantum phase-space distribution functions over a family of phase-space manifolds. We show that under some conditions the resulting marginals are always nonnegative. © 1999 Published by Elsevier Science B.V. All rights reserved.

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Phase-space representations of quantum mechanics have proven to be very useful in many areas, particularly in statistical physics and quantum optics (for review see, e.g., [1–3]). The main feature of the phase-space approach is the possibility of expressing quantum-mechanical expectation values in the same way as it is done in classical statistical mechanics, employing integration over the phase space Γ :

$$\langle \mathscr{A} \rangle = \int_{\Gamma} \mathrm{d} p \, \mathrm{d} q \, a(p,q) \, \rho(p,q) \tag{1}$$

The functions a(p,q) and $\rho(p,q)$ in the integrand represent the observable quantity \mathscr{A} and the appropriate phase-space distribution function describing the state of the system considered, respectively.

It is well-known that quantum phase-space distribution functions may assume negative values and hence they cannot be directly interpreted as probability densities in the usual meaning. To improve this situation, various 'marginalization' or 'averaging' procedures leading to proper probability densities have been suggested, especially for the Wigner distribution function [4]. The most obvious one seems to be the integrating out some of the variables, as it is done in probability theory (cf., e.g., [5]). Unfortunately, such marginals are not always positive and /or correct from the physical point of view (cf., e.g., [2]). Moreover, even the correct marginal position and momentum distributions are not sufficient to reconstruct the quantum state [6], therefore such simple marginalization is a one-way transformation only.

Recently, there has been a renewed interest in this subject, in connection with the tomographic reconstruction of quantum states, proposed first in the

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context of the Wigner distribution function by Bertrand and Bertrand [7] and shortly after by Vogel and Risken [8]. In this case the respective marginals were defined as phase-space line integrals (Radon transforms) of the Wigner distribution function $\rho_W(p,q)$:

$$w(x,\theta) = \frac{1}{(2\pi)^2} \int_{\Gamma} dp \, dq \, \delta(x - q\cos\theta - p\sin\theta)$$
$$\times \rho_W(p,q) \tag{2}$$

For a recent review on this topic see, e.g. [9], and [10].

In this Letter we will discuss marginalization of phase-space distributions through integration over a family of phase-space manifolds $\mathfrak{M}(\boldsymbol{\xi})$ parametrized by $\boldsymbol{\xi} = (\xi_1, \xi_2, \dots, \xi_n)$

$$\mu(\xi) = \int_{\mathfrak{M}(\xi)} \mathrm{d}p \,\mathrm{d}q \,\rho(p,q) \tag{3}$$

Such transformations are generalizations of the Radon transform used in quantum state tomography [13] and were intensively studied in the field of integral geometry [11,12]. In the context of quantum phase-space distribution functions they were, to the best of our knowledge, first discussed by the present author [14].

We will perform our considerations within the framework of Δ -representations introduced by Srinivas and Wolf [15] and studied further by many authors (see, e.g., [16,17]). This class contains all particular phase-space representations of quantum mechanics being of practical interest, including the Weyl–Wigner–Moyal one as the simplest and also most regular case.

For simplicity sake, we restrict ourselves in the following to the case when $\Gamma \equiv \mathbb{R}^2$ and when $\mathfrak{M}(\xi)$ is a family of sufficiently regular curves in the phase-space plane, described by the equation $\varphi(p,q;\xi) = 0$. We assume also that the phase-space function $\varphi(p,q;\xi)$ corresponds to a 'quadrature observable' \mathscr{F} , represented alternatively by a quantum mechanical operator \hat{F} , related to $\varphi(p,q;\xi)$ according to the correspondence rules specific for the chosen Δ -representation, which we will express concisely by using the convenient \triangleq relation sign as $\hat{F} \triangleq \varphi(p,q;\xi)$.

Under these assumptions, we could rewrite Eq. (3) in the following form:

$$\mu(\xi) = \int_{\Gamma} \mathrm{d}p \,\mathrm{d}q \,\delta(\varphi(p,q;\xi)) \,\rho(p,q) \tag{4}$$

where $\delta(\varphi(p,q;\xi))$ is the δ -distribution concentrated on that curve. Using the integral representation of the δ -distribution with the exponential expanded into power series we get:

$$\mu(\xi) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}x \sum_{k=0}^{\infty} \frac{(\mathrm{i}x)^k}{k!} \phi(\xi, k) \tag{5}$$

where

$$\phi(\xi,k) = \int_{\Gamma} \mathrm{d}p \,\mathrm{d}q \,\varphi^k(p,q;\xi) \,\rho(p,q) \tag{6}$$

The last equation has the form an expectation value with the function $\varphi(p,q;\xi)$ in *k*th power, which in general case does *not* correspond to $\langle \mathscr{F}^k \rangle =$ $\operatorname{Tr}\left[\hat{F}^k \hat{\rho}\right]$, where $\hat{\rho}$ is the density operator. It is caused by the fact that phase-space functions corresponding to operator products are nonlocal and noncommutative ' \bigstar_{Δ} -products' of the respective components, not the ordinary pointwise function products, i.e., if $\hat{A} \triangleq a(p,q)$ and $\hat{B} \triangleq b(p,q)$ then $\hat{A}\hat{B} \triangleq$ $(a\bigstar_{\Delta}b)(p,q)$.

Let us assume now that $\varphi(p,q;\xi)$ was chosen in such ingenious way that for any k the k-fold \bigstar_{Δ^-} product for the given Δ -representation is in this particular case equal to the ordinary pointwise k-fold product. Let further $\hat{\rho} = \sum_{ij} c_i c_j^* |i\rangle \langle j|$ be the expansion of the density operator into the dynamics $|i\rangle \langle j|$ of (orthonormal) eigenvectors $|i\rangle$ of the quadrature operator \hat{F} corresponding to the eigenvalue λ_i . Then we have:

$$\phi(\xi,k) = \operatorname{Tr}\left[\hat{F}^k \hat{\rho}\right] = \sum_i \lambda_i^k |c_i|^2 \tag{7}$$

Inserting Eq. (7) back into Eq. (5) we get, after some algebra, an explicitly nonnegative expression:

$$\mu(\xi) = \sum_{i} |c_{i}|^{2} \delta(\lambda_{i})$$
(8)

Therefore, we have shown that the following theorem holds for any Δ -representation of quantum mechanics:

Theorem. Let $\mathfrak{M}(\xi)$ be a family of phase-space manifolds parametrized by $\xi \in \mathbb{R}^n$, defined by the

equation $\varphi(p,q;\xi) = 0$, where φ is a sufficiently smooth function.

If for any $k \in \mathbb{N}$

$$\underbrace{\varphi \star_{\Delta} \varphi \star_{\Delta} \dots \star_{\Delta} \varphi}_{k-\text{times}} = (\varphi)^k \tag{9}$$

then the quantity

$$\mu(\xi) = \int_{\mathfrak{M}(\xi)} \mathrm{d}p \, \mathrm{d}q \, \rho_{\Delta}(p,q)$$

is nonnegative for any phase-space distribution $\rho_{\Delta}(p,q)$.

As an illustration, let us consider some examples evolving commonly employed phase-space representations.

a. Weyl–Wigner–Moyal representation. We adopt here the following definition of the respective \bigstar_{W} -product [18]:

$$(a \bigstar_{W} b)(p,q) = a(p,q) \exp\left\{\frac{\hbar}{2i}\left(\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p}\right)\right\}b(p,q)$$
(10)

It could be verified by a direct calculation that the function:

$$\chi(p,q;\xi) = \xi_1 p + \xi_2 q + \xi_3 \tag{11}$$

where $\xi_i \in \mathbb{R}$, fulfills the requirement contained in Eq. (9).

This particular case corresponds exactly to the so-called 'symplectic tomography', introduced and investigated extensively by Mancini, Man'ko and Tombesi [19–23] in the context of various approaches to quantum tomography. The respective integral transform is invertible and therefore the resulting marginal distribution could be even used to establish a classical-like description of quantum mechanics [23].

The nonnegativity of the integral transform $\mu(\xi)$ for all Wigner distribution functions (WDFs) implies (cf., e.g. [2], par. 2.1), that $\delta(\chi(p,q;\xi))$ could be regarded as a (generalized) WDF (cf [1]. pp. 366–367 for another derivation and discussion). It could be shown (cf., e.g., Appendix C in Ref. [25]) that

 $\delta(\xi_1 p + \xi_2 q + \xi_3)$ are the *only* δ -shaped WDFs, which in turn indicates that there are *no* nonlinear curves for which Eq. (4) is nonnegative for all possible WDFs. On the other hand, it is evident from the form of Eq. (10) that any nonlinear term in $\chi(p,q;\xi)$ will break Eq. (9).

The invariance of WDFs under affine symplectic phase-space transformations (cf., e.g., [26,27]) and the respective equivariance of the \bigstar_W -product enables one to simplify the things considerably. Namely, by using such transformations the quantity $\chi(p,q;\xi)$ in Eq. (11) could be expressed as a multiple of the new momentum p' (or the new position q') which trivializes the evaluation of Eq. (4). Moreover, the equality $\chi \bigstar_W \dots \bigstar_W \chi = \chi^k$ can be then transformed to $p'\bigstar_W \dots \bigstar_W p' = p'^k$ (or to $q'\bigstar_W \dots \bigstar_W q' = q'^k$) which is fulfilled for the Weyl–Wigner–Moyal and some other phase-space representations [28], including the standard and antistandard representations discussed below.

b. Standard and Antistandard representations. The respective ★-products can be defined here as follows [24]:

$$a \bigstar_{s} b)(p,q) = a(p,q) \exp\left\{-i\hbar\left(\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}\right)\right\} b(p,q) \qquad (12)$$

for the standard representation, and

$$(a \star_{A} b)(p,q) = a(p,q) \exp\left\{i\hbar\left(\frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p}\right)\right\}b(p,q)$$
(13)

for the antistandard one.

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It could be easily verified that the function $\chi(p,q;\xi)$ defined in Eq. (11) above may fulfill the requirement stated in Eq. (9) only when one of the parameters, ξ_1 or ξ_2 , is equal to zero. The resulting integral transforms are here rather trivial and noninvertible, e.g.:

$$\mu_{\mathrm{S}}(\xi) = \int_{\Gamma} \mathrm{d}p \,\mathrm{d}q \,\delta(\xi_{2}q + \xi_{3})\rho_{\mathrm{S}}(p,q)$$
$$= \int_{\Gamma} \mathrm{d}p \,\rho_{\mathrm{S}}\left(p, -\frac{\xi_{3}}{\xi_{2}}\right) \tag{14}$$

which is, up to rescaling, equivalent to integrating out one of the variables in the respective distribution function $\rho(p,q)$.

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