Probability density functions of quantum mechanical observable uncertainties

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Abstract
We study the uncertainties of quantum mechanical observables, quantified by the standard deviation (square root of variance) in Haar-distributed random pure states. We derive analytically the probability density functions (PDFs) of the uncertainties of arbitrary qubit observables. Based on these PDFs, the uncertainty regions of the observables are characterized by the support of the PDFs. The state-independent uncertainty relations are then transformed into the optimization problems over uncertainty regions, which opens a new vista for studying state-independent uncertainty relations. Our results may be generalized to multiple observable cases in higher dimensional spaces.

Keywords: uncertainty of observable, probability density function, uncertainty region, state-independent uncertainty relation

(Some figures may appear in colour only in the online journal)

1. Introduction

The uncertainty principle rules out the possibility to obtain precise measurement outcomes simultaneously when one measures two incomparable observables at the same time. Since the uncertainty relation is satisfied by the position and momentum [1], various uncertainty relations have been extensively investigated [2–7]. On the occasion of celebrating the 125th anniversary of the academic journal ‘Science’, the magazine listed 125 challenging scientific problems [8]. The 21st problem asks: Do deeper principles underlie quantum uncertainty and nonlocality? As uncertainty relations play significant roles in entanglement detection [9–14] and quantum nonlocality [15], and many others, it is desirable to explore the mathematical structures and physical implications of uncertainties in more detail from various perspectives.

The state-dependent Robertson–Schrödinger uncertainty relation [16–19] is of the form:

\[(\Delta_{\rho} A)^2 (\Delta_{\rho} B)^2 \geq \frac{1}{4} \langle [A, B] \rangle_{\rho}^2\]

\(-\langle A \rangle_{\rho} \langle B \rangle_{\rho}^2 + \langle [A, B] \rangle_{\rho}^2,\)

where \([A, B] := AB + BA\), \([A, B] := AB - BA\), and \((\Delta_{\rho} X)^2 \equiv \text{Tr}(X^2 \rho) - \text{Tr}(X \rho)^2\) is the variance of \(X\) with respect to the state \(\rho\), \(X = A, B\).

Recently, state-independent uncertainty relations have been investigated [10, 12], which have direct applications to entanglement detection. In order to get state-independent uncertainty relations, one considers the sum of the variances and solves the following optimization problems:

\[\text{Var}_{\rho}(A) + \text{Var}_{\rho}(B) \geq \min_{\rho \in \mathcal{D}(C^2)} (\text{Var}_{\rho}(A) + \text{Var}_{\rho}(B)),\]

\[(\Delta_{\rho} A + \Delta_{\rho} B)^2 \geq \min_{\rho \in \mathcal{D}(C^2)} (\Delta_{\rho} A + \Delta_{\rho} B),\]

where \(\text{Var}_{\rho}(X) = (\Delta_{\rho} X)^2\) is the variance of the observable \(X\) associated with state \(\rho \in \mathcal{D}(C^2)\).

Efforts have been devoted to providing quantitative uncertainty bounds for the above inequalities [20]. However, searching for such uncertainty bounds may not be the best way to get new uncertainty relations [21]. Recently, Busch and Reardon-Smith proposed to consider the uncertainty region [20] of two observables \(A\) and \(B\), instead of finding the bounds based on some particular choice of uncertainty functional, typically such as the product or sum of uncertainties [22]. Once we can identify what the structures of
uncertainty regions are, we can infer specific information about the state with minimal uncertainty in some sense. In view of this, the above two optimization problems (1) and (2) become

$$\min_{\rho \in \mathcal{D}(\mathbb{C}^d)} \{ \text{Var}_\rho(A) + \text{Var}_\rho(B) \}$$

$$= \min \{ x^2 + y^2 : (x, y) \in \mathcal{U}^{(m)}_{\Delta_A, \Delta_B} \},$$

$$\min_{\rho \in \mathcal{D}(\mathbb{C}^d)} \{ \Delta_\rho A + \Delta_\rho B \}$$

$$= \min \{ x + y : (x, y) \in \mathcal{U}^{(m)}_{\Delta_A, \Delta_B} \},$$

where $\mathcal{U}^{(m)}_{\Delta_A, \Delta_B}$ is the so-called uncertainty region of two observables $A$ and $B$ defined by

$$\mathcal{U}^{(m)}_{\Delta_A, \Delta_B} = \{ (\Delta_\rho A, \Delta_\rho B) \in \mathbb{R}_+^2 : \rho \in \mathcal{D}(\mathbb{C}^d) \}.$$  

Random matrix theory or probability theory are powerful tools in quantum information theory. Recently, the non-additivity of quantum channel capacity [23] has been cracked via probabilistic tools. The Duistermaat–Heckman measure on moment polytope has been used to derive the probability distribution density of one-body quantum marginal states of multipartite random quantum states [24, 25] and that of classical probability mixture of random quantum states [26, 27]. As a function of random quantum pure states, the probability density function (PDF) of the quantum expectation value of an observable is also analytical calculated [28]. Motivated by these works, we investigate the joint PDFs of uncertainties of observables. By doing so, we find that it is not necessarily to solve directly the uncertainty regions of observables. It is sufficient to identify the support of such PDF because PDF vanishes exactly beyond the uncertainty regions. Thus all the problems are reduced to compute the PDF of uncertainties of observables since all information concerning uncertainty regions and state-independent uncertainty relations are encoded in such PDFs. In [29] we have studied such PDFs for the random mixed quantum state ensembles, where all problems concerning qubit observables are completely solved, i.e. analytical formulae of the PDFs of uncertainties are obtained, and the characterization of uncertainty regions over which the optimization problems for state-independent lower bound of the sum of variances is presented. In this paper, we will focus on the same problem for random pure quantum state ensembles.

Let $\delta(x)$ be delta function [30] defined by

$$\delta(x) = \begin{cases} +\infty, & \text{if } x = 0; \\ 0, & \text{if } x = 0. \end{cases}$$

One has $\langle \delta, f \rangle := \int_{\mathbb{R}} f(x) \delta(x) \, dx = f(0)$. Denote by $\delta_a(x) := \delta(x - a)$. Then $\langle \delta_a, f \rangle = f(a)$. Let $Z(g) := \{ x \in D(g) : g(x) = 0 \}$ be the zero set of function $g(x)$ with its domain $D(g)$. We will use the following definition.

**Definition 1.** [31, 32]

If $g : \mathbb{R} \to \mathbb{R}$ is a smooth function (the first derivative $g'$ is a continuous function) such that $Z(\gamma) \cap Z(\gamma') = \emptyset$, then the composite $\delta g$ is defined by:

$$\delta(g(x)) = \sum_{x \in Z(g)} \frac{1}{|g'(x)|} \delta_x.$$  

2. Uncertainty regions of observables

We can extend the notion of the uncertainty region of two observables $A$ and $B$, put forward in [20], into that of multiple observables.

**Definition 2.** Let $(A_1, \ldots, A_n)$ be an $n$-tuple of qubit observables acting on $\mathbb{C}^d$. The uncertainty region of such $n$-tuple $(A_1, \ldots, A_n)$, for the mixed quantum state ensemble, is defined by

$$\mathcal{U}^{(n)}_{\Delta A_1, \ldots, \Delta A_n} := \{ (\Delta_\rho A_1, \ldots, \Delta_\rho A_n) \in \mathbb{R}_+^n : \rho \in \mathcal{D}(\mathbb{C}^d) \}.$$  

Similarly, the uncertainty region of such $n$-tuple $(A_1, \ldots, A_n)$, for the pure quantum state ensemble, is defined by

$$\mathcal{U}^{(n)}_{\Delta A_1, \ldots, \Delta A_n} := \{ (\Delta_\rho A_1, \ldots, \Delta_\rho A_n) \in \mathbb{R}_+^n : |\psi \rangle \in \mathbb{C}^d \}.$$  

Apparently, $\mathcal{U}^{(n)}_{\Delta A_1, \ldots, \Delta A_n} \subset \mathcal{U}^{(m)}_{\Delta A_1, \ldots, \Delta A_m}.$

Note that our definition of the uncertainty region is different from the one given in [2]. In the above definition, we use the standard deviation instead of variance.

Next, we will show that $\mathcal{U}^{(m)}_{\Delta A_1, \ldots, \Delta A_m}$ is contained in the supercube in $\mathbb{R}_+^m$. To this end, we study the following sets $\mathcal{P}(A) = \{ \text{Var}_\rho(A) : |\psi \rangle \in \mathbb{C}^d \}$ and $\mathcal{M}(A) = \{ \text{Var}_\rho(A) : \rho \in \mathcal{D}(\mathbb{C}^d) \}$ for a qudit observable $A$ acting on $\mathbb{C}^d$. The relationship between both sets $\mathcal{P}(A)$ and $\mathcal{M}(A)$ is summarized in the following proposition.

**Proposition 1.** It holds that

$$\mathcal{P}(A) = \mathcal{M}(A) = \text{conv}(\mathcal{P}(A))$$

is a closed interval $[0, \text{max}_\psi \text{Var}_\rho(A)]$.

**Proof.** Note that $\mathcal{P}(A) \subset \mathcal{M}(A) \subset \text{conv}(\mathcal{P}(A))$. Here the first inclusion is apparent; the second inclusion follows immediately from the result obtained in [33]: for any density matrix $\rho \in \mathcal{D}(\mathbb{C}^d)$ and a qudit observable $A$, there is a pure state ensemble decomposition $\rho = \sum_j p_j |\psi_j \rangle \langle \psi_j |$ such that

$$\text{Var}_\rho(A) = \sum_j p_j \text{Var}_\rho(A_j).$$

Since all pure states on $\mathbb{C}^d$ can be generated via a fixed $\psi_0$ and the whole unitary group $U(d)$, it follows that

$$\mathcal{P}(A) = \text{im}(\Phi),$$

where the mapping $\Phi : U(d) \to \mathcal{P}(A)$ is defined by $\Phi(U) = \text{Var}_{\psi_0}(A)$. This mapping $\Phi$ is surjective and continuous. Due to the fact that $U(d)$ is a compact Lie group,
we see that \( \Phi \) can attain maximal and minimal values over the unitary group \( U(d) \). In fact, \( \min_{U(d)} \Phi = 0 \). This can be seen if we take some \( U \) such that \( U|\psi_k\rangle = \Phi(U|\psi_k\rangle) = \Phi(k) \). Since \( U(d) \) is also connected, then \( \im(\Phi) = \Phi(U(d)) \) is also connected, thus \( \im(\Phi) = [0, \max_{U(d)} \Phi] \). This amounts to saying that \( \mathcal{P}(A) \) is a closed interval \([0, \max_{U(d)} \Phi]\) which means that \( \mathcal{P}(A) \) is a compact and convex set, i.e.
\[
\mathcal{P}(A) = \text{conv}(\mathcal{P}(A)).
\]
Therefore
\[
\mathcal{P}(A) = \mathcal{M}(A) = \text{conv}(\mathcal{P}(A)) = [0, \max \Phi_{U(d)}] = [0, \max \text{Var}_p(A)].
\]
This completes the proof. \( \square \)

Next, we determine \( \max_{p \in \mathcal{D}(C^d)} \text{Var}_p(A) \) for an observable \( A \). To this end, we recall the following \((d-1)\)-dimensional probability simplex, which is defined by
\[
\Delta_{d-1} := \{ p = (p_1, \ldots, p_d) \in \mathbb{R}^d : p_k \geq 0, \forall k \in [d], \sum_{j=1}^d p_j = 1 \}.
\]
The interior of \( \Delta_{d-1} \) is denoted by \( \Delta_{d-1}^\circ := \{ p = (p_1, \ldots, p_d) \in \mathbb{R}^d : p_k > 0, \forall k \in [d], \sum_{j=1}^d p_j = 1 \} \).

This indicates that a point \( x \) in the boundary \( \partial \Delta_{d-1} \) means that there must be at least a component \( x_i = 0 \) for some \( i \in [d] \), where \([d] := \{1, 2, \ldots, d\} \). Now we separate the boundary of \( \partial \Delta_{d-1} \) into the union of the following subsets:
\[
\partial \Delta_{d-1} = \bigcup_{j=1}^d F_j,
\]
where \( F_j := \{ x \in \partial \Delta_{d-1} : x_j = 0 \} \). Although the following result is known in 1935 [34], we still include our proof for completeness.

**Proposition 2.** Assume that \( A \) is an observable acting on \( C^d \).

Denote the vector consisting of eigenvalues of \( A \) by \( \lambda(A) \) with components being \( \lambda_1(A) \leq \cdots \leq \lambda_d(A) \). It holds that
\[
\max \{ \text{Var}_p(A) : p \in \mathcal{D}(C^d) \} = \frac{1}{4} (\lambda_{\text{max}}(A) - \lambda_{\text{min}}(A))^2.
\]
Here \( \lambda_{\text{min}}(A) = \lambda_1(A) \) and \( \lambda_{\text{max}}(A) = \lambda_d(A) \).

**Proof.** Assume that \( a := \lambda(A) \) where \( a_j := \lambda_j(A) \). Note that \( \text{Var}_p(A) = \text{Tr}(A^2 p) - \text{Tr}(A p)^2 = (a_i^2 D_U \lambda(p)) - (a_i D_U \lambda(p))^2 \), where \( a = (a_1, \ldots, a_d)^\top \), \( a_i^2 = (a_i^2, \ldots, a_i^2)^\top \), and \( D_U = U \sigma U \) (here \( \sigma \) stands for Schur product, i.e. entrywise product), and \( \lambda(p) = (\lambda_1(p), \ldots, \lambda_d(p))^\top \). Denote \( x := D_U \lambda(p) \in \Delta_{d-1} := \{ p = (p_1, \ldots, p_d) \in \mathbb{R}^d : \sum_{j=1}^d p_j = 1 \} \).

the \((d-1)\)-dimensional probability simplex. Then
\[
\text{Var}_p(A) = \langle a, x \rangle - \langle a, x \rangle^2 = \sum_{j=1}^d a_j^2 x_j - \left( \sum_{j=1}^d a_j x_j \right)^2 = \left( \sum_{j=1}^d a_j x_j \right)^2 = f(x).
\]

(i) If \( d = 2 \),
\[
f(x_1, x_2) = a_1^2 x_1 + a_2^2 x_2 - (a_1 x_1 + a_2 x_2)^2 = a_1^2 x_1 + a_2^2 (1 - x_1) - (a_1 x_1 + a_2 (1 - x_2))^2 = (a_2 - a_1)^2 \left[ \frac{1}{4} - \left( x_1 - \frac{1}{2} \right)^2 \right] \leq \frac{1}{4} (a_2 - a_1)^2,
\]

implying that \( f_{\text{max}} = \frac{1}{2} (a_2 - a_1)^2 \) when \( x_1 = x_2 = \frac{1}{2} \).

(ii) If \( d \geq 3 \), without loss of generality, we assume that \( a_1 < a_2 < \cdots < a_d \), we will show that the function \( f \) takes its maximal value on the point \( x_1, x_2, \ldots, x_{d-1}, x_d = (\frac{1}{2}, 0, \ldots, 0, \frac{1}{2}) \), with the maximal value being \( \frac{1}{4} (a_d - a_1)^2 = \frac{1}{4} (\lambda_{\text{max}}(A) - \lambda_{\text{min}}(A))^2 \). Then, using the Lagrangian multiplier method, we let
\[
L(x_1, x_2, \ldots, x_d, \lambda) = \sum_{i=1}^d a_i^2 x_i - \sum_{i=1}^d a_i x_i + \lambda \left( \sum_{i=1}^d x_i - 1 \right).
\]

Thus
\[
\frac{\partial L}{\partial x_i} = a_i^2 - 2a_i \sum_{i=1}^d a_i x_i + \lambda, \quad (i = 1, \ldots, d),
\]
\[
\frac{\partial L}{\partial \lambda} = \sum_{i=1}^d x_i - 1 = 0.
\]

Denote \( m := \sum_{i=1}^d a_i x_i \). Because (4) holds for all \( i = 1, \ldots, d \), we see that
\[
\lambda = -a_2 + 2a_1 m - a_1^2 + 2a_1 m,
\]
that is, \( m = a_2 + a_1 \) and \( \lambda = a_1 a_2 \) for all distinct indices \( i \) and \( j \). Furthermore, for all distinct indices \( i \) and \( j \), the system of equations \( \sum_{i=1}^d a_i x_i = m = a_2 + a_1 \) have no solution on \( \Delta_{d-1} \). Hence there is no stationary point on \( \Delta_{d-1} \), and thus \( f_{\text{max}} \) is obtained on the boundary \( \partial \Delta_{d-1} \) of \( \Delta_{d-1} \). Suppose, by induction, that the conclusion holds for the case where \( d = k \geq 2 \), i.e. the function \( f \) takes its maximal value
Proposition 3. Let \((A_1, \ldots, A_n)\) be an \(n\)-tuple of qudit observables acting on \(\mathbb{C}^d\). Denote \(v(A_k) := \frac{1}{2} (\lambda_{\max}(A_k) - \lambda_{\min}(A_k))\), where \(k = 1, \ldots, n\) and \(\lambda_{\max}, \lambda_{\min}(A_k)\) stands for the maximal/minimal eigenvalue of \(A_k\). Then
\[
U^{(\min)}_{\Delta A_1, \ldots, \Delta A_n} \subset [0, v(A_1)] \times \cdots \times [0, v(A_n)].
\]

Proof. The proof is easily obtained by combining proposition 1 and proposition 2. □

3. PDFs of expectation values and uncertainties of qudit observables

Assume \(A\) is a non-degenerate positive matrix with eigenvalues \(\lambda_1(A) < \cdots < \lambda_d(A)\), denoted by \(\lambda(A) = (\lambda_1(A), \ldots, \lambda_d(A))\). In view of the specialty of pure state ensemble and noting propositions 1 and 2, we will consider only the variances of observable \(A\) over pure states. In fact, the same problem is also considered very recently for mixed states [29]. Then the PDF of \((A|\psi) := \langle \psi|A|\psi\rangle\) is defined by
\[
f^{(d)}_{\langle A|}(r) := \int \delta(r - \langle A|_\psi) d\mu(\psi).
\]
Here \(d\mu(\psi)\) is the so-called uniform probability measure, which is invariant under the unitary rotations, and can be realized in the following way:
\[
d\mu(\psi) = \frac{\Gamma(d)}{2\pi^d} \delta(1 - \|\psi\|)[d\psi],
\]
where \([d\psi] = \prod_{i=1}^{d} dx_i dy_i\) for \(\psi_i = x_i + iy_i(k = 1, \ldots, d)\), and \(\Gamma(\cdot)\) is the Gamma function. Thus
\[
f^{(d)}_{\langle A|}(r) = \Gamma(d) \int_{\mathbb{R}^d} \delta(r - \sum_{i=1}^{d} \lambda_i(A) r_i) \delta \times \left(1 - \sum_{i=1}^{d} r_i\right)^d \prod_{i=1}^{d} dr_i.
\]

For completeness, we will give a different proof of it although the following result is already obtained in [28]:

Proposition 4. For a given quantum observable \(A\) with simple spectrum \(\lambda(A) = (\lambda_1(A), \ldots, \lambda_d(A))\), where \(\lambda_1(A) < \cdots < \lambda_d(A)\), the PDF of \(\langle A|\psi\rangle\), where \(\psi\) a Haar-distributed random pure state on \(\mathbb{C}^d\), is given by the following:
\[
f^{(d)}_{\langle A|}(r) = (-1)^{d-i}(d - 1) \times \sum_{i=1}^{d} \prod_{j \neq i} (\lambda_i(A) - \lambda_j(A)) H(r - \lambda_i(A)),
\]
where \(i := \{1, 2, \ldots, d\}\) \(\backslash\{i\}\) and \(H\) is the so-called Heaviside function, defined by \(H(t) = 1\) if \(t > 0\), 0 otherwise. Thus the support of \(f^{(d)}_{\langle A|}(r)\) is the closed interval \([\lambda_1(A), \lambda_d(A)]\). In particular, for \(d = 2\), we have
\[
f^{(2)}_{\langle A|}(r) = \frac{1}{\lambda_2(A) - \lambda_1(A)} H(r - \lambda_1(A)) - H(r - \lambda_2(A)).
\]
Still by performing Laplace transformation \((t \to x)\) of \(F_t(t)\):
\[
\mathcal{L}(F_t)(x) = \Gamma(d) \int \exp \left( -x \sum_{i=1}^{d} \lambda_i(A) r_i \right) \times \exp \left( -x \sum_{i=1}^{d} r_i \right)^d \prod_{i=1}^{d} dr_i \\
= \Gamma(d) \prod_{i=1}^{d} \exp \left( -x \lambda_i(A) \right) + x \prod_{i=1}^{d} \exp \left( -x r_i \right)^d \\
= \Gamma(d) \prod_{i=1}^{d} \exp \left( -x (\lambda_i(A) - \lambda_j(A)) \right),
\]

implying that [35]
\[
F_t(t) = \Gamma(d) \sum_{i=1}^{d} \exp(-\lambda_i(A) \cdot t) \prod_{j \neq i} (\lambda_j(A) - \lambda_i(A)),
\]

where \(i \in \{1, \ldots, d\} \setminus \{i\}\). Thus
\[
\mathcal{L}(F_t^{(d)}(s)) = F_t(1)
\]
\[
= \Gamma(d) \sum_{i=1}^{d} \exp(-\lambda_i(A) \cdot s) \prod_{j \neq i} (\lambda_j(A) - \lambda_i(A)).
\]

Therefore, we get that
\[
f^{(d)}_A(r) = (-1)^{d-1}(d - 1) \times \prod_{i=1}^{d} H(r - \lambda_i(A))(r - \lambda_j(A))^{d-2} \prod_{j \neq i} (\lambda_j(A) - \lambda_i(A)),
\]
where \(H(r - \lambda_i(A))\) is the so-called Heaviside function, defined by \(H(t) = 1\) if \(t > 0\); otherwise \(0\). The support of this pdf is the closed interval \([l, u]\) where
\[
l = \min\{\lambda_i(A) : i = 1, \ldots, d\},
\]
\[
u = \max\{\lambda_i(A) : i = 1, \ldots, d\}.
\]

The normalization of \(f^{(d)}_A(r)\) (i.e. \(\int f^{(d)}_A(r) dr = 1\)) can be checked by assuming \(\lambda_1 < \lambda_2 < \cdots < \lambda_d\), then \([l, u] = [\lambda_1, \lambda_d]\) since \(f^{(d)}_A(r)\) is a symmetric of \(\lambda_i\)'s.

### 3.1. The case for one qubit observable

Let us now turn to the qubit observables. Any qubit observable \(A\), which may be parameterized as
\[
A = a_0 1 + a \cdot \sigma, \quad (a_0, a) \in \mathbb{R}^3,
\]
where \(1\) is the identity matrix on the qubit Hilbert space \(\mathbb{C}^2\), and \(\sigma = (\sigma_1, \sigma_2, \sigma_3)\) is the vector of the standard Pauli matrices:
\[
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

Without loss of generality, we assume that our qubit observables are of simple eigenvalues, otherwise the problem is trivial. Thus the two eigenvalues of \(A\) are
\[
\lambda_k(A) = a_0 + (-1)^k a, \quad k = 1, 2,
\]
with \(a := |a| = \sqrt{a_1^2 + a_2^2 + a_3^2} > 0\) being the length of vector \(a = (a_1, a_2, a_3) \in \mathbb{R}^3\). Thus (5) becomes
\[
f^{(2)}_A(r) = \frac{1}{\lambda_2(A) - \lambda_1(A)} \times [H(r - \lambda_1(A)) - H(r - \lambda_2(A))].
\]

**Theorem 1.** For the qubit observable \(A\) defined by equation (6), the PDF of \(\Delta_\psi A\), where \(\psi\) is a Haar-distributed random pure state on \(\mathbb{C}^2\), is given by
\[
f^{(2)}_\Delta A(x) = \frac{x}{|a| \sqrt{|a|^2 - x^2}}, \quad x \in [0, |a|).
\]

**Proof.** Note that
\[
\delta(r^2 - r_0^2) = \frac{1}{2|r_0|}(\delta(r - r_0) + \delta(r + r_0)).
\]

For \(x \geq 0\), because
\[
\delta(x^2 - \Delta_\psi A^2) = \frac{1}{2x}[\delta(x + \Delta_\psi A) + \delta(x - \Delta_\psi A)] = \frac{1}{2x} \delta(x - \Delta_\psi A),
\]
we see that
\[
f^{(2)}_\Delta A(x) = \int \delta(x - \Delta_\psi A) d\mu(\psi) = 2x \int \delta(x^2 - \Delta^2_\psi A) d\mu(\psi).
\]

For any complex \(2 \times 2\) matrix \(A\), \(A^2 = \text{Tr}(A)A - \text{det}(A)1\).

Then \(\Delta^2_\psi A = (\psi - \lambda_1(A))((\lambda_2(A) - \lambda_1(A))\psi - \lambda_1(A))\)
\[
\delta(x^2 - \Delta^2_\psi A) = \delta(x^2 - (\psi - \lambda_1(A))(\lambda_2(A) - \lambda_1(A)))
\]
\[
\times (\lambda_2(A) - \lambda_1(A)) d\mu(\psi).
\]

In particular, we see that
\[
f^{(2)}_\Delta A(x) = 2x \int_{\lambda_1(A)}^{\lambda_2(A)} d\mu(\psi)
\times \delta(x^2 - (\psi - \lambda_1(A))(\lambda_2(A) - \lambda_1(A)))
\times \delta(x^2 - (\psi - \lambda_1(A))(\lambda_2(A) - r))\iint_{\lambda_2(A) - \lambda_1(A)}.
\]

Denote \(f_r(r) = x^2 - (r - \lambda_1(A))(\lambda_2(A) - r)\). Thus
\[
\delta f_r(r) = 2r - \lambda_1(A) - \lambda_2(A).\]

Then \(f_r(r) = 0\) has two distinct roots in \([\lambda_1(A), \lambda_2(A)]\) if and only if \(x \in \left[0, \frac{\sqrt{V_2(\lambda(A))}}{2}\right]\), where \(V_2(\lambda(A)) = \lambda_2(A) - \lambda_1(A)\). Now the roots are given by
\[
r_{\pm}(x) = \frac{\lambda_1(A) + \lambda_2(A) \pm \sqrt{V_2(\lambda(A))^2 - 4x^2}}{2}.
\]
Thus
\[ \delta(f_x(r)) = \frac{1}{|\partial_{r=x}f_x(r)|} \delta_{r=x} + \frac{1}{|\partial_{r=x}f_x(r)|} \delta_{r=x}, \]
implying that
\[ f_{\Delta x}^2(x) = \frac{4\pi}{V_2(\lambda(A)) \sqrt{V_2(\lambda(A))^2 - 4\pi^2}}. \]
Now for \( A = a_0 I + a \cdot \sigma \), we have \( V_2(\lambda(A)) = 2|a| \).
Substituting this into the above expression, we get the desired result:
\[ f_{\Delta x}^2(x) = \frac{x}{|a| \sqrt{|a|^2 - x^2}}, \]
where \( x \in [0, |a|] \). This is the desired result. \( \square \)

### 3.2. The case for two-qubit observables

Let \( A = a_0 + a \cdot \sigma \) and \( B = b_0 + b \cdot \sigma \)
\[ f_{\Delta A, \Delta B}^2(r, s) = \int \delta(r - \langle \psi | A | \psi \rangle) \delta(s - \langle \psi | B | \psi \rangle) \mu(\psi) \]
\[ \times \int \exp(-i\langle \psi | (\alpha A + \beta B) | \psi \rangle) \mu(\psi), \]
where
\[ \int \exp(-i\langle \psi | (\alpha A + \beta B) | \psi \rangle) \mu(\psi) \]
\[ = \int_{\lambda = (\alpha A + \beta B)} \exp(-ir)f_2(t) dt \]
\[ = \frac{1}{2|\alpha A + \beta B|^2} \int_{\lambda = (\alpha A + \beta B)} \exp(-it) dt \]
\[ = \exp(-i(a_0 \alpha + b_0 \beta)) \sin |\alpha A + \beta B| \]
for
\[ \lambda = (\alpha A + \beta B) = \alpha a_0 + \beta b_0 \pm |\alpha A + \beta B|. \]

Now that
\[ f_{\Delta A, \Delta B}^2(r) = \frac{1}{\lambda_2 - \lambda_1} (H(r - \lambda_1) - H(r - \lambda_2)), \]
therefore
\[ f_{\Delta A, \Delta B}^2(r, s) = \frac{1}{(2\pi)^2} \int_{\beta} \sin |\alpha A + \beta B|, \]
(i) If \([a, b]\) is linearly independent, then the following matrix \( T_{a, b} \) is invertible, and thus
\[ \left( \begin{array}{c} \alpha \\ \beta \end{array} \right) = T_{a, b}^{-1} \left( \begin{array}{c} \alpha' \\ \beta' \end{array} \right), \]
where \( T_{a, b} = \left( \begin{array}{cc} \langle a, a \rangle & \langle a, b \rangle \\ \langle b, a \rangle & \langle b, b \rangle \end{array} \right) \).

Thus we see that
\[ f_{\Delta A, \Delta B}^2(r, s) = \frac{1}{(2\pi)^2} \frac{1}{\det(T_{a, b})} \int_{\beta} \sin |\alpha A + \beta B|, \]
\[ \times \exp(i(r - a_0)\alpha + (s - b_0)\beta) \sin \sqrt{\alpha + \beta} \]
\[ = \frac{1}{(2\pi)^2} \frac{1}{\det(T_{a, b})} \int_0^{2\pi} dt \sin t \int_0^{2\pi} d\theta \]
\[ \times \exp(i(r - a_0)\alpha + (s - b_0)\beta) \sin \sqrt{\alpha + \beta} \]
\[ \times (r - a_0)^2 + (s - b_0)^2, \]
where \( J_0(z) \) is the so-called Bessel function of the first kind, defined by
\[ J_0(z) = \frac{1}{\pi} \int_0^\pi \cos(c \cos \theta) d\theta. \]

Therefore
\[ f_{\Delta A, \Delta B}^2(r, s) = \frac{1}{2\pi} \frac{1}{\det(T_{a, b})} \int_0^{2\pi} dt \sin t J_0 \]
\[ \times \left( t \cdot \sqrt{(r - a_0, s - b_0)T_{a, b}^{-1}(r - a_0, s - b_0)} \right), \]
where
\[ \int_0^\infty J_0(\lambda t) \sin(t) dt = \frac{1}{\sqrt{1 - \lambda^2}} H(1 - |\lambda|). \]

Therefore
\[ f_{\Delta A, \Delta B}^2(r, s) = \frac{H(1 - \omega_{A, B}(r, s))}{2\pi \det(T_{a, b})(1 - \omega_{A, B}(r, s))}, \]
where
\[ \omega_{A, B}(r, s) = \sqrt{(r - a_0, s - b_0)T_{a, b}^{-1}(r - a_0, s - b_0)}. \]
Thus
\[ f_{A,B}^{(2)}(r,s) = \frac{(1 - \omega_{A,B}(r,s))}{\sqrt{\text{det}(T_{a,b})(1 - \omega_{A,B}(r,s))}} \]

Proposition 5. For a pair of qubit observables \( A = a_0 1 + a \cdot \sigma \) and \( B = b_0 1 + b \cdot \sigma \), (i) if \( \{a, b\} \) is linearly independent, then the pdf of \((A)_{\psi}, (B)_{\psi}\), where \( \psi \in \mathbb{C}^2 \) is a Haar-distributed pure state, is given by
\[ f_{(A), (B)}^{(2)}(r,s) = \frac{H(1 - \omega_{A,B}(r,s))}{2\pi \sqrt{\text{det}(T_{a,b})(1 - \omega_{A,B}(r,s))}} \]

(ii) If \( \{a, b\} \) is linearly dependent, without loss of generality, let \( b = \kappa \cdot a \), then
\[ f_{(A), (B)}^{(2)}(r,s) = \delta((s - b_0) - \kappa(r - a_0))f_{(A)}^{(2)}(r) \]

From proposition 5, we can directly infer the results obtained in [36, 37].

We now turn to a pair of qubit observables
\[ A = a_0 1 + a \cdot \sigma, \quad B = b_0 1 + b \cdot \sigma, \quad (a_0, a), (b_0, b) \in \mathbb{R}^4 \]

whose uncertainty region
\[ \mathcal{U}_{A,B} := \{(\Delta_A, \Delta_B) \in \mathbb{R}^2 : |\psi\rangle \in \mathbb{C}^2\} \]

was proposed by Busch and Reardon-Smith [20] in the mixed state case. We consider the probability distribution density
\[ f_{(A), (B)}^{(2)}(x, y) = \int \delta(x - \Delta_A)\delta(y - \Delta_B)d\mu(\psi), \]
on the uncertainty region defined by equation (10). Denote
\[ T_{A,B} := \begin{pmatrix} (a, a) & (a, b) \\ (b, a) & (b, b) \end{pmatrix} \]

Theorem 2. The joint probability distribution density of the uncertainties \((\Delta_A, \Delta_B)\) for a pair of qubit observables defined by equation (9), where \( \psi \) is a Haar-distributed random pure state on \( \mathbb{C}^2 \), is given by
\[ f_{(A), (B)}^{(2)}(x, y) = \frac{2xy \sum_{x \in \{0,1\}} f_{(A), (B)}^{(2)}(r_x(x), s_y(y))}{\sqrt{(a^2 - x^2)(b^2 - y^2)}} \]

where \( a = |a| > 0, b = |b| > 0, \quad r_x(x) = a_0 \pm \sqrt{a^2 - x^2}, \quad s_y(y) = b_0 \pm \sqrt{b^2 - y^2}. \)

Proof. Note that in the proof of theorem 1, we have already obtained that
\[ \delta(x^2 - \Delta_A^2) = \delta(x^2 - (r - \lambda_A)) \]
\[ \times \delta(\lambda_A(r) - r) = \delta(f_x(r)), \]
where \( f_x(r) := x^2 - (r - \lambda_A)(\lambda_A(r) - r). \) Similarly,
\[ \delta(y^2 - \Delta_B^2) = \delta(g_y(s)), \]
where \( g_y(s) := y^2 - (s - \lambda_B)(\lambda_B(s) - s). \)

Again, by using (7), we get that
\[ f_{(A), (B)}^{(2)}(x, y) = 4xy \int \delta(x^2 - \Delta_A^2)\delta(y^2 - \Delta_B^2)d\mu(\psi) \]
\[ = 4xy \int dxdy f_{(A), (B)}^{(2)}(r, s) \delta(f_x(r))\delta(g_y(s)), \]
where \( f_{(A), (B)}^{(2)}(r, s) \) is determined by proposition 5. Hence
\[ \delta(f_x(r)) = \frac{1}{|\partial_{r,x}f_x(r)|} \delta_{r,x} + \frac{1}{|\partial_{r,s}f_x(r)|} \delta_{r,s}, \]
\[ \delta(g_y(s)) = \frac{1}{|\partial_{s,x}g_y(s)|} \delta_{s,x} + \frac{1}{|\partial_{s,y}g_y(s)|} \delta_{s,y} \]

From the above, we have already known that
\[ \delta(f_x(r))\delta(g_y(s)) \]
\[ = \frac{\delta_{r,s} + \delta_{r,x} + \delta_{r,s,x} + \delta_{r,x,y}}{4\sqrt{(a^2 - x^2)(b^2 - y^2)}}. \]

Based on this observation, we get that
\[ f_{(A), (B)}^{(2)}(x, y) = \frac{xy}{\sqrt{(a^2 - x^2)(b^2 - y^2)}} \times \sum_{i,j \in \{0,1\}} f_{(A), (B)}^{(2)}(r_i(x), s_j(y)). \]
It is easily checked that $\omega_{A,B}(\cdot, \cdot)$, defined in (8), satisfies that
\[
\omega_{A,B}(r(x), s(y)) = \omega_{A,B}(r(x), s(y)),
\]
\[
\omega_{A,B}(r(x), s(y)) = \omega_{A,B}(r(x), s(y)).
\]
These lead to the fact that
\[
\sum_{i,j \in \{\pm\}} f_{A,B}^{(2)}(r_i(x), s_j(y)) = 2
\]
\[
\times \sum_{j \in \{\pm\}} f_{A,B}^{(2)}(r_j(x), s_j(y)).
\]
Therefore
\[
f_{A,B}^{(2)}(x, y) = \frac{2\chi \sum_{j \in \{\pm\}} f_{A,B}^{(2)}(r_j(x), s_j(y))}{\sqrt{(a^2 - x^2)(b^2 - y^2)}}.
\]
We get the desired result.

### 3.3. The case for three-qubit observables

We now turn to the case where there are three-qubit observables
\[
A = a_01 + a \cdot \sigma, \quad B = b_01 + b \cdot \sigma, \quad C = c_01 + c \cdot \sigma
\]
whose uncertainty region
\[
U_{A,B,C} := \{(\Delta_x A, \Delta_x B, \Delta_x C) \in \mathbb{R}_+^3 : |\psi\rangle \in C^2\}. \quad (12)
\]
We define the probability distribution density
\[
f_{A,B,C}^{(2)}(x, y, z) = \int \delta(x - \Delta_x A)\delta(y - \Delta_x B)\delta(z - \Delta_x C)d\mu(\psi),
\]
on the uncertainty region defined by equation (12). Denote
\[
T_{a,b,c} := \begin{pmatrix} (a, a) & \langle a, b \rangle & \langle a, c \rangle \\ (b, a) & \langle b, b \rangle & \langle b, c \rangle \\ (c, a) & \langle c, b \rangle & \langle c, c \rangle \end{pmatrix}.
\]
Again note that $T_{a,b,c}$ is also a semidefinite positive matrix. We find that rank($T_{a,b,c}$) ≤ 3. There are three cases that would be possible: rank($T_{a,b,c}$) = 1, 2, 3. Thus $T_{a,b,c}$ is invertible (i.e. rank($T_{a,b,c}$) = 3) if and only if $\{a, b, c\}$ linearly independent. In such case, we write
\[
\omega_{A,B,C}(r, s, t) := \sqrt{(r - a_0, s - b_0, t - c_0)^T T_{a,b,c} (r - a_0, s - b_0, t - c_0)}. \quad (13)
\]
In order to calculate $f_{A,B,C}^{(2)}$, essentially we need to derive the joint probability distribution density of $(|A\rangle_\psi, |B\rangle_\psi, |C\rangle_\psi)$, which is defined by
\[
f_{A,B,C}^{(2)}(r, s, t) := \int \delta(r - |A\rangle_\psi)\delta(s - |B\rangle_\psi)\delta(t - |C\rangle_\psi)d\mu(\psi).
\]
We have the following result:

**Proposition 6.** For three-qubit observables, given by equation (11), (i) if rank($T_{a,b,c}$) = 3, i.e. $\{a, b, c\}$ is linearly independent, then the joint probability distribution density of $(|A\rangle_\psi, |B\rangle_\psi, |C\rangle_\psi)$, where $\psi$ is a Haar-distributed random pure state on $C^2$, is given by the following:
\[
f_{A,B,C}^{(2)}(r, s, t) = \frac{1}{4\pi \sqrt{\det(T_{a,b,c})}} \delta(1 - \omega_{A,B,C}(r, s, t)). \quad (13)
\]
(ii) If rank($T_{a,b,c}$) = 2, i.e. $\{a, b, c\}$ is linearly independent and $c = \kappa_a \cdot a + \kappa_b \cdot b$ for some $\kappa_a$ and $\kappa_b$ with $\kappa_a \kappa_b = 0$, then
\[
f_{A,B,C}^{(2)}(r, s, t) = \delta((t - c_0) - \kappa_a(r - a_0) - \kappa_b(s - b_0))f_{A,B}^{(2)}(r, s).
\]
(iii) If rank($T_{a,b,c}$) = 1, i.e. $\{a, b, c\}$ is linearly dependent, without loss of generality, we assume that $\{a, b\}$ is linearly independent and $b = \kappa_{ba} \cdot a$, $c = \kappa_{ca} \cdot a$ for some $\kappa_{ba}$ and $\kappa_{ca}$ with $\kappa_{ba} \kappa_{ca} = 0$, then
\[
f_{A,B,C}^{(2)}(r, s, t) = \delta((s - b_0) - \kappa_{ba}(r - a_0) - \kappa_{ca}(s - b_0))f_{A,B}^{(2)}(r, s).
\]

**Proof.**

(i) If rank($T_{a,b,c}$) = 3, then $T_{a,b,c}$ is invertible. By using Bloch representation, $|\psi\rangle = \frac{1}{2}(1 + u \cdot \sigma)$, where $|u| = 1$. Then for $(r, s, t) = (|A\rangle_\psi, |B\rangle_\psi, |C\rangle_\psi) = (a_0 + \langle u, a \rangle, b_0 + \langle u, b \rangle, \langle u, c \rangle)$, we see that $(r - a_0, s - b_0, t - c_0) = (|u, a \rangle, \langle u, b \rangle, \langle u, c \rangle)$.

Denote $Q := (a, b, c)$, which is a $3 \times 3$ invertible real matrix due to the fact that $\{a, b, c\}$ is linearly independent. Then $T_{a,b,c} = Q^T Q$ and $(r - a_0, s - b_0, t - c_0) = (|u, Q\rangle, |u, Q\rangle, |u, Q\rangle)$, which means that
\[
\omega_{A,B,C}(r, s, t) = \sqrt{|u| Q^T (Q^T Q)^{-1} Q^T |u|} = |u| = 1.
\]

This tells us an interesting fact that $(|A\rangle_\psi, |B\rangle_\psi, |C\rangle_\psi)$ lies at the boundary surface of the ellipsoid $\omega_{A,B,C}(r, s, t) = 1$, i.e. $\omega_{A,B,C}(r, s, t) = 1$. This indicates that the PDF of $(|A\rangle_\psi, |B\rangle_\psi, |C\rangle_\psi)$ satisfies that
\[
f_{A,B,C}^{(2)}(r, s, t) \propto \delta(1 - \omega_{A,B,C}(r, s, t)).
\]

Next, we calculate the following integral:
\[
\int_{\mathbb{R}^3} \delta(1 - \omega_{A,B,C}(r, s, t))drdsdt = 4\pi \sqrt{\det(T_{a,b,c})}.
\]
Apparently
\[
\int_{\mathbb{R}^3} \delta(1 - \sqrt{|x| T_{a,b,c} |x|}) |dx| = \int_{\mathbb{R}^3} \delta(1 - \sqrt{|x| T_{a,b,c} |x|}) |dx|.
\]
Here $x = (r - a_0, s - b_0, t - c_0)$ and $[dx] = drdsdt$. Indeed, by using the spectral decomposition theorem for the Hermitian matrix $A$, we get that there is an orthogonal matrix $O \in O(3)$ such that $T_{a,b,c} = O^T \Lambda \Lambda (\lambda_0, \lambda_2, \lambda_3) O$ where $\lambda_k > 0 (k = 1, 2, 3)$. Thus

$$\omega_{A,B,C}(r, s, t) = \langle O|x|\delta(\lambda_1^{-1}, \lambda_2^{-1}, \lambda_3^{-1})|Ox\rangle$$

where $y = Ox$. Thus

$$\int_{\mathbb{R}^3} \delta(1 - \omega_{A,B,C}(r, s, t)) drdsdt$$

Let $z = \delta(\lambda_1^{-1/2}, \lambda_2^{-1/2}, \lambda_3^{-1/2})y$. Then $[dz] = \frac{1}{\sqrt{\lambda_1 \lambda_2 \lambda_3}}[dy]$ and $\int_{\mathbb{R}^3} \delta(1 - \omega_{A,B,C}(r, s, t)) drdsdt = \sqrt{\det(T_{a,b,c})} \int_{\mathbb{R}^3} \delta(1 - |z|)[dz] = 4\sqrt{\det(T_{a,b,c})}$. Finally, we get that

$$f^{(2)}_{A,B,C}(r, s, t) = \frac{1}{4\sqrt{\det(T_{a,b,c})}} \delta(1 - \omega_{A,B,C}(r, s, t)).$$

(ii) If $\text{rank}(T_{a,b,c}) = 2$, then $[a, b, c]$ is linearly dependent. Without loss of generality, we assume that $[a, b]$ is independent. Now $c = \kappa_a a + \kappa_b b$ for some $\kappa_a, \kappa_b \in \mathbb{R}$ with $\kappa_a \kappa_b \neq 0$. Thus

$$t - c_0 \equiv (C) - c_0 = \langle \psi|c|\psi\rangle = \kappa_a \langle \psi|a|\psi\rangle + \kappa_b \langle \psi|b|\psi\rangle = \kappa_a (t - a_0) + \kappa_b (s - b_0).$$

Therefore we get that

$$f^{(2)}_{A,B,C}(r, s, t) = \delta((t - c_0)$$

$$- \kappa_a (t - a_0) - \kappa_b (s - b_0)) f^{(2)}_{A,B}(r, s).$$

(iii) If $\text{rank}(T_{a,b,c}) = 1$, then $[a, b, c]$ is linearly dependent. Without loss of generality, we assume that $a$ is linearly independent and $b = \kappa_{ba} a, c = \kappa_{ca} a$ for some $\kappa_{ba}$ and $\kappa_{ca}$ with $\kappa_{ba}\kappa_{ca} = 0$. Then we get the desired result by mimicking the proof in (ii).

Theorem 3. The joint probability distribution density of $(\Delta_A, \Delta_B, \Delta_C)$ for a triple of qubit observables defined by equation (11), where $|\psi\rangle$ is a Haar-distributed random pure state on $\mathbb{C}^2$, is given by

$$f^{(2)}_{A,B,C}(x, y, z) = \frac{2xyz}{(a^2 - x^2)(b^2 - y^2)(c^2 - z^2)}$$

$$\times \sum_{j,k \in \{\pm\}} f^{(2)}_{A_j,B_j,C_j}(r_s(x), s_j(y), t_k(z)),$$

where $f^{(2)}_{A_j,B_j,C_j}(r, s, t)$ is the joint probability distribution density of the expectation values $(A_j, B_j, C_j)$, which is determined by equation (13) in proposition 6; and

$$r_s(x) = a_0 \pm \sqrt{a^2 - x^2},$$

$$s_j(y) = b_0 \pm \sqrt{b^2 - y^2},$$

$$t_k(z) = c_0 \pm \sqrt{c^2 - z^2}.$$

Proof. Note that

$$f^{(2)}_{A,B,C}(x, y, z) = \int \delta(x - \Delta_A) \delta(y - \Delta_B) \delta(z - \Delta_C) d\mu(\psi)$$

$$= 8xyz \int \delta(x^2 - \Delta_A^2) \cdot \delta(y^2 - \Delta_B^2) \cdot \delta(z^2 - \Delta_C^2) d\mu(\psi).$$

Again using the method in the proof of theorem 1, we have already obtained that

$$\delta(x^2 - \Delta_A^2) \cdot \delta(y^2 - \Delta_B^2) \cdot \delta(z^2 - \Delta_C^2)$$

$$= \delta(f_r(x)) \delta(g_s(y)) \delta(h_t(z)),$$

where

$$f_r(x) = x^2 - (r - \lambda_1(A))(\lambda_2(A) - r),$$

$$g_s(y) = y^2 - (s - \lambda_1(B))(\lambda_2(B) - s),$$

$$h_t(z) = z^2 - (t - \lambda_1(C))(\lambda_2(C) - t).$$

Then

$$f^{(2)}_{A,B,C}(x, y, z) = 8xyz$$

$$\times \int \delta(f_r(x)) \delta(g_s(y)) \delta(h_t(z)) f^{(2)}_{A_j,B_j,C_j}(r_s(x), s_j(y), t_k(z)) drdsdt.$$

Furthermore, we have

$$\delta(f_r(x)) \delta(g_s(y)) \delta(h_t(z))$$

$$= \frac{4xyz}{\sqrt{(a^2 - x^2)(b^2 - y^2)(c^2 - z^2)}},$$

Based on this observation, we get that

$$f^{(2)}_{A,B,C}(x, y, z) = \frac{xyz}{\sqrt{(a^2 - x^2)(b^2 - y^2)(c^2 - z^2)}}$$

$$\times \sum_{j,k \in \{\pm\}} \delta(f_r(x)) \delta(g_s(y)) \delta(h_t(z)) f^{(2)}_{A_j,B_j,C_j}(r_s(x), s_j(y), t_k(z)).$$
Thus
\[
f_{\Delta A \Delta B \Delta C}^{(2)}(x, y, z) = \frac{\alpha \sqrt{2 \pi}}{\sqrt{(a^2 - x^2)(b^2 - y^2)(c^2 - z^2)}}.
\]

It is easily seen that
\[
\begin{align*}
f_{\Delta A \Delta B \Delta C}^{(2)}(x, y, z) &= \frac{\alpha \sqrt{2 \pi}}{\sqrt{(a^2 - x^2)(b^2 - y^2)(c^2 - z^2)}}.
\end{align*}
\]

The desired result is obtained.

Note that the PDFs of uncertainties of multiple qubit observables (more than three) will be reduced into the three situations above, as shown in [29]. Here we will omit it here.

4. PDF of uncertainty of a single qubit observable

Assume $A$ is a non-degenerate positive matrix with eigenvalues $\lambda_i(A) = a_i(k = 1, \ldots, d)$ with $a_1 > \cdots > a_d$, denoted by $V_d(a) = \prod_{a_i < a_j} (a_i - a_j)$. Due to the following relation $\Delta_A A^2 = (\langle \psi|A^2|\psi\rangle - (\langle \psi|A|\psi\rangle)^2$, i.e. the variance of $A$ is the function of $r = \langle \psi|A|\psi\rangle$ and $s = \langle \psi|A^2|\psi\rangle$, where $|\psi\rangle$ is a Haar-distributed pure state. Thus firstly we derive the joint PDF of $\langle \psi|A|\psi\rangle$, $\langle \psi|A^2|\psi\rangle$, defined by
\[
f_{\Delta A \Delta A^2}^{(3)}(r, s) = \int \delta(r - \langle \psi|A|\psi\rangle)\delta(s - \langle \psi|A^2|\psi\rangle) d\mu(\rho).
\]

By performing Laplace transformation $(r, s) \rightarrow (\alpha, \beta)$ to $f_{\Delta A \Delta A^2}^{(3)}(r, s)$, we get that
\[
L^\alpha(f_{\Delta A \Delta A^2}^{(3)})(\alpha, \beta)
\]
\[
= \int \exp(-\langle \psi|\alpha A + \beta A^2|\psi\rangle) d\mu(\psi)
\]
\[
= \int \exp(-z) f_{\Delta A \Delta A^2}^{(3)}(z) dz,
\]

where $f_{\Delta A \Delta A^2}^{(3)}(z)$ is determined by proposition 4:
\[
f_{\Delta A \Delta A^2}^{(3)}(z) = \frac{\Gamma(3)}{V_3(a)}.
\]

Theoretically, we can calculate the above integral for any finite natural number $d$, but instead, we will focus on the case where $d = 3, 4$. We use Mathematica to do this tedious job. By simplifying the results obtained via the Laplace transformation/inverse Laplace transformation in Mathematica, we get the following results without details.

Theorem 4. For a given qubit observable $A$, acting on $\mathbb{C}^3$, with their eigenvalues $a_1 < a_2 < a_3$, the joint pdf of $(\langle A|\psi\rangle, \langle A^2|\psi\rangle)$, where $|\psi\rangle \in \mathbb{C}^3$, is given by
\[
f_{\Delta A \Delta A^2}^{(3)}(r, s) = \frac{\Gamma(3)}{V_3(a)},
\]
on $D = D_1 \cup D_2$ for
\[
D_1 = \{(r, s); a_1 \leq r \leq a_2, (a_1 + a_2)r - a_1 a_2 \leq s \leq (a_1 + a_2)r - a_1 a_3\},
\]
\[
D_2 = \{(r, s); a_2 \leq r \leq a_3, (a_2 + a_3)r - a_2 a_3 \leq s \leq (a_2 + a_3)r - a_2 a_1\};
\]

and $f_{\Delta A \Delta A^2}^{(3)}(r, s) = 0$ otherwise. Thus
\[
f_{\Delta A \Delta A^2}^{(3)}(r, s) = \frac{2\Gamma(3)}{V_3(a)} x \quad (\forall (r, s) \in R),
\]

where $R = R_1 \cup R_2$ with
\[
R_1 = \{(r, s); a_1 \leq r \leq a_2, \sqrt{(a_2 - r)(r - a_1)} \leq s \leq \sqrt{(a_3 - r)(r - a_1)}\}
\]
\[
R_2 = \{(r, s); a_2 \leq r \leq a_3, \sqrt{(a_3 - r)(r - a_2)} \leq s \leq \sqrt{(a_3 - r)(r - a_1)}\};
\]

and $f_{\Delta A \Delta A^2}^{(3)}(r, s) = 0$ otherwise. Moreover, we get that
\[
f_{\Delta A}^{(3)}(x) = \frac{4\Gamma(3)}{V_3(a)} x \left(\chi_{[0, \frac{a_2 - a_1}{2}]}(x) \delta_{\epsilon_31}(x) - \chi_{[0, \frac{a_3 - a_1}{2}]}(x) \delta_{\epsilon_21}(x)\right)
\]

where $x \in \left[0, \frac{a_1 - a_2}{2}\right]$ and $\chi_S(x)$ is the indicator of the set $S$, i.e. $\chi_S(x) = 1$ if $x \in S$, and $\chi_S(x) = 0$ if $x \notin S$;
\[
\epsilon_{\beta}(x) = \sqrt{\left(\frac{a_1 - a_2}{2}\right)^2 - x^2}.
\]
Remark 2. Denote by $D_1 = \bigcup_{i=1}^{2} D_1^{(i)}$, $D_2 = \bigcup_{j=1}^{6} D_2^{(j)}$, and $D_3 = \bigcup_{k=1}^{2} D_3^{(k)}$, respectively. Thus
\[
D_1 = \{ (r, s) : a_1 \leq r \leq a_2, \varphi_{1,2}(r) \leq s \leq \varphi_{1,4}(r) \},
\]
\[
D_2 = \{ (r, s) : a_1 \leq r \leq a_3, \varphi_{2,3}(r) \leq s \leq \varphi_{2,4}(r) \},
\]
\[
D_3 = \{ (r, s) : a_3 \leq r \leq a_4, \varphi_{2,4}(r) \leq s \leq \varphi_{4,4}(r) \},
\]
and $f_{(A), (A')}^{(4)}(r, s) = 0$ otherwise.

Remark 2. Denote by $D_1 = \bigcup_{i=1}^{2} D_1^{(i)}$, $D_2 = \bigcup_{j=1}^{6} D_2^{(j)}$, and $D_3 = \bigcup_{k=1}^{2} D_3^{(k)}$, respectively. Thus
\[
D_1 = \{ (r, s) : a_1 \leq r \leq a_2, \varphi_{1,2}(r) \leq s \leq \varphi_{1,4}(r) \},
\]
\[
D_2 = \{ (r, s) : a_1 \leq r \leq a_3, \varphi_{2,3}(r) \leq s \leq \varphi_{2,4}(r) \},
\]
\[
D_3 = \{ (r, s) : a_3 \leq r \leq a_4, \varphi_{2,4}(r) \leq s \leq \varphi_{4,4}(r) \},
\]
and $f_{(A), (A')}^{(4)}(r, s) = 0$ otherwise.
and \( f^{(4)}_{\Delta A}(r, x) = 0 \) otherwise. Moreover \( f^{(4)}_{\Delta A}(x) \) can be identified as
\[
\begin{align*}
\mathcal{D}(x) = \frac{4^4}{V_4(a)} & \chi[(a_4 - a_3)\chi(0, \frac{a_4 - a_3}{a_4 - a_2})\chi(0, \frac{a_4 - a_3}{a_4 - a_2})]d_3(x) \\
&+ (a_4 - a_3)\chi(0, \frac{a_4 - a_3}{a_4 - a_2})\chi(0, \frac{a_4 - a_3}{a_4 - a_2})d_3(x) \\
&- (a_4 - a_3)\chi(0, \frac{a_4 - a_3}{a_4 - a_2})\chi(0, \frac{a_4 - a_3}{a_4 - a_2})d_3(x) \\
&+ (a_4 - a_3)\chi(0, \frac{a_4 - a_3}{a_4 - a_2})\chi(0, \frac{a_4 - a_3}{a_4 - a_2})d_3(x) \\
&+ (a_4 - a_3)\chi(0, \frac{a_4 - a_3}{a_4 - a_2})\chi(0, \frac{a_4 - a_3}{a_4 - a_2})d_3(x).
\end{align*}
\]

Here the meanings of the notations \( \chi \) and \( \varepsilon_{ij} \) can be found in theorem 4.

**Remark 3.** Denote by \( R_1 = \bigcup_{i=1}^{3} R_i^{(1)} \), \( R_2 = \bigcup_{i=1}^{6} R_i^{(2)} \), and \( R_3 = \bigcup_{i=1}^{6} R_i^{(3)} \), respectively. Thus
\[
\begin{align*}
R_1 &= \{(r, x): a_1 \leq r \leq a_2, \sqrt{(a_2 - r)(r - a_1)} \\
&\quad \leq x \leq \sqrt{(a_4 - r)(r - a_3)}\}, \\
R_2 &= \{(r, x): a_2 \leq r \leq a_3, \sqrt{(a_4 - r)(r - a_2)} \\
&\quad \leq x \leq \sqrt{(a_4 - r)(r - a_3)}\}, \\
R_3 &= \{(r, x): a_3 \leq r \leq a_4, \sqrt{(a_4 - r)(r - a_3)} \\
&\quad \leq x \leq \sqrt{(a_4 - r)(r - a_4)}\}.
\end{align*}
\]

This implies that the support of \( f^{(4)}_{\Delta A} \) is just \( R_1 \cup R_2 \cup R_3 \), i.e. \( \text{supp}(f^{(4)}_{\Delta A}) = R_1 \cup R_2 \cup R_3 \). We draw the plot of the support of \( f^{(4)}_{\Delta A}(r, x) \), where \( d = 3, 4 \), in figure 1 as below:

(a) The support of \( f^{(3)}_{(A', \Delta A)}(r, x) \), where \( \lambda(A) = (1, 3, 9) \)

(b) The support of \( f^{(4)}_{(A', \Delta A)}(r, x) \), where \( \lambda(A) = (1, 3, 9, 27) \)

**Figure 1.** Plots of the supports of \( f^{(d)}_{(A', \Delta A)}(r, x) \) for qudit observables \( A \).

In addition, deriving the joint PDF of two uncertainties \((\Delta A, \Delta B)\) of two qudit observables \( A \) and \( B \), \( f^{(d)}_{\Delta A, \Delta B} \) is very complicated. This is not the goal of the present paper.

**Example 1.** For a qudit observable \( A \), acting on \( \mathbb{C}^q \), with the eigenvalues \( \lambda(A) = (1, 3, 9, 27) \). Still employing the notation in (14) here:
\[
\begin{align*}
\varepsilon_{12}(x) &= \sqrt{1 - x^2}, \\
\varepsilon_{13}(x) &= \sqrt{4^2 - x^2}, \\
\varepsilon_{14}(x) &= \sqrt{13^2 - x^2}, \\
\varepsilon_{23}(x) &= \sqrt{3^2 - x^2}, \\
\varepsilon_{24}(x) &= \sqrt{12^2 - x^2}, \\
\varepsilon_{34}(x) &= \sqrt{9^2 - x^2}.
\end{align*}
\]

Then from corollary 1, using marginal integral, we can derive the PDF of \( \Delta A \) that

(i) If \( x \in [0, 1] \),
\[
\begin{align*}
f^{(4)}_{\Delta A}(x) &= \frac{x}{33696} (9\varepsilon_{12}^3(x) + 13\varepsilon_{13}^3(x) \\
&- 12\varepsilon_{13}^3(x) + \varepsilon_{34}^3(x) - 4\varepsilon_{24}^3(x) + 3\varepsilon_{14}^3(x)).
\end{align*}
\]

(ii) If \( x \in [1, 3] \),
\[
\begin{align*}
f^{(4)}_{\Delta A}(x) &= \frac{x}{33696} (13\varepsilon_{23}^3(x) - 12\varepsilon_{13}^3(x) \\
&+ \varepsilon_{34}^3(x) - 4\varepsilon_{24}^3(x) + 3\varepsilon_{14}^3(x)).
\end{align*}
\]

(iii) If \( x \in [3, 4] \),
\[
\begin{align*}
f^{(4)}_{\Delta A}(x) &= \frac{x}{33696} (-12\varepsilon_{13}^3(x) \\
&+ \varepsilon_{34}^3(x) - 4\varepsilon_{24}^3(x) + 3\varepsilon_{14}^3(x)).
\end{align*}
\]

(iv) If \( x \in [4, 9] \),
\[
\begin{align*}
f^{(4)}_{\Delta A}(x) &= \frac{x}{33696} (\varepsilon_{34}^3(x) - 4\varepsilon_{24}^3(x) + 3\varepsilon_{14}^3(x)).
\end{align*}
\]
Theorem 6. For a qudit observable $A$, acting on $\mathbb{C}^d$, with eigenvalues $\lambda(A) = (a_1, \ldots, a_d)$, where $a_1 < \cdots < a_d$, the supports of the PDFs of $f_{\lambda(A), (A^t)}^d((r, s))$ and $f_{\lambda(A), \Delta A}^d((r, x))$, respectively, given by the following:

$$\text{supp}(f_{\lambda(A), (A^t)}^d((r, s))) = \bigcup_{k=1}^{d-1} F_{k,k+1},$$

where

$$F_{k,k+1} := \{(r, s); a_k \leq r \leq a_{k+1},$$
$$\varphi_{k,k+1}(r) \leq s \leq \varphi_{1,d}(r)\};$$

$$\text{supp}(f_{\lambda(A), \Delta A}^d) = \bigcup_{k=1}^{d-1} V_{k,k+1},$$

where

$$V_{k,k+1} := \{(r, x); a_k \leq r \leq a_{k+1},$$
$$\sqrt{(a_{k+1} - r)(r - a_k)} \leq x \leq \sqrt{(a_d - r)(r - a_1)}\}.$$

Proof. Without loss of generality, we assume that $A = \text{diag}(a_1, \ldots, a_d)$ with $a_1 < \cdots < a_d$. Let $|\psi\rangle = (\psi_1, \ldots, \psi_d) \in \mathbb{C}^d$ be a pure state and $r_k = |\psi_k|^2$. Thus $(r_1, \ldots, r_d)$ is a $d$-dimensional probability vector. Then

$$r = \langle A \rangle = \sum_{k=1}^{d} a_k r_k \quad \text{and} \quad s = \langle A^t \rangle = \sum_{k=1}^{d} a_k^2 r_k.$$

Thus, for each $k \in \{1, \ldots, d - 1\}$,

$$s - \varphi_{k,k+1}(r) = \sum_{i=1}^{d} a_i^2 r_i - (a_k + a_{k+1}) \sum_{i=1}^{d} a_i r_i + a_k a_{k+1}$$

$$= \sum_{i=1}^{d} a_i^2 r_i - (a_k + a_{k+1}) \sum_{i=1}^{d} a_i r_i + a_k a_{k+1}$$

$$= \sum_{i=1}^{d} (a_i - a_k)(a_i - a_{k+1}) r_i.$$

Note that $a_1 < \cdots < a_d$ and $r_i \geq 0$ for each $i = 1, \ldots, d$. We see that, when $i = k, k + 1$, $(a_i - a_k)(a_i - a_{k+1}) r_i = 0$, and $(a_i - a_k)(a_i - a_{k+1}) r_i \geq 0$ otherwise. This means that $s \geq \varphi_{k,k+1}(r)$; and this inequality is saturated if $(r_i, r_{k+1}) = (t, 1 - t)$ for $t \in (0, 1)$ and $r_i = 0$ for $i \neq k, k + 1$. Similarly, we can easily get that $s \leq \varphi_{1,d}(r)$. Denote

$$F_{k,k+1} := \{(r, s); a_k \leq r \leq a_{k+1},$$
$$\varphi_{k,k+1}(r) \leq s \leq \varphi_{1,d}(r)\}.$$

Hence

$$\text{supp}(f_{\lambda(A), (A^t)}^d) = \bigcup_{k=1}^{d-1} F_{k,k+1}.$$

Now, for $x = \Delta_A A$, we see that $s = r^2 + x^2$. By employing the support of $f_{\lambda(A), (A^t)}^d$, we can derive the support of
$f^{(d)}_{A \Delta A}(r, x)$ as follows: Denote
\[ V_{k+1} = \{(r, x) : a_k \leq r \leq a_{k+1}, \sqrt{(a_{k+1} - r)(r - a_k)} \leq x \leq \sqrt{(a_d - r)(r - a_k)}\}, \]
then
\[ \varphi_{k+1}(r) \leq s = r^2 + x^2 \leq \varphi_{1,d}(r) \]
\[ \iff (r, x) \in V_{k+1}. \]
Therefore the support of $f^{(d)}_{A \Delta A}(r, x)$ is given by
\[ \text{supp}(f^{(d)}_{A \Delta A}) = \bigcup_{k=1}^{d-1} V_{k+1}. \]
This completes the proof.

For the joint PDF of uncertainties of multiple qudit observables acting on $\mathbb{C}^d (d \geq 3)$, say, a pair of qudit observables $(A, B)$, deriving the joint PDF $f^{(d)}_{A \Delta A}(x, y)$ is very complicated because there is much difficulty in calculating the Laplace transformation/inverse Laplace transformation of $f^{(d)}_{A \Delta A}(x, y)$. The reason is that we still cannot figure out what the relationship between $\lambda(A + B)$, $\lambda(A)$, and $\lambda(B)$ is varied $(\alpha, \beta) \in \mathbb{R}^2$. A fresh method to do this is expected to discover in the future.

5. Discussion and concluding remarks

Recall that the support $\text{supp}(f)$ of a function $f$ is given by the closure of the subset of preimage for which $f$ does not vanish. From theorem 1, we see that the support of $f^{(2)}_{A \Delta A}$ is closed interval $[0, |A|]$. This is inconsistent with the fact that $\Delta_{r}A \in [0, \nu(A)]$, where $\nu(A) := \frac{1}{2}(\lambda_{\text{max}}(A) - \lambda_{\text{min}}(A))$ and $|\psi\rangle$ is any pure state.

From proposition 5 and theorem 2, we can infer that, for $d = 2$, each element in $\mathcal{U}^{(m)}_{A \Delta A,B}$ is just the solution of the following inequality:
\[
|b|^2 x^2 + |a|^2 y^2 + 2|a, b| \times \sqrt{|a|^2 - x^2} (|b|^2 - y^2) \geq |a|^2 |b|^2 + |a, b|^2,
\]
which is exactly the one we obtained in [29] for mixed states. This indicates that, in the qubit situation, we have that

**Proposition 7.** For a pair of qubit observables $(A, B)$ acting on $\mathbb{C}^2$, it holds that
\[ \mathcal{U}^{(q)}_{A \Delta A,B} = \mathcal{U}^{(m)}_{A \Delta A,B}. \]

One may wonder if this identity holds for general $d \geq 2$, as the variance of $A$ with respect to a mixed state can always be decomposed as a convex combination of some variances of $A$ associated with pure states, see equation (3).

For multiple qudit observables $A_k (k = 1, \ldots, n)$ acting on $\mathbb{C}^d$, comparing the set $\mathcal{U}^{(d)}_{A_1, \ldots, A_n}$ with the set $\mathcal{U}^{(m)}_{A_1, \ldots, A_n}$ is an interesting problem. Unfortunately, our theorem 3, together with the result obtained in [29], indicates that $\mathcal{U}^{(m)}_{A_1, \Delta A_2, \ldots, A_n} = \mathcal{U}^{(p)}_{A_1, \Delta A_2, \ldots, A_n}$ does not hold in general. In fact, $\partial \mathcal{U}^{(m)}_{A_1, \Delta A_2, \ldots, A_n} = \partial \mathcal{U}^{(p)}_{A_1, \Delta A_2, \ldots, A_n}$ in the qubit situations, that is, the boundary surface of $\mathcal{U}^{(m)}_{A_1, \Delta A_2, \ldots, A_n}$ is just $\mathcal{U}^{(p)}_{A_1, \Delta A_2, \ldots, A_n}$ in the qubit situations. This also indicates that the following inclusion is proper in general for multiple observables,
\[ \mathcal{U}^{(q)}_{A_1, \ldots, A_n} \subsetneq \mathcal{U}^{(m)}_{A_1, \ldots, A_n}. \]
Based on this, two extreme cases: $\mathcal{U}^{(q)}_{A_1, \ldots, A_n} = \mathcal{U}^{(m)}_{A_1, \ldots, A_n}$ or $\mathcal{U}^{(q)}_{A_1, \ldots, A_n} = \partial \mathcal{U}^{(m)}_{A_1, \ldots, A_n}$, should be characterized.

In addition, we also see that once we obtain the uncertainty regions for observables $A_k$, we can infer additive uncertainty relations such as
\[ \sum_{k=1}^{n} (\Delta_{A_k})^2 \geq \min_{\rho \in \mathcal{D}(\mathbb{C}^d)} \sum_{k=1}^{n} (\Delta_{A_k})^2 \]
\[ = \min \left\{ \sum_{k=1}^{n} \chi^2 : (\chi_1, \ldots, \chi_n) \in \mathcal{U}^{(m)}_{A_1, \ldots, A_n} \right\}. \]

Analogous optimal problems can also be considered for $\mathcal{U}^{(q)}_{A_1, \ldots, A_n}$. These results can be used to detect entanglement [10, 12]. The current results and the results in [29] together give the complete solutions to the uncertainty region and uncertainty relations for qubit observables.

We hope the results obtained in the present paper can shed new light on the related problems in quantum information theory. Our approach may be applied to the study of PDFs in higher dimensional spaces. It would also be interesting to apply PDFs to measurement and/or quantum channel uncertainty relations.

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