On the Wigner distribution of the reduced density matrix

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Consider a bipartite quantum system consisting of two subsystems A and B. The reduced density matrix of A a is obtained by taking the partial trace with respect to B. In this work we will show that the Wigner distribution of this reduced density matrix is obtained by integrating the total Wigner distribution with respect to the phase space variables corresponding to the subsystem B. The proof we give is rigorous (as opposed to those found in the literature) and makes use of the Weyl–Wigner–Moyal phase space formalism. Our main result is applied to general Gaussian mixed states, of which it gives a particularly simple and precise description. We also briefly discuss the purification of a mixed from the Wigner formalism point of view.

1. Introduction

A quantum state is abstractly defined as a non-negative operator with trace one on some Hilbert space [1, 3, 5, 7]. In this paper we will assume that this Hilbert space is $L^2(\mathbb{R}^n)$ (the square integrable functions). We will deal with a bipartite system consisting of two parts A and B with respective Hilbert spaces $L^2(\mathbb{R}^{n_A})$ and $L^2(\mathbb{R}^{n_B})$ (such systems play a central role in the study of quantum entanglement). We denote by $\mathcal{L}_1(L^2(\mathbb{R}^n))$ (resp. $\mathcal{L}_1(L^2(\mathbb{R}^{n_A}))$) the spaces of trace-class operators on $L^2(\mathbb{R}^n)$ (*resp.* on $L^2(\mathbb{R}^{n_A})$). Setting $n = n_A + n_B$ there exists [12] a unique mapping

$$\mathrm{Tr}^B : \mathcal{L}_1(L^2(\mathbb{R}^n)) \longrightarrow \mathcal{L}_1(L^2(\mathbb{R}^{n_A}))$$
$$\widehat{\rho} \longmapsto \widehat{\rho}^A = \mathrm{Tr}^B(\widehat{\rho})$$

such that for every $\widehat{Q}^A \in \mathcal{B}(L^2(\mathbb{R}^{n_A}))$ (the bounded operators) the identity

$$\tag{1} \mathrm{Tr}(\widehat{\rho}(\widehat{Q}^A \otimes \widehat{I}^B)) = \mathrm{Tr}(\widehat{\rho}^A \widehat{Q}^A)$$

holds for all $\widehat{\rho} \in \mathcal{L}_1(L^2(\mathbb{R}^n))$ where $\widehat{I}^B$ is the identity on $L^2(\mathbb{R}^{n_B})$ (the left-hand side of (1) is well defined since $\mathcal{L}_1(L^2(\mathbb{R}^n))$ is a two-sided ideal in $\mathcal{B}(L^2(\mathbb{R}^n))$). The map Tr^B is called "partial trace with respect to B". Of particular interest is the case where $\widehat{\rho}$ has trace one and is positive semi-definite: $\widehat{\rho} \geq 0$, because then $\widehat{\rho}$ is a quantum density matrix and the operator $\widehat{\rho}^A = \mathrm{Tr}^B(\widehat{\rho})$ is the reduced density matrix on $L^2(\mathbb{R}^{n_A})$.

The aim of this paper is to show that the reduced density matrix $\widehat{\rho}^A$ can be determined in a very easy and explicit way if one applies the Weyl–Wigner–Moyal phase space formalism [9, 17] to the Wigner distribution [11] of the full density matrix $\widehat{\rho}$. In fact, we are going to prove the following result, where we use the notation $z = (z_A, z_B)$, $z_A = (x_A, p_A)$, $z_B = (x_B, p_B)$ for the phase space variables:

Theorem 1. *Let $\widehat{\rho} \in \mathcal{L}_1(L^2(\mathbb{R}^n))$ be a density operator and*

$$(2) \qquad \rho(z) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}py} \langle x + \tfrac{1}{2}y|\widehat{\rho}|x - \tfrac{1}{2}y\rangle dy$$

its Wigner distribution ($x = (x_A, x_B)$). If ρ decreases sufficiently fast at infinity (as described in Lemma 2) then the Wigner distribution of the reduced density matrix $\widehat{\rho}^A = \mathrm{Tr}^B(\widehat{\rho})$ is

$$(3) \qquad \rho^A(z_A) = \int_{\mathbb{R}^{2n_B}} \rho(z_A, z_B) dz_B.$$

As a simple illustration we will apply this result to Gaussian mixed states. We also consider the purification of a density matrix $\rho^A \in \mathcal{L}_1(L^2(\mathbb{R}^{n_A}))$; this will lead us to a new property of the Wigner function. Namely, we show that for every normalized $\psi \in L^2(\mathbb{R}^n)$ there exists an orthonormal basis (ϕ_j^A) of $L^2(\mathbb{R}^{n_A})$ and numbers $\lambda_j \geq 0$, $\sum_j \lambda_j = 1$, such that

$$(4) \qquad \int_{\mathbb{R}^{2n_B}} W\psi(z_A, z_B) dz_B = \sum_j \lambda_j W^A \phi_j^A(z_A) .$$

2. Preliminaries

A density operator $\widehat{\rho}$ on $L^2(\mathbb{R}^n)$ is a compact self-adjoint operator hence the spectral theorem ensures us of the existence of an orthonormal set of vectors

(ψ_j) in $L^2(\mathbb{R}^n)$ and of positive constants λ_j summing up to one such that

$$(5) \qquad \widehat{\rho} = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j| .$$

Since for every index k we have $\widehat{\rho}|\psi_k\rangle = \lambda_k|\psi_k\rangle$ the λ_j are the eigenvalues of $\widehat{\rho}$ and the $|\psi_j\rangle$ the corresponding eigenvectors. Inserting this sum into definition (2) of the Wigner distribution we get

$$(6) \qquad \rho(x,p) = \left(\tfrac{1}{2\pi\hbar}\right)^n \sum_j \lambda_j \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}py}\langle x + \tfrac{1}{2}y|\psi_j\rangle\langle\psi_j|x - \tfrac{1}{2}y\rangle dy$$

(we are using in this formula the standard splitting $x = (x_A, x_B)$, $p = (p_A, p_B)$). Since we have

$$\langle x + \tfrac{1}{2}y|\psi_j\rangle = \psi_j(x + \tfrac{1}{2}y) \ , \ \langle\psi_j|x - \tfrac{1}{2}y\rangle = \psi_j^*(x - \tfrac{1}{2}y),$$

it follows that

$$\left(\tfrac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}py}\langle x + \tfrac{1}{2}y|\psi_j\rangle\langle\psi_j|x - \tfrac{1}{2}y\rangle dy = W\psi_j(x,p)$$

where

$$(7) \qquad W\psi_j(x,p) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}py}\psi_j(x + \tfrac{1}{2}y)\psi_j^*(x - \tfrac{1}{2}y)dy$$

is the usual Wigner transform [4, 18] of ψ_j. The Wigner distribution of the density matrix $\widehat{\rho}$ is thus a convex sum of Wigner transforms [5]:

$$\rho(x,p) = \sum_j \lambda_j W\psi_j(x,p).$$

Let now $W(\phi, \psi)$ be the cross-Wigner transform [18] of $\phi, \psi \in L^2(\mathbb{R}^n)$. By definition [4]

$$(8) \qquad W(\phi, \psi)(x,p) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}py}\phi(x + \tfrac{1}{2}y)\psi^*(x - \tfrac{1}{2}y)dy$$

hence, in particular, $W(\psi, \psi) = W\psi$. We recall the following classical formula from Weyl calculus [3, 4]: if $\widehat{Q}$ is a bounded operator on $L^2(\mathbb{R}^n)$ then,

setting $z = (x, p)$,

$$(9) \qquad \langle \phi | \widehat{Q} \psi \rangle = \int_{\mathbb{R}^{2n}} q(z) W(\phi, \psi)(z) dz$$

where $q(z)$ is the Weyl symbol of $\widehat{Q}$, that is,

$$(10) \qquad q(x, p) = \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar} py} \langle x + \tfrac{1}{2} y | \widehat{Q} | x - \tfrac{1}{2} y \rangle dy \ .$$

We will use he notation $\widehat{Q} = \mathrm{Op_W}(q)$ to denote the Weyl operator with symbol q; formally

$$(11) \qquad \mathrm{Op_W}(q)\psi(x) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar} p(x-yy)} q(\tfrac{1}{2}(x+y), p) \psi(y) dp dy.$$

Comparison with formula (2) shows that the Wigner distribution of a density matrix is just the Weyl symbol of that density matrix divided by $(2\pi\hbar)^n$, that is,

$$(12) \qquad \widehat{\rho} = (2\pi\hbar)^n \, \mathrm{Op_W}(\rho) \ .$$

We will use the following criterion due to Shubin ([14], p. 203) for determining whether a given function on phase space is the Weyl symbol of an operator:

Lemma 2. *Assume that $q \in C^\infty(\mathbb{R}^{2n})$ and that there exist for every multi-index $\alpha \in \mathbb{N}^n$ a constant $C_\alpha > 0$ such that*

$$(13) \qquad |\partial_z^\alpha q(z)| \le C_\alpha (1 + |z|^2)^{(m-|\alpha|)/2}.$$

If $m < -2n$, then $\widehat{Q} = \mathrm{Op_W}(q)$ is of trace class and we have

$$(14) \qquad \mathrm{Tr}(\widehat{Q}) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^{2n}} q(z) dz$$

where the integral is absolutely convergent.

In particular, if ρ satisfies the conditions above then the operator $\widehat{\rho} = (2\pi\hbar)^n \operatorname{Op_W}(\rho)$ is of trace class and its trace is given by the formula

$$(15) \qquad \operatorname{Tr}(\widehat{\rho}) = \int_{\mathbb{R}^{2n}} \rho(z)dz$$

(this formula is often sloppily used in the literature, but one should be aware of the fact that it only holds under rather stringent conditions on ρ; see our discussion and the references in [3, 5]).

3. Proof of Theorem 1

We will again use the notation $z_A = (x_A, p_A)$, $z_B = (x_B, p_B)$, and $z = (z_A, z_B)$.

The partial trace operator (1) can be explicitly calculated [12] using the formula

$$(16) \qquad \langle \phi^A | \widehat{\rho}^A \psi^A \rangle_A = \sum_j \langle \phi^A \otimes \phi_j^B | \widehat{\rho}(\psi^A \otimes \phi_j^B) \rangle$$

where $\psi^A, \phi^A \in L^2(\mathbb{R}^{n_A})$ and (ϕ_j^B) is an arbitrary orthonormal basis of $L^2(\mathbb{R}^{n_B})$; $\langle \cdot | \cdot \rangle_A$ is the bra-ket on $L^2(\mathbb{R}^{n_A})$. Taking into account the relations $\widehat{\rho}^A = (2\pi\hbar)^{n_A} \operatorname{Op_W}(\rho^A)$ and $\widehat{\rho} = (2\pi\hbar)^n \operatorname{Op_W}(\rho)$ we have, in view of formula (9),

$$(17) \qquad \langle \phi^A | \widehat{\rho}^A \psi^A \rangle_A = (2\pi\hbar)^{n_A} \int_{\mathbb{R}^{2n_A}} \rho^A(z_A) W^A(\phi^A, \psi^A)(z_A) dz_A$$

(18)
$$\langle \phi^A \otimes \phi_j^B | \widehat{\rho}(\psi^A \otimes \phi_j^B) \rangle = (2\pi\hbar)^n \int_{\mathbb{R}^{2n}} \rho(z) W(\phi^A \otimes \phi_j^B, \psi^A \otimes \phi_j^B)(z) dz$$

where $W^A(\phi^A, \psi^A)$ is the cross-Wigner transform on $L^2(\mathbb{R}^{n_A})$. In view of the obvious tensor product property

$$W(\phi^A \otimes \phi_j^B, \psi^A \otimes \phi_j^B) = W^A(\phi^A, \psi^A) \otimes W^B \phi_j^B$$

the identity (18) becomes

$$\langle \phi^A \otimes \phi_j^B | \widehat{\rho}(\psi^A \otimes \phi_j^B) \rangle = (2\pi\hbar)^n \int_{\mathbb{R}^{2n_A}} \left[\int_{\mathbb{R}^{2n_B}} \rho(z) W^B \phi_j^B(z_B) dz_B \right] \\ \times W^A(\phi^A, \psi^A)(z_A) dz_A$$

and comparison with the equality (17) shows that we have

$$(2\pi\hbar)^{n_A}\rho^A(z_A) = (2\pi\hbar)^n \sum_j \int_{\mathbb{R}^{2n_B}} \rho(z_A, z_B) W^B \phi_j^B(z_B)dz_B \ ,$$

that is, since $n = n_A + n_B$,

$$(19) \qquad \rho^A(z_A) = (2\pi\hbar)^{n_B} \sum_j \int_{\mathbb{R}^{2n_B}} \rho(z_A, z_B) W^B \phi_j^B(z_B)dz_B \ .$$

There remains to prove that the right-hand side of this equality is just the integral $\int_{\mathbb{R}^{2n_B}} \rho(z_A, z_B)dz_B$. Let us freeze the value of z_A and set $f(z_B) = \rho(z_A, z_B)$. Since we are assuming that ρ satisfies the Shubin estimates (13) we have, for some $m < -n/2$,

$$|\partial_{z_B}^\beta f(z_B)| \leq C_\beta (1 + |z_A|^2 + |z_B|^2)^{m-|\beta|/2}$$
$$\leq C_\beta (1 + |z_B|^2)^{m-|\beta|/2}.$$

The inequality $m < -n/2$ *de facto* implies that $m < -n_B/2$ hence it follows from Lemma 2 that the operator $\widehat{F} = \mathrm{Op_W}(f)$ is of trace class on $L^2(\mathbb{R}^{2n_B})$ and that its trace is the absolutely convergent integral

$$(20) \qquad \mathrm{Tr}(\widehat{F}) = \left(\tfrac{1}{2\pi\hbar}\right)^{n_B} \int_{\mathbb{R}^{2n_B}} f(z_B)dz_B \ .$$

Returning to the identity (19) we have, for every z_A,

$$\rho^A(z_A) = \sum_j \int_{\mathbb{R}^{2n_B}} f(z_B) W^B \phi_j^B(z_B)dz_B$$
$$= \sum_j \langle \phi_j^B | \widehat{F} \phi_j^B \rangle$$
$$= \mathrm{Tr}(\widehat{F})$$

the last identity being just the algebraic definition of the trace of a positive semi-definite trace class operator [1, 3] in terms of an (arbitrary) orthonormal basis (ϕ_j^B). Taking (20), (19), and the definition of the function f into account, we get

$$\rho^A(z_A) = \int_{\mathbb{R}^{2n_B}} \rho(z_A, z_B)dz_B$$

which was to be proven.

4. Application to Gaussian states

A (centered) Gaussian quantum state has Wigner distribution

$$(21) \qquad \rho(z) = \frac{1}{(2\pi)^n \sqrt{\det \Sigma}} e^{-\frac{1}{2} z^T \Sigma^{-1} z}$$

where the covariance matrix Σ is symmetric positive definite and of dimension $2n \times 2n$ (we will write for short $\Sigma > 0$). The uncertainty principle imposes that, in addition, Σ must satisfies the condition [3, 10, 15]

$$\Sigma + \frac{i\hbar}{2} J \geq 0$$

where J is the standard symplectic matrix in the phase space splitting $z = (z_A, z_B)$, that is, $J = J_A \oplus J_B$ with

$$J_A = \begin{pmatrix} 0_{n_A \times n_A} & I_{n_A \times n_A} \\ -I_{n_A \times n_A} & I_{n_A \times n_A} \end{pmatrix} \ , \ J_B = \begin{pmatrix} 0_{n_B \times n_B} & I_{n_B \times n_B} \\ -I_{n_B \times n_B} & I_{n_B \times n_B} \end{pmatrix}.$$

The purity of the corresponding state $\widehat{\rho}$ is given by the formula ([3])

$$\mathrm{Tr}(\widehat{\rho}^2) = \left(\tfrac{\hbar}{2}\right)^n (\det \Sigma)^{-1/2}$$

and we have $\mathrm{Tr}(\widehat{\rho}^2) = 1$ (e.g.. $\widehat{\rho}$ is a pure state) if and only if $\Sigma = \frac{\hbar}{2} S^T S$ for some symplectic matrix S (i.e. $S^T J S = J$). We will write the covariance matrix as

$$(22) \qquad \Sigma = \begin{pmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{pmatrix} \text{ with } \Sigma_{BA} = \Sigma_{AB}^T$$

the blocks $\Sigma_{AA}, \Sigma_{AB}, \Sigma_{BA}, \Sigma_{BB}$ having dimensions $2n_A \times 2n_A$, $2n_A \times 2n_B$, $2n_B \times 2n_A$, $2n_B \times 2n_B$, respectively. A calculation involving Gaussian integrals [2, 6] shows that the partial trace $\widehat{\rho}^A$ is a Gaussian state with Wigner distribution

$$(23) \qquad \rho_A(z_A) = \frac{1}{(2\pi)^{n_A} \sqrt{\det \Sigma_{AA}}} e^{-\frac{1}{\hbar} z_A^T (\Sigma_{AA}^{-1}) z_A} \ .$$

This can easily be seen by reducing the problem to the case where the covariance matrix (22) is block diagonal

$$\begin{pmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{pmatrix} = \begin{pmatrix} H^T & 0 \\ 0 & K^T \end{pmatrix} \begin{pmatrix} \Sigma'_{AA} & 0 \\ 0 & \Sigma'_{BB} \end{pmatrix} \begin{pmatrix} H & 0 \\ 0 & K \end{pmatrix}$$

with $H \in O(2n_A)$, $K \in O(2n_B)$. In particular we have

$$\text{Tr}[(\widehat{\rho}^A)^2] = \left(\tfrac{\hbar}{2}\right)^n (\det \Sigma_{AA})^{-1/2}$$

hence $\widehat{\rho}_A$ is a pure state if and only if $\det \Sigma_{AA} = (\hbar/2)^{2n}$; this is the case if and only if $\Sigma_{AA} = \tfrac{\hbar}{2} S_A^T S_A$ where S_A is a symplectic matrix in $\mathbb{R}^{2n_A}$.

5. Purification

We recall the following: let $\widehat{\rho}^A \in \mathcal{L}_1(L^2(\mathbb{R}^{n_A}))$ be a density matrix of rank $r \leq \infty$. Then there exists a Hilbert space H_B with $\dim H_B = r$ and a pure state $|\psi\rangle$ such that $|\psi\rangle\langle\psi| \in \mathcal{L}_1(L^2(\mathbb{R}^{n_A}) \otimes H_B)$ and $\widehat{\rho}^A = \text{Tr}^B(|\psi\rangle\langle\psi|)$ (we assume throughout that $W\psi$ satisfies the conditions of Lemma 2). The state $|\psi\rangle\langle\psi|$, which is not uniquely defined, is called a *purification* of $\widehat{\rho}^A$. In what follows we assume that $\widehat{\rho}^A$ has maximal rank $r = \infty$ and we identify H_B with $L^2(\mathbb{R}^{n_B})$. The purification is constructed as follows: one starts with the spectral decomposition

$$\widehat{\rho}^A = \sum_j \lambda_j |\phi_j^A\rangle\langle\phi_j^A| \quad, \quad \sum_j \lambda_j = 1 \quad, \quad \lambda_j \geqq 0$$

and one then defines $\psi \in L^2(\mathbb{R}^{n_A}) \otimes L^2(\mathbb{R}^{n_B})$ by its Schmidt decomposition [12]

$$(24) \qquad \psi = \sum_j \sqrt{\lambda_j} \phi_j^A \otimes \phi_j^B \quad, \quad \sum_j \lambda_j = \langle\psi|\psi\rangle = 1 .$$

We have

$$(25) \qquad \widehat{\rho}^A = \text{Tr}^B(|\psi\rangle\langle\psi|) = \sum_j \lambda_j |\phi_j^A\rangle\langle\phi_j^A|$$

so, by Theorem 1, the Wigner distribution $\rho^A(z_A)$ of $\widehat{\rho}^A$ is

$$(26) \qquad \int_{\mathbb{R}^{2n_B}} W\psi(z_A, z_B) dz_B = \sum_j \lambda_j W^A \phi_j^A(z_A)$$

which is formula (4).

6. Concluding remarks

The main result of this work is the partial trace formula (3) in Theorem 1. While this formula is hardly surprising (and seems to be part of the "folklore" in physics), its proof is not trivial, and we have been unable to find a rigorous treatment thereof in the literature (mathematical or physical); mentions of this result can be found in [8, 13, 16], however no proof whatsoever is given in these references. This result is particularly important when one uses methods from harmonic analysis in phase space to study problems in quantum mechanics. From our point of view, this approach is more fruitful than abstract operator theory because it leads to quantities that can be explicitly calculated (either directly, or using numerical algorithms). Theorem 1 and its consequences (as shortly outlined in the rest of the article) could be instrumental in advancing the study of entanglement and entropy of partial states because it allows direct explicit calculations involving the Weyl expression of these partial states (in [2] we used formula (3) without proof to study the separability of Gaussian States).

There has been no data generated or analyzed in his work. Neither is there any conflict of interest.

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