

Uncertainty regions of observables and state-independent uncertainty relations

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Abstract

The optimal state-independent lower bounds for the sum of variances or deviations of observables are of significance for the growing number of experiments that reach the uncertainty limited regime. We present a framework for computing the tight uncertainty relations of variance or deviation via determining the uncertainty regions, which are formed by the tuples of two or more of quantum observables in random quantum states induced from the uniform Haar measure on the purified states. From the analytical formulae of these uncertainty regions, we present state-independent uncertainty inequalities satisfied by the sum of variances or deviations of two, three and arbitrary many observables, from which experimentally friend entanglement detection criteria are derived for bipartite and tripartite systems.

Keywords Uncertainty of observable \cdot Probability density function \cdot Uncertainty region \cdot State-independent uncertainty relation \cdot Harish–Chandra–Itzykson–Züber integral

Contents

1	ntroduction	2
2	Main results	3
3	Proofs of main results	10

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3.1	Proof of Lemma 2.1.	 			 													10
3.2	Proof of formula (2.6)	 			 													22
3.3	Proof of Theorem 2.2	 			 													23
3.4	Proof of Lemma 2.3 .	 			 													26
3.5	Proof of Theorem 2.4	 			 													34
3.6	Proof of Lemma 2.5 .	 																35
3.7	Proof of Theorem 2.6	 																39
Refere	ences	 		•								•						41

1 Introduction

The uncertainty principle, apart from serving as a hallmark of the quantum world, has wide applications and implications in both theoretical and practical investigations of quantum mechanics. Ever since its birth in 1927 [1], various uncertainty relations, as concrete realizations of the uncertainty principle, have been extensively and intensively studied. In particular, recently, the state-independent uncertainty relations have attracted a lot of attentions [2–7]. Whether deeper principles underlie quantum uncertainty and nonlocality has been listed as one of the challenging scientific problems on the occasion of celebrating the 125th anniversary of the academical journal *Science* [8]. Thus, it is of fundamental significance to explore the intrinsic uncertainty of given quantum mechanical observables due to its connections with entanglement detection [9–14] and quantum nonlocality [15].

The most celebrated uncertainty relation was initially conceived for position and momentum observables by Heisenberg [1]. A general form was the Robertson–Schrödinger uncertainty relation [16–19]:

$$(\Delta_{\rho} \boldsymbol{A})^{2} (\Delta_{\rho} \boldsymbol{B})^{2} \geq \frac{1}{4} (\langle \{\boldsymbol{A}_{0}, \boldsymbol{B}_{0}\} \rangle_{\rho}^{2} + \langle [\boldsymbol{A}, \boldsymbol{B}] \rangle_{\rho}^{2}),$$

where $\langle X \rangle_{\rho} = \text{Tr} (X\rho)$ is the expectation value of X with respect to the state ρ , $(\Delta_{\rho}A)^2 = (\langle A^2 \rangle_{\rho} - \langle A \rangle_{\rho}^2)$ is the corresponding variance of A, $A_0 = A - \langle A \rangle_{\rho}$, $B_0 = B - \langle B \rangle_{\rho}$, $\{A, B\} = AB + BA$ and [A, B] = AB - BA denote the anti-commutator (symmetric Jordan product) and commutator (anti-symmetric Lie product), respectively.

Although the above uncertainty relation captures certain features of the uncertainty principle in a very appealing, intuitive and succinct way, the state-dependent lower bound and the variances capture limited information of uncertainty for given pair of observables. Recently, Busch and Reardon-Smitha proposed to consider the uncertainty region of two observables *A* and *B* instead of finding bounds on some particular choice of uncertainty functionals [20], which provides apparently more information about the uncertainty of the two observables *A* and *B*. Later some Vasudevrao *et al* also followed this line and conducted specific computations about uncertainty regions [21].

In this paper, we use the probability theory and random matrices to study the uncertainty regions of two, three and multiple qubit observables. The probabilistic method and random matrix theory have many useful applications such as in evaluating the average entropy of a subsystem [22–25], studying the non-additivity of quantum channel capacity [26] and random quantum pure states [27–31]. Motivated by these works, we derive analytical formulas concerning the expectation and uncertainty (variance) of quantum observables in random quantum states. We identify the uncertainty regions as the supports of such probability distribution functions. From these analytical results on uncertainty regions, we present the optimal state-independent lower bounds for the sum of variances or the deviations, which are just the optimization problems over the uncertainty regions. The paper is organized as follows. In Sect. 2, we present our main results, their proofs are developed in Sect. 3.

2 Main results

A qubit observable can be parameterized as $A = a_0 \mathbb{1} + \boldsymbol{a} \cdot \boldsymbol{\sigma}$, $(a_0, \boldsymbol{a}) \in \mathbb{R}^4$, where $\mathbb{1}$ is the identity matrix on the qubit Hilbert space \mathbb{C}^2 , and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of the standard Pauli matrices. The two eigenvalues of A are $\lambda_k(A) = a_0 + (-1)^k |\boldsymbol{a}|$ (k = 1, 2) with $|\boldsymbol{a}| = (a_1^2 + a_2^2 + a_3^2)^{1/2} > 0$ the length of the vector $\boldsymbol{a} = (a_1, a_2, a_3) \in \mathbb{R}^3$.

Any qubit state ρ can be purified to a pure state on $\mathbb{C}^2 \otimes \mathbb{C}^2$. The set of pure states on $\mathbb{C}^2 \otimes \mathbb{C}^2$ can be represented as $\{U|\Phi\rangle : U \in U(\mathbb{C}^2 \otimes \mathbb{C}^2)\}$ with $|\Phi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ any fixed pure state, and $U(\mathbb{C}^2 \otimes \mathbb{C}^2)$ the full unitary group on $\mathbb{C}^2 \otimes \mathbb{C}^2$, endowed with the standard Haar measure. Denote $D(\mathbb{C}^2)$ the set of all quantum (pure or mixed) states on \mathbb{C}^2 . The probability measure $d\mu(\rho)$ can be derived from this Haar measure by taking partial trace over \mathbb{C}^2 of the pure states on $\mathbb{C}^2 \otimes \mathbb{C}^2$.

Let A_k (k = 1, ..., n) be a set of qubit observables. The uncertainty region $U_{\Delta A_1,...,\Delta A_n}$ of an *n*-tuple of uncertainties ΔA_k is defined by

$$\left\{ (\Delta_{\rho} A_1, \dots, \Delta_{\rho} A_n) \in \mathbb{R}^n_{\geq 0} : \rho \in \mathcal{D}(\mathbb{C}^2) \right\}.$$
 (2.1)

Here, $\mathbb{R}_{\geq 0} = [0, +\infty)$. From (2.1), tight state-independent variance and deviation uncertainty relations can be obtained,

$$\sum_{k=1}^{n} (\Delta_{\rho} A_{k})^{2} \ge \min_{(x_{1},\dots,x_{n}) \in \mathcal{U}_{\Delta A_{1},\dots,\Delta A_{n}}} \sum_{k=1}^{n} x_{k}^{2},$$

$$(2.2)$$

$$\sum_{k=1}^{n} \Delta_{\rho} A_{k} \geq \min_{(x_{1},\dots,x_{n}) \in \mathcal{U}_{\Delta} A_{1},\dots,\Delta A_{n}} \sum_{k=1}^{n} x_{k}.$$
(2.3)

We first investigate the uncertainty regions for a pair of observables $\mathbf{A} = a_0 \mathbb{1} + \mathbf{a} \cdot \boldsymbol{\sigma}$ and $\mathbf{B} = b_0 \mathbb{1} + \mathbf{b} \cdot \boldsymbol{\sigma}$ with $(a_0, \mathbf{a}), (b_0, \mathbf{b}) \in \mathbb{R}^4$. Denote

$$T_{a,b} = \left(egin{array}{cc} \langle a,a
angle & \langle a,b
angle \\ \langle b,a
angle & \langle b,b
angle \end{array}
ight).$$

Lemma 2.1 The uncertainty region $\mathcal{U}_{\Delta A, \Delta B} = \left\{ (\Delta_{\rho} A, \Delta_{\rho} B) \in \mathbb{R}^2_{\geq 0} : \rho \in D(\mathbb{C}^2) \right\}$ of A and B is determined by the following inequality:

$$|\boldsymbol{b}|^{2} x^{2} + |\boldsymbol{a}|^{2} y^{2} + 2 |\langle \boldsymbol{a}, \boldsymbol{b} \rangle |\sqrt{(|\boldsymbol{a}|^{2} - x^{2})(|\boldsymbol{b}|^{2} - y^{2})} \ge |\boldsymbol{a}|^{2} |\boldsymbol{b}|^{2} + \langle \boldsymbol{a}, \boldsymbol{b} \rangle^{2},$$
(2.4)

where $x \in [0, |\mathbf{a}|]$, $y \in [0, |\mathbf{b}|]$ and $\{\mathbf{a}, \mathbf{b}\}$ is linearly independent.

From Lemma 2.1, the boundary curve of the uncertainty region $U_{\Delta A, \Delta B}$ is easily obtained. Clearly, the boundary curve equations are independent of (a_0, b_0) . Denote θ the angle between a and b. We see that, for |a| = |b| = 1,

$$x^{2} + y^{2} + 2|\cos\theta|\sqrt{(1-x^{2})(1-y^{2})} \ge 1 + \cos^{2}\theta.$$
 (2.5)

In particular, for $\theta \in \left\{\frac{\pi}{16}, \frac{\pi}{8}, \frac{\pi}{4}, \frac{3\pi}{8}, \frac{7\pi}{16}, \frac{\pi}{2}\right\}$, our result covers that in [3,20] perfectly. Obviously, $\mathcal{U}_{\Delta A, \Delta B} \equiv \mathcal{U}(\theta)$ is determined only by the angle θ between \boldsymbol{a} and \boldsymbol{b} if $|\boldsymbol{a}| = |\boldsymbol{b}| = 1$, and $\mathcal{U}(\theta) = \mathcal{U}(\pi - \theta)$ for $\theta \in [0, \pi]$. Moreover, we can also get the volume (the area for the two-dimensional domain) of the uncertainty region $\mathcal{U}(\theta)(\theta \in [0, \pi/2])$,

$$\operatorname{vol}(\mathcal{U}(\theta)) = \frac{1}{2}(\pi - 3\theta)\sin\theta - \cos\theta + 1.$$
(2.6)

Hence, in general, $\operatorname{vol}(\mathcal{U}_{\Delta A,\Delta B}) = |\mathbf{a}| |\mathbf{b}| \operatorname{vol}(\mathcal{U}(\theta))$. From (2.6), we have that the maximal uncertainty region is attained at $\theta_0 \simeq 0.741758 < \frac{\pi}{4}$,

$$\max_{\theta \in [0,\pi/2]} \operatorname{vol}[\mathcal{U}(\theta)] = \operatorname{vol}[\mathcal{U}(\theta_0)] \simeq 0.572244.$$

From the uncertainty region given in Lemma 2.1, we can derive the optimal *state-independent* lower bound for the sum of variances $(\Delta_{\rho} A)^2 + (\Delta_{\rho} B)^2$ and the sum of standard deviation $\Delta_{\rho} A + \Delta_{\rho} B$.

Theorem 2.2 *The sum of the variances and the standard deviations satisfy the following tight inequalities with state-independent lower bounds,*

$$(\Delta_{\rho} A)^{2} + (\Delta_{\rho} B)^{2} \ge \min\left\{x^{2} + y^{2} : (x, y) \in \mathcal{U}_{\Delta A, \Delta B}\right\} = \lambda_{\min}(\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}}) \quad (2.7)$$

and

$$\Delta_{\rho} \boldsymbol{A} + \Delta_{\rho} \boldsymbol{B} \ge \min\left\{ \boldsymbol{x} + \boldsymbol{y} : (\boldsymbol{x}, \boldsymbol{y}) \in \mathcal{U}_{\Delta \boldsymbol{A}, \Delta \boldsymbol{B}} \right\} = \frac{|\boldsymbol{a} \times \boldsymbol{b}|}{\max(|\boldsymbol{a}|, |\boldsymbol{b}|)}, \quad (2.8)$$

where $\lambda_{\min}(T_{a,b})$ stands for the minimal eigenvalue of $T_{a,b}$.



Fig. 1 The uncertainty region $U_{\Delta A,\Delta B}$ in Lemma 2.1 and those points where the minimizations in Theorem 2.2 are achieved

In particular, if |a| = |b| = 1, (2.7) and (2.8) are reduced to

$$(\Delta_{\rho} A)^{2} + (\Delta_{\rho} B)^{2} \ge 1 - |\langle a, b \rangle|,$$

$$\Delta_{\rho} A + \Delta_{\rho} B \ge |a \times b|.$$

Note that $[A, B] = AB - BA = 2i(a \times b) \cdot \sigma$, $|\langle a, b \rangle| = |\cos \theta|$ and $|a \times b| = |\sin \theta|$. One recovers the uncertainty relations [20],

$$(\Delta_{\rho} \boldsymbol{A})^{2} + (\Delta_{\rho} \boldsymbol{B})^{2} \ge 1 - \sqrt{1 - \frac{1}{4} \| [\boldsymbol{A}, \boldsymbol{B}] \|^{2}},$$
$$\Delta_{\rho} \boldsymbol{A} + \Delta_{\rho} \boldsymbol{B} \ge \frac{1}{2} \| [\boldsymbol{A}, \boldsymbol{B}] \|.$$

As an illustration, in Fig. 1 we plot for any fixed angle $\theta \in (0, \frac{\pi}{2})$ the uncertainty region $\mathcal{U}_{\Delta A, \Delta B}$ given in Lemma 2.1 and those points where the minimizations in Theorem 2.2 are achieved, where the coordinate of the red point is $(\sqrt{(1-\cos\theta)/2}, \sqrt{(1-\cos\theta)/2})$, and the coordinates of the two purple points are $(\sin\theta, 0)$ and $(0, \sin\theta)$, respectively.

We now turn to the uncertainty region for a triple (A, B, C) of qubit observables $A = a_0 \mathbb{1} + a \cdot \sigma$, $B = b_0 \mathbb{1} + b \cdot \sigma$ and $C = c_0 \mathbb{1} + c \cdot \sigma$ with (a_0, a) , (b_0, b) , $(c_0, c) \in \mathbb{R}^4$, and $\{a, b, c\}$ being linearly independent. Denote $u_{\epsilon_b, \epsilon_c}(x, y, z) =$

$$T_{a,b,c} = \begin{pmatrix} \langle a,a \rangle & \langle a,b \rangle & \langle a,c \rangle \\ \langle b,a \rangle & \langle b,b \rangle & \langle b,c \rangle \\ \langle c,a \rangle & \langle c,b \rangle & \langle c,c \rangle \end{pmatrix}.$$

Let γ , β and α be the angles between a and b, a and c, b and c, respectively, where α , β , $\gamma \in (0, \pi)$. Set $\phi(t_1, t_2, t_3) = \cos(t_1) - \cos(t_2)\cos(t_3)$. We have the following result:

Lemma 2.3 The uncertainty region $\mathcal{U}_{\Delta A, \Delta B, \Delta C} = \left\{ (\Delta_{\rho} A, \Delta_{\rho} B, \Delta_{\rho} C) \in \mathbb{R}^{3}_{\geq 0} : \rho \in D(\mathbb{C}^{2}) \right\}$ is determined by the following inequality:

$$\boldsymbol{u}_{\epsilon_b,\epsilon_c}(x, y, z)\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}}^{-1}\boldsymbol{u}_{\epsilon_b,\epsilon_c}^{\mathsf{T}}(x, y, z) \leqslant 1,$$
(2.9)

where $\epsilon_b, \epsilon_c \in \{\pm 1\}$ are independent of each other, which is given by the union of solutions of the following inequalities if $|\mathbf{a}| = |\mathbf{b}| = |\mathbf{c}| = 1$:

$$\begin{aligned} \left| \phi(\gamma, \alpha, \beta) \sqrt{1 - x^2} + \epsilon \phi(\alpha, \beta, \gamma) \sqrt{1 - z^2} \right| \sqrt{1 - y^2} \\ + \epsilon \phi(\beta, \gamma, \alpha) \sqrt{(1 - z^2)(1 - x^2)} \\ + \frac{1}{2} \left[\sin^2(\alpha) x^2 + \sin^2(\beta) y^2 + \sin^2(\gamma) z^2 \right] \ge 1 - \cos(\alpha) \cos(\beta) \cos(\gamma) 2.10) \end{aligned}$$

under the conditions $\alpha < \beta + \gamma$, $\beta < \gamma + \alpha$, $\gamma < \alpha + \beta$ and $\alpha + \beta + \gamma < 2\pi$, where $\epsilon \equiv \epsilon_c \in \{\pm 1\}$.

In particular, e.g., for $\alpha = \beta = \gamma = \frac{\pi}{2}$, the uncertainty region is just $\{(x, y, z) \in \mathbb{R}^3_{\geq 0} : x^2 + y^2 + z^2 \geq 2\} \cap [0, 1]^3$. Clearly, our equations include the results in [20] as special cases, see Fig. 2.

Analogously, the state-independent lower bound for $(\Delta_{\rho} A)^2 + (\Delta_{\rho} B)^2 + (\Delta_{\rho} C)^2$ can be obtained from (2.10).

Theorem 2.4 The variances of the observables A, B and C satisfy

$$(\Delta_{\rho} A)^{2} + (\Delta_{\rho} B)^{2} + (\Delta_{\rho} C)^{2} \ge \min\{x^{2} + y^{2} + z^{2} : (x, y, z) \in \mathcal{U}_{\Delta A, \Delta B, \Delta C}\}$$

= Tr (*T_{a,b,c}*) - \lambda_{max}(*T_{a,b,c}*), (2.11)

where $\lambda_{\max}(T_{a,b,c})$ stands for the maximal eigenvalue of $T_{a,b,c}$.

We analyze the state-independent lower bound of (2.11) in two cases:

(i) If α = β = γ = θ ∈ [0, π/2], then the three eigenvalues of T_{a,b,c} are given by {1 - cos θ, 1 - cos θ, 1 + 2 cos θ}, namely, the maximal eigenvalue is λ_{max}(T_{a,b,c}) = 1 + 2 cos θ. Therefore, the uncertainty relation (2.11) simply becomes (Δ_ρA)² + (Δ_ρB)² + (Δ_ρC)² ≥ 2(1 - cos θ);



Fig. 2 The uncertainty regions $\mathcal{U}_{\Delta A, \Delta B, \Delta C} \equiv \mathcal{U}(\alpha, \beta, \gamma)$ for a triple of qubit observables $A = a_0 \mathbb{1} + a \cdot \sigma$, $B = b_0 \mathbb{1} + b \cdot \sigma$ and $C = c_0 \mathbb{1} + c \cdot \sigma$, where |a| = |b| = |c| = 1, $\langle a, b \rangle = \cos \gamma$, $\langle a, c \rangle = \cos \beta$ and $\langle b, c \rangle = \cos \alpha$

(ii) If $\beta = \gamma = \frac{\pi}{2}$ and $\alpha \in [0, \pi/2]$, the three eigenvalues of $T_{a,b,c}$ are $\{1, 1 - \cos \alpha, 1 + \cos \alpha\}$. The maximal eigenvalue is $\lambda_{\max}(T_{a,b,c}) = 1 + \cos \alpha$. In this case, the uncertainty relation (2.11) becomes $(\Delta_{\rho}A)^2 + (\Delta_{\rho}B)^2 + (\Delta_{\rho}C)^2 \ge 2 - \cos \alpha$.

We consider now the uncertainty regions for multiple qubit observables. For an *n*-tuple of qubit observables (A_1, \ldots, A_n) , where $A_k = a_0^{(k)} \mathbb{1} + a_k \cdot \sigma$ with $(a_0^{(k)}, a_k) \in \mathbb{R}^4$, $k = 1, \ldots, n$, denote $T_{a_1, \ldots, a_n} = (\langle a_i, a_j \rangle)$. Note that $\{a_1, a_2, \ldots, a_n\}$ has at most three vectors that are linearly independent. Without loss of generality, we assume $\{a_1, a_2, a_3\}$ is linearly independent. The rest vectors can be linearly expressed by $\{a_1, a_2, a_3\}$, $a_l = \kappa_{l1}a_1 + \kappa_{l2}a_2 + \kappa_{l3}a_3$, for

some coefficients
$$\kappa_{lj}$$
, $l = 4, \cdots, n, j = 1, 2, 3$. Set $u_{\epsilon_1, \epsilon_2, \epsilon_3}(x_1, x_2, x_3) = \left(\epsilon_1 \sqrt{|a_1|^2 - x_1^2}, \epsilon_2 \sqrt{|a_2|^2 - x_2^2}, \epsilon_3 \sqrt{|a_3|^2 - x_3^2}\right).$

Lemma 2.5 The uncertainty region $U_{\Delta A_1,...,\Delta A_n}$ of an n-tuple of qubit observables $(A_1,...,A_n)$ is determined by $(x_1,...,x_n) \in U_{\Delta A_1,...,\Delta A_n}$ satisfying

$$\begin{cases} \boldsymbol{u}_{\epsilon_{1},\epsilon_{2},\epsilon_{3}}(x_{1}, x_{2}, x_{3}) \boldsymbol{T}_{\boldsymbol{a}_{1},\boldsymbol{a}_{2},\boldsymbol{a}_{3}}^{-1} \boldsymbol{u}_{\epsilon_{1},\epsilon_{2},\epsilon_{3}}^{\mathsf{T}}(x_{1}, x_{2}, x_{3}) \leqslant 1 \\ \epsilon_{l} \sqrt{|\boldsymbol{a}_{l}|^{2} - x_{l}^{2}} = \sum_{j=1}^{3} \kappa_{lj} \epsilon_{j} \sqrt{|\boldsymbol{a}_{j}|^{2} - x_{j}^{2}} \end{cases}$$

 $\forall l = 4, ..., n$, where $\epsilon_k \in \{\pm 1\}$, $x_k \in [0, |a_k|], k = 1, ..., n$.

Correspondingly, we have the following result:

Theorem 2.6 *The variances of the observables* A_k (k = 1, ..., n) *satisfy*

$$\sum_{k=1}^{n} (\Delta_{\rho} A_{k})^{2} \ge \min_{(x_{1},...,x_{n}) \in \mathcal{U}_{\Delta A_{1},...,\Delta A_{n}}} \sum_{k=1}^{n} x_{k}^{2} = \operatorname{Tr}\left(\boldsymbol{T}_{\boldsymbol{a}_{1},...,\boldsymbol{a}_{n}}\right) - \lambda_{\max}(\boldsymbol{T}_{\boldsymbol{a}_{1},...,\boldsymbol{a}_{n}}),$$
(2.12)

where $\lambda_{\max}(T_{a_1,\dots,a_n})$ stands for the maximal eigenvalue of T_{a_1,\dots,a_n} .

As applications of our state-independent uncertainty relations, we consider the entanglement detection. As shown in [9,11,12], every state-independent uncertainty relation gives rise to a nonlinear entanglement witness. We consider the tripartite scenario: three parties, Alice, Bob and Charlie perform local measurements A_i , B_i and C_i , where i = 1, 2, 3, on an unknown tripartite quantum state $\rho_{ABC} \equiv \rho$, acting on $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$, respectively. Their goal is to decide if ρ is fully separable or not. They measure the composite observables M_i (i = 1, 2, 3) given by

$$\boldsymbol{M}_i = \boldsymbol{A}_i \otimes \mathbb{1}_{BC} + \mathbb{1}_A \otimes \boldsymbol{B}_i \otimes \mathbb{1}_C + \mathbb{1}_{AB} \otimes \boldsymbol{C}_i.$$

Note that

$$\begin{aligned} (\Delta_{\rho} \boldsymbol{M}_{i})^{2} &= 2(\mathrm{Tr} \left(\boldsymbol{A}_{i} \otimes \boldsymbol{B}_{i} \rho_{AB}\right) - \mathrm{Tr} \left(\boldsymbol{A}_{i} \rho_{A}\right) \mathrm{Tr} \left(\boldsymbol{B}_{i} \rho_{B}\right)) \\ &+ 2(\mathrm{Tr} \left(\boldsymbol{B}_{i} \otimes \boldsymbol{C}_{i} \rho_{BC}\right) - \mathrm{Tr} \left(\boldsymbol{B}_{i} \rho_{B}\right) \mathrm{Tr} \left(\boldsymbol{C}_{i} \rho_{C}\right)) \\ &+ 2(\mathrm{Tr} \left(\boldsymbol{A}_{i} \otimes \boldsymbol{C}_{i} \rho_{AC}\right) - \mathrm{Tr} \left(\boldsymbol{A}_{i} \rho_{A}\right) \mathrm{Tr} \left(\boldsymbol{C}_{i} \rho_{C}\right)) \\ &+ (\Delta_{\rho_{A}} \boldsymbol{A}_{i})^{2} + (\Delta_{\rho_{B}} \boldsymbol{B}_{i})^{2} + (\Delta_{\rho_{C}} \boldsymbol{C}_{i})^{2}. \end{aligned}$$

If ρ is of the form, $\rho = \rho_A \otimes \rho_B \otimes \rho_C$, then $\Delta_{\rho}^2 M_i = \Delta_{\rho_A}^2 A_i + \Delta_{\rho_B}^2 B_i + \Delta_{\rho_C}^2 C_i$. Thus, for fully separable states $\rho = \sum_k p_k \rho_k$, where $\rho_k = \rho_{k,A} \otimes \rho_{k,B} \otimes \rho_{k,C}$, we get

$$\Delta_{\rho}^2 \boldsymbol{M}_1 + \Delta_{\rho}^2 \boldsymbol{M}_2 + \Delta_{\rho}^2 \boldsymbol{M}_3$$

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$$\geq \sum_{k} p_{k} \left(\Delta_{\rho_{k}}^{2} \boldsymbol{M}_{1} + \Delta_{\rho_{k}}^{2} \boldsymbol{M}_{2} + \Delta_{\rho_{k}}^{2} \boldsymbol{M}_{3} \right)$$

$$= \sum_{k} p_{k} \left(\Delta_{\rho_{k,A}}^{2} \boldsymbol{A}_{1} + \Delta_{\rho_{k,A}}^{2} \boldsymbol{A}_{2} + \Delta_{\rho_{k,A}}^{2} \boldsymbol{A}_{3} \right)$$

$$+ \sum_{k} p_{k} \left(\Delta_{\rho_{k,B}}^{2} \boldsymbol{B}_{1} + \Delta_{\rho_{k,B}}^{2} \boldsymbol{B}_{2} + \Delta_{\rho_{k,B}}^{2} \boldsymbol{B}_{3} \right)$$

$$+ \sum_{k} p_{k} \left(\Delta_{\rho_{k,C}}^{2} \boldsymbol{C}_{1} + \Delta_{\rho_{k,C}}^{2} \boldsymbol{C}_{2} + \Delta_{\rho_{k,C}}^{2} \boldsymbol{C}_{3} \right)$$

Denote $m_X^{(3)} = \min\{x^2 + y^2 + z^2 : (x, y, z) \in \mathcal{U}_{\Delta X_1, \Delta X_2, \Delta X_3}\}, X = A, B, C$, the optimal uncertainty bounds given by Theorem 2.4 for the observable triples (A_1, A_2, A_3) , (B_1, B_2, B_3) and (C_1, C_2, C_3) , respectively. We have

Theorem 2.7 If a tripartite state ρ is fully separable, then

$$\Delta_{\rho}^{2} \boldsymbol{M}_{1} + \Delta_{\rho}^{2} \boldsymbol{M}_{2} + \Delta_{\rho}^{2} \boldsymbol{M}_{3} \ge m_{A}^{(3)} + m_{B}^{(3)} + m_{C}^{(3)}.$$
(2.13)

From Theorem 2.7, one has that if (2.13) is violated, ρ must be entangled. In addition, denote

$$m_M^{(3)} = \min_{\rho \in \mathcal{D}(\mathbb{C}^2)} \left(\Delta_{\rho}^2 \boldsymbol{M}_1 + \Delta_{\rho}^2 \boldsymbol{M}_2 + \Delta_{\rho}^2 \boldsymbol{M}_3 \right),$$

the uncertainty bound for the observable triple (M_1, M_2, M_3) . We have that if ρ is not fully separable, then

$$m_A^{(3)} + m_B^{(3)} + m_C^{(3)} > \Delta_{\rho}^2 M_1 + \Delta_{\rho}^2 M_2 + \Delta_{\rho}^2 M_3 \ge m_M^{(3)}.$$

Instead of three measurements, we may also consider two measurements with three observables each. Denote $m_X^{(2)} = \min\{x^2 + y^2 : (x, y) \in \mathcal{U}_{\Delta X_1, \Delta X_2}\}$ (X = A, B, C) the optimal uncertainty bounds for the observables pairs (A_1, A_2) , (B_1, B_2) and (C_1, C_2) , respectively, given by Theorem 2.2. Similarly, we get

$$\Delta_{\rho}^{2} \boldsymbol{M}_{1} + \Delta_{\rho}^{2} \boldsymbol{M}_{2} \ge m_{A}^{(2)} + m_{B}^{(2)} + m_{C}^{(2)}.$$
(2.14)

If Eq. (2.14) is violated, ρ must be entangled. Let $m_M^{(2)}$ be the uncertainty bound for the observable pair (M_1, M_2) . We can draw a new criterion that ρ is entangled for

$$m_A^{(2)} + m_B^{(2)} + m_C^{(2)} > \Delta_\rho^2 M_1 + \Delta_\rho^2 M_2 \ge m_M^{(2)}.$$

In [12], the authors considered the entanglement detect for bipartite scenario with two measurements and obtained that

$$\Delta_{\rho}^{2} M_{1} + \Delta_{\rho}^{2} M_{2} \ge m_{A}^{(2)} + m_{B}^{(2)}.$$
(2.15)

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From Theorem 2.7, we can also consider the entanglement detect for bipartite systems with three measurements,

$$\boldsymbol{M}_i = \boldsymbol{A}_i \otimes \mathbb{1} + \mathbb{1} \otimes \boldsymbol{B}_i, \quad i = 1, 2, 3.$$

We have

$$\Delta_{\rho}^{2} M_{1} + \Delta_{\rho}^{2} M_{2} + \Delta_{\rho}^{2} M_{3} \ge m_{A}^{(3)} + m_{B}^{(3)}, \qquad (2.16)$$

where $m_A^{(3)}$ and $m_B^{(3)}$ are the ones given in Theorem 2. The criterion (2.16) is a new one that is different from (2.15) given in [12].

We have investigated uncertainty relations of quantum observables in a random quantum state, by deriving explicitly the probability distribution densities of uncertainty for two, three and multiple qubit observables. As the supports of these density functions, the uncertainty regions are analytically derived. The advantage of the probabilistic approach used in the paper is that it gives a unified framework from which one can obtain the correlations (PDF) among uncertainties of multiple observables and derive analytically the uncertainty regions. Various state-independent uncertainty relations may be derived from the uncertainty regions. Throughout this paper, we have focused on qubit observables. Our framework may be also applied to the case of qudit observables with random mixed quantum state ensembles.

3 Proofs of main results

3.1 Proof of Lemma 2.1

The proof of Lemma 2.1 will be essentially recognized as a series of Propositions 3.1–3.8. Note that in the proof of Lemma 2.1, we directly use Propositions 3.7 and 3.8, which are in fact based on the previous Propositions 3.1–3.6.

Proposition 3.1 (Harish–Chandra–Itzykson–Züber integral [32]) Let *A* and *B* be $n \times n$ Hermitian matrices with eigenvalues $\lambda_1(A) < \cdots < \lambda_n(A)$ and $\lambda_1(B) < \cdots < \lambda_n(B)$, then

$$\int_{\mathcal{U}(\mathbb{C}^n)} e^{z \operatorname{Tr} \left(A U B U^{\dagger} \right)} \mathrm{d} \mu_{\operatorname{Haar}}(U) = C_n \frac{\operatorname{det} \left(e^{z \lambda_i(A) \lambda_j(B)} \right)}{z^{\binom{n}{2}} V(\lambda(A)) V(\lambda(B))} \quad (\forall z \in \mathbb{C} \setminus \{0\})$$

where $d\mu_{\text{Haar}}$ is the Haar measure on the unitary group $U(\mathbb{C}^n)$, $C_n = \prod_{k=1}^n \Gamma(k)$, and $V(\lambda(A)) = \prod_{1 \leq i < j \leq n} (\lambda_j(A) - \lambda_i(A))$ is the so-called Vandermonde determinant.

Any state $\rho \in D(\mathbb{C}^n)$, the set of all quantum states (pure or mixed) on \mathbb{C}^n , can be purified to a bipartite pure state on $\mathbb{C}^n \otimes \mathbb{C}^n$. The set of pure states on $\mathbb{C}^n \otimes \mathbb{C}^n$ can be represented as $\{U | \Phi \rangle : U \in U(\mathbb{C}^n \otimes \mathbb{C}^n)\}$ with $|\Phi\rangle \in \mathbb{C}^n \otimes \mathbb{C}^n$ any fixed pure state and $U(\mathbb{C}^n \otimes \mathbb{C}^n)$ the full unitary group on $\mathbb{C}^n \otimes \mathbb{C}^n$, which is endowed with the standard Haar measure. The induced measure $d\mu(\rho)$ on $D(\mathbb{C}^n)$ is derived from the above Haar

$$d\mu(\rho) = d\nu(\lambda) \times d\mu_{\text{Haar}}(\boldsymbol{U}),$$

where [33], for $0 < \lambda_1 < \cdots < \lambda_n < 1$,

$$\mathrm{d}\nu(\boldsymbol{\lambda}) = N_n \cdot \delta\Big(1 - \sum_{j=1}^n \lambda_j\Big) V^2(\lambda) \prod_{j=1}^n \mathrm{d}\lambda_j$$

is the Lebesgue measure supported on the simplex

$$P_+ := \left\{ (\lambda_1, \lambda_2, \dots, \lambda_n) : 0 < \lambda_1 < \lambda_2 < \dots < \lambda_n < 1, \sum_{j=1}^n \lambda_j = 1 \right\},\$$

where

$$N_n = \frac{\Gamma(n+1)\Gamma(n^2)}{\prod_{j=0}^{n-1}\Gamma(n-j+1)\Gamma(n-j)},$$

and $\delta(\cdot)$ is the Dirac delta function. As usual,

$$\langle \delta, f \rangle = \int_{\mathbb{R}} \delta(x) f(x) dx = f(0),$$

and $\delta_a(x) = \delta(x - a), \langle \delta_a, f \rangle = f(a)$. Denote the zero set of a function $g : \mathbb{R} \to \mathbb{R}$ as $Z(g) = \{x \in \mathbb{R} : g(x) = 0\}$. If $g : \mathbb{R} \to \mathbb{R}$ is a function with continuous derivative such that $Z(g) \cap Z(g') = \emptyset$, then [34]

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

Proposition 3.2 Let A be a non-degenerate positive matrix with eigenvalues $\lambda_1(A) < \cdots < \lambda_n(A)$ and $\lambda(A) = (\lambda_1(A), \ldots, \lambda_n(A))$, then

$$\int_{\mathcal{D}(\mathbb{C}^n)} e^{-i\alpha \operatorname{Tr}(\boldsymbol{A}\rho)} \mathrm{d}\mu(\rho) = \frac{C_n \cdot N_n}{(-i\alpha)^{\binom{n}{2}} V(\lambda(\boldsymbol{A}))} \int_{P_+} \prod_{j=1}^n \mathrm{d}\lambda_j V(\lambda) \det(e^{-i\alpha\lambda_i(\boldsymbol{A})\lambda_j}).$$

Proof Since $d\mu(\rho) = d\nu(\lambda) \times d\mu_{\text{Haar}}(U)$, it follows from Proposition 3.1 that

$$\begin{split} \int_{\mathrm{D}(\mathbb{C}^n)} e^{-\mathrm{i}\alpha \operatorname{Tr}(A\rho)} \mathrm{d}\mu(\rho) &= \int_{P_+} \mathrm{d}\nu(\lambda) \int_{\mathrm{U}(n)} \mathrm{d}\mu_{\mathrm{Haar}}(U) e^{-\mathrm{i}\alpha \operatorname{Tr}(AU\Lambda U^{\dagger})} \\ &= C_n \int_{P_+} \mathrm{d}\nu(\lambda) \frac{\det\left(e^{-\mathrm{i}\alpha\lambda_i(A)\lambda_j}\right)}{(-\mathrm{i}\alpha)^{\binom{n}{2}} V(\lambda(A)) V(\lambda)} \\ &= \frac{C_n}{(-\mathrm{i}\alpha)^{\binom{n}{2}} V(\lambda(A))} \int_{P_+} \mathrm{d}\nu(\lambda) \frac{\det\left(e^{-\mathrm{i}\alpha\lambda_i(A)\lambda_j}\right)}{V(\lambda)} \\ &= \frac{C_n \cdot N_n}{(-\mathrm{i}\alpha)^{\binom{n}{2}} V(\lambda(A))} \int_{P_+} \prod_{j=1}^n \mathrm{d}\lambda_j V(\lambda) \det\left(e^{-\mathrm{i}\alpha\lambda_i(A)\lambda_j}\right), \end{split}$$

which is the desired identity.

Any qubit observable A can be parameterized as

$$\boldsymbol{A} = a_0 \mathbb{1} + \boldsymbol{a} \cdot \boldsymbol{\sigma}, \qquad (a_0, \boldsymbol{a}) \in \mathbb{R}^4,$$

where $\mathbb{1}$ is the identity matrix on the qubit Hilbert space \mathbb{C}^2 , and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ 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 observable A has simple eigenvalues

$$\lambda_k(\mathbf{A}) = a_0 + (-1)^k |\mathbf{a}|, \quad k = 1, 2$$

with $|\mathbf{a}| = \sqrt{a_1^2 + a_2^2 + a_3^2} > 0$ being the length of vector $\mathbf{a} = (a_1, a_2, a_3) \in \mathbb{R}^3$.

Proposition 3.3 For the qubit observable A as above, we have

$$\int_{\mathcal{D}(\mathbb{C}^2)} e^{-i\operatorname{Tr}(\boldsymbol{A}\rho)} \mathrm{d}\mu(\rho) = 3e^{-ia_0} \frac{\sin(|\boldsymbol{a}|) - |\boldsymbol{a}|\cos(|\boldsymbol{a}|)}{|\boldsymbol{a}|^3}.$$

Proof From Proposition 3.2, we have

$$\begin{split} \int_{\mathcal{D}(\mathbb{C}^2)} e^{-i\operatorname{Tr}(A\rho)} d\mu(\rho) &= \frac{C_2 \cdot N_2}{(-i)V(\lambda(A))} \int \prod_{j=1}^2 d\lambda_j \delta\Big(1 - \sum_{j=1}^2 \lambda_j\Big) V(\lambda) \det(e^{-i\alpha\lambda_i(A)\lambda_j}) \\ &= \frac{3i}{|a|} \int_0^{\frac{1}{2}} d\lambda_1 (1 - 2\lambda_1) \left| \begin{array}{c} e^{-i(a_0 - |a|)\lambda_1} & e^{-i(a_0 - |a|)(1 - \lambda_1)} \\ e^{-i(a_0 + |a|)\lambda_1} & e^{-i(a_0 + |a|)(1 - \lambda_1)} \end{array} \right| \\ &= 3e^{-ia_0} \frac{\sin(|a|) - |a|\cos(|a|)}{|a|^3}. \end{split}$$

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This completes the proof.

Now, we derive the probability density functions of uncertainties of observables. We first derive the probability density of the mean value for an observable. Let A be a non-degenerate Hermitian matrix with eigenvalues $\lambda_1(A) < \cdots < \lambda_n(A)$ and $\lambda(A) = (\lambda_1(A), \dots, \lambda_n(A))$. The probability density function of the mean value $\langle A \rangle_{\rho} = \text{Tr} (A\rho)$ is defined as

$$f_{\langle A \rangle}(r) = \int_{\mathcal{D}(\mathbb{C}^n)} \delta(r - \langle A \rangle_{\rho}) \mathrm{d}\mu(\rho).$$

By using the integral representation of the Dirac delta function, $\delta(r) = \frac{1}{2\pi} \int d\alpha e^{ir\alpha}$, we have

$$f_{\langle A \rangle}(r) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\alpha e^{\mathrm{i}r\alpha} \int_{\mathrm{D}(\mathbb{C}^2)} \mathrm{d}\mu(\rho) e^{-\mathrm{i}\alpha \operatorname{Tr}(A\rho)}.$$

By combining Propositions 3.1 and 3.2, we have

$$f_{\langle A \rangle}(r) = \frac{C_n \cdot N_n}{2\pi V(\lambda(A))} \int_{\mathbb{R}} (-i\alpha)^{-\binom{n}{2}} e^{ir\alpha} I_n(\alpha) d\alpha,$$

where

$$I_n(\alpha) = \int_{P_+} \prod_{j=1}^n \mathrm{d}\lambda_j V(\boldsymbol{\lambda}) \det(e^{-\mathrm{i}\alpha\lambda_i(\boldsymbol{A})\lambda_j}).$$

Since the integration is over the simplex P_+ , which can be represented as

$$\begin{cases} 0 < \lambda_1 < \frac{1}{n} \\ \lambda_k < \lambda_{k+1} < \frac{1 - (\lambda_1 + \dots + \lambda_k)}{n - k}, \quad k = 1, \dots, n - 2, \\ \lambda_n = 1 - (\lambda_1 + \dots + \lambda_{n-1}) \end{cases}$$

using the last identity to replace λ_n in the integrand $V(\lambda) \det \left(e^{-i\alpha\lambda_i(A)\lambda_j}\right) = \det \left(\sum_{k=1}^n \lambda_k^{i-1} e^{-i\alpha\lambda_k\lambda_j(A)}\right)$, the integral $I_n(\alpha)$ is reduced to

$$I_n(\alpha) = \int_0^{\frac{1}{n}} \mathrm{d}\lambda_1 \int_{\lambda_1}^{\frac{1-\lambda_1}{n-1}} \mathrm{d}\lambda_2 \cdots \int_{\lambda_{n-2}}^{\frac{1-(\lambda_1+\cdots+\lambda_{n-2})}{2}} \mathrm{d}\lambda_{n-1} \det\Big(\sum_{k=1}^n \lambda_k^{i-1} e^{-\mathrm{i}\alpha\lambda_k\lambda_j(A)}\Big).$$

Proposition 3.4 For a given qubit observable **A** with simple spectrum $\lambda(\mathbf{A}) = (\lambda_1(\mathbf{A}), \lambda_2(\mathbf{A}))$ with $\lambda_1(\mathbf{A}) < \lambda_2(\mathbf{A}))$, the probability distribution density of $\langle \mathbf{A} \rangle_{\rho} =$

Tr $(A\rho)$, where ρ is resulted from partially tracing over a subsystem \mathbb{C}^2 of a Haardistributed random pure state on $\mathbb{C}^2 \otimes \mathbb{C}^2$, is given by

$$f_{\langle A \rangle}(r) = \frac{3!}{V^3(\lambda(A))} (r - \lambda_1(A))(\lambda_2(A) - r) (H(r - \lambda_1(A)) - H(r - \lambda_2(A))),$$

where *H* is the Heaviside function. The support of $f_{\langle A \rangle}(r)$ is the closed interval $[\lambda_1(A), \lambda_2(A)]$.

Proof In particular, when n = 2, we have $C_2 = 1$ and $N_2 = 6$, therefore

$$I_{2}(\alpha) = \int_{0}^{\frac{1}{2}} d\lambda_{1}(1-2\lambda_{1}) \left| \begin{array}{c} e^{-i\alpha\lambda_{1}(A)\lambda_{1}} & e^{-i\alpha\lambda_{1}(A)(1-\lambda_{1})} \\ e^{-i\alpha\lambda_{2}(A)\lambda_{1}} & e^{-i\alpha\lambda_{2}(A)(1-\lambda_{1})} \end{array} \right| \\ = \frac{1}{(\lambda_{2}(A) - \lambda_{1}(A))^{2}\alpha^{2}} \sum_{k=1}^{2} e^{-i\lambda_{k}(A)\alpha} (i(\lambda_{2}(A) - \lambda_{1}(A))\alpha + (-1)^{k}2),$$

and

$$f_{\langle A \rangle}(r) = \frac{3!}{2\pi V^3(\lambda(A))} \int_{\mathbb{R}} \mathrm{d}\alpha \alpha^{-3} e^{\mathrm{i}r\alpha} \sum_{k=1}^2 e^{-\mathrm{i}\lambda_k(A)\alpha} ((\lambda_1(A) - \lambda_2(A))\alpha + (-1)^k 2\mathrm{i}).$$

Let $\varphi(\alpha) = \alpha^{-3} e^{ir\alpha} \sum_{k=1}^{2} e^{-i\lambda_k(A)\alpha} ((\lambda_1(A), -\lambda_2(A))\alpha + (-1)^k 2i)$ and $H(\cdot)$ be the Heaviside function, then

$$\int_{\mathbb{R}} \varphi(\alpha) d\alpha = \int_{0}^{\infty} (\varphi(\alpha) + \varphi(-\alpha)) d\alpha$$

= $2\pi (\lambda_2(A) - r)(r - \lambda_1(A)) (H(r - \lambda_1(A)) - H(r - \lambda_2(A))),$

and we come to the result.

Proposition 3.5 For any qubit observable $\mathbf{A} = a_0 \mathbb{1} + \mathbf{a} \cdot \boldsymbol{\sigma}$, $(a_0, \mathbf{a}) \in \mathbb{R}^4$, the probability distribution density of the uncertainty $\Delta_{\rho} \mathbf{A}$, where ρ is resulted from partially tracing over a subsystem \mathbb{C}^2 of a Haar-distributed random pure state on $\mathbb{C}^2 \otimes \mathbb{C}^2$, is given by

$$f_{\Delta A}(x) = \frac{3x^3}{2 |a|^3 \sqrt{|a|^2 - x^2}}.$$

Proof From $\delta(r^2 - r_0^2) = \frac{1}{2|r_0|} (\delta(r - r_0) + \delta(r + r_0))$, we conclude that

$$\delta(x^2 - (\Delta_{\rho} A)^2) = \frac{1}{2x} (\delta(x + \Delta_{\rho} A) + \delta(x - \Delta_{\rho} A)) = \frac{1}{2x} \delta(x - \Delta_{\rho} A), \qquad x \ge 0.$$

For any complex 2×2 matrix *A*,

$$A^{2} = \operatorname{Tr}(A) A - \det(A)\mathbb{1}, \quad \det(A) = \frac{(\operatorname{Tr} A)^{2} - \operatorname{Tr}(A^{2})}{2},$$

and thus

$$\delta\left(x^2 - (\Delta_{\rho}A)^2\right) = \delta\left(x^2 + \det(A) - \operatorname{Tr}(A)\langle A \rangle_{\rho} + \langle A \rangle_{\rho}^2\right).$$

Consequently,

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$$\begin{split} f_{\Delta A}(x) &= \int_{\mathcal{D}(\mathbb{C}^2)} \mathrm{d}\mu(\rho)\delta(x - \Delta_{\rho}A) \\ &= 2x \int_{\mathcal{D}(\mathbb{C}^2)} \mathrm{d}\mu(\rho)\delta\left(x^2 - (\Delta_{\rho}A)^2\right) \\ &= 2x \int_{\mathbb{R}} \mathrm{d}r\delta\left(\left(x^2 + \det(A)\right) - \operatorname{Tr}(A)r + r^2\right) \int_{\mathcal{D}(\mathbb{C}^2)} \mathrm{d}\mu(\rho)\delta(r - \langle A \rangle_{\rho}) \\ &= 2x \int_{\mathbb{R}} \mathrm{d}rf_{\langle A \rangle}(r)\delta\left(x^2 + \det(A) - \operatorname{Tr}(A)r + r^2\right) \\ &= 2x \int_{\lambda_1(A)}^{\lambda_2(A)} \mathrm{d}rf_{\langle A \rangle}(r)\delta\left(x^2 + \lambda_1(A)\lambda_2(A) - (\lambda_1(A) + \lambda_2(A))r + r^2\right) \\ &= \frac{12x}{V^3(\lambda(A))} \int_{\lambda_1(A)}^{\lambda_2(A)} \mathrm{d}r(r - \lambda_1(A))(\lambda_2(A) - r)\delta\left(x^2 - (r - \lambda_1(A))(\lambda_2(A) - r)\right). \end{split}$$

where we used Proposition 3.4 in the last equality. For $A = a_0 \mathbb{1} + \boldsymbol{a} \cdot \boldsymbol{\sigma}$, we have $V(\lambda(\boldsymbol{A})) = 2 |\boldsymbol{a}|$. For any fixed *x*, let $g_x(r) = x^2 - (r - \lambda_1(\boldsymbol{A}))(\lambda_2(\boldsymbol{A}) - r)$, then $g'_x(r) = \partial_r g_x(r) = 2r - \lambda_1(\boldsymbol{A}) - \lambda_2(\boldsymbol{A})$. For fixed *x*, the equation $g_x(r) = 0$ has two distinct roots

$$r_{\pm}(x) = \frac{\lambda_1(A) + \lambda_2(A) \pm \sqrt{V^2(\lambda(A)) - 4x^2}}{2} = a_0 \pm \sqrt{|a|^2 - x^2}$$

in $[\lambda_1(A), \lambda_2(A)]$ if and only if $x \in [0, V(\lambda(A))/2)$. In this case,

$$\delta(g_{x}(r)) = \frac{1}{|g'_{x}(r_{+}(x))|} \delta_{r_{+}(x)} + \frac{1}{|g'_{x}(r_{-}(x))|} \delta_{r_{-}(x)},$$

which implies that

$$f_{\Delta A}(x) = \frac{12x}{V^3(\lambda(A))} \left(\frac{(r_+(x) - \lambda_1(A))(\lambda_2(A) - r_+(x))}{2r_+(x) - \lambda_1(A) - \lambda_2(A)} + \frac{(r_-(x) - \lambda_1(A))(\lambda_2(A) - r_-(x))}{\lambda_1(A) + \lambda_2(A) - 2r_-(x)} \right)$$
$$= \frac{24x^3}{V^3(\lambda(A))\sqrt{V(\lambda(A))^2 - 4x^2}} = \frac{3x^3}{2 |a|^3 \sqrt{|a|^2 - x^2}}.$$

This completes the proof.

Proposition 3.6 Let $J_0(z) = \frac{1}{\pi} \int_0^{\pi} \cos(z \cos \theta) d\theta$ be the Bessel function of first kind. Then, we have the following identity:

$$\int_0^\infty \frac{\sin q - q \cos q}{q^2} J_0(\lambda q) \mathrm{d}q = \begin{cases} \sqrt{1 - \lambda^2}, & \text{if } |\lambda| < 1; \\ 0, & \text{if } |\lambda| \ge 1. \end{cases}$$

Proof Denote

$$\Phi(\lambda) = \int_0^\infty \frac{\sin q - q \cos q}{q^2} J_0(\lambda q) dq \quad (\forall \lambda \in \mathbb{R}).$$

Clearly, $\Phi(\lambda)$ is even and

$$\Phi(0) = \int_0^\infty \frac{\sin q - q \cos q}{q^2} d\tau = -\frac{\sin q}{q} \Big|_0^\infty = 1.$$

Without loss of generality, we assume that $\lambda > 0$, then

$$\begin{split} \Phi(\lambda) &= -\int_0^\infty d\left(\frac{\sin q}{q}\right) J_0(\lambda q) \\ &= -J_0(\lambda q) \frac{\sin q}{q} \Big|_0^\infty + \int_0^\infty \frac{\sin q}{q} d(J_0(\lambda q)) \\ &= 1 - \lambda \int_0^\infty \frac{\sin q}{q} J_1(\lambda q) dq, \end{split}$$

where $J_1(z) = \frac{1}{\pi} \int_0^{\pi} d\theta \cos \theta \sin(z \cos \theta)$. Noting that

$$\int_0^\infty \frac{\sin q}{q} J_1(\lambda q) \mathrm{d}q = \begin{cases} \frac{1 - \sqrt{1 - \lambda^2}}{\lambda}, & \lambda \in (0, 1) \\ \frac{1}{\lambda}, & \lambda \in [1, +\infty) \end{cases}$$

we get

$$\Phi(\lambda) = \begin{cases} \sqrt{1 - \lambda^2}, & \text{if } |\lambda| < 1; \\ 0, & \text{if } |\lambda| \ge 1. \end{cases}$$

This completes the proof.

Recall that a support of a function f, defined on the domain D(f), is defined by

$$\operatorname{supp}(f) = \overline{\{x \in D(f) : f(x) \neq 0\}}.$$

That is, the closure of the subset of D(f) in which f does not vanish. From this, we see that $\operatorname{supp}(f_{\Delta A}) = [0, |a|].$

Before we study the probability distribution density

$$f_{\Delta \boldsymbol{A},\Delta \boldsymbol{B}}(\boldsymbol{x},\boldsymbol{y}) = \int_{\mathrm{D}(\mathbb{C}^2)} \delta(\boldsymbol{x} - \Delta_{\rho} \boldsymbol{A}) \delta(\boldsymbol{y} - \Delta_{\rho} \boldsymbol{B}) \mathrm{d}\mu(\rho)$$

of the uncertainties $(\Delta_{\rho} A, \Delta_{\rho} B)$ for a pair of qubit observables A, B, we first consider the joint probability distribution density

$$f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle}(r, s) = \int_{\mathcal{D}(\mathbb{C}^2)} \delta(r - \langle \boldsymbol{A} \rangle_{\rho}) \delta(s - \langle \boldsymbol{B} \rangle_{\rho}) \mathrm{d}\mu(\rho)$$

of the mean values $(\langle A \rangle_{\rho}, \langle B \rangle_{\rho})$, where ρ is resulted from partially tracing over a subsystem \mathbb{C}^2 of a Haar-distributed random pure state on $\mathbb{C}^2 \otimes \mathbb{C}^2$.

Proposition 3.7 Let $A = a_0 \mathbb{1} + a \cdot \sigma$, $B = b_0 \mathbb{1} + b \cdot \sigma$, $(a_0, a), (b_0, b) \in \mathbb{R}^4$ be a pair of qubit observables. Let

$$T_{a,b} = \begin{pmatrix} \langle a, a \rangle & \langle a, b \rangle \\ \langle b, a \rangle & \langle b, b \rangle \end{pmatrix}.$$

(i) If $\{a, b\}$ is linearly independent, then

$$f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle}(\boldsymbol{r}, \boldsymbol{s}) = \frac{3}{2\pi\sqrt{\det(\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}})}} \sqrt{1 - \omega_{\boldsymbol{A}, \boldsymbol{B}}^2(\boldsymbol{r}, \boldsymbol{s})} H(1 - \omega_{\boldsymbol{A}, \boldsymbol{B}}(\boldsymbol{r}, \boldsymbol{s})),$$

where $\omega_{A,B}(r,s) = \sqrt{(r-a_0,s-b_0)T_{a,b}^{-1}(r-a_0,s-b_0)^{T}}$.

(ii) If $\{a, b\}$ is linearly dependent, without loss of generality, we assume that $b = \kappa \cdot a$ for some nonzero κ , then

$$f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle}(r, s) = \delta((s - b_0) - \kappa(r - a_0)) f_{\langle \boldsymbol{A} \rangle}(r),$$

where $f_{\langle A \rangle}(r)$ is from Proposition 3.4.

Proof By using integral representation of delta function twice, we get

$$f_{\langle \boldsymbol{A}\rangle,\langle \boldsymbol{B}\rangle}(\boldsymbol{r},s) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \mathrm{d}\alpha \mathrm{d}\beta e^{\mathrm{i}(\boldsymbol{r}\alpha+s\beta)} \int_{\mathrm{D}(\mathbb{C}^2)} \mathrm{d}\mu(\rho) e^{-\mathrm{i}\operatorname{Tr}((\alpha \boldsymbol{A}+\beta \boldsymbol{B})\rho)},$$

and by Proposition 3.3, we have get

$$\int_{\mathcal{D}(\mathbb{C}^2)} e^{-i\operatorname{Tr}((\alpha A + \beta B)\rho)} d\mu(\rho)$$

= $3e^{-i(a_0\alpha + b_0\beta)} \frac{\sin(|\alpha a + \beta b|) - |\alpha a + \beta b| \cos(|\alpha a + \beta b|)}{|\alpha a + \beta b|^3}$

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Thus,

$$f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle}(\boldsymbol{r}, \boldsymbol{s}) = \frac{3}{(2\pi)^2} \int_{\mathbb{R}^2} d\alpha d\beta e^{i((\boldsymbol{r}-\boldsymbol{a}_0)\alpha + (\boldsymbol{s}-\boldsymbol{b}_0)\beta)} \\ \frac{\sin(|\alpha \boldsymbol{a} + \beta \boldsymbol{b}|) - |\alpha \boldsymbol{a} + \beta \boldsymbol{b}| \cos(|\alpha \boldsymbol{a} + \beta \boldsymbol{b}|)}{|\alpha \boldsymbol{a} + \beta \boldsymbol{b}|^3}.$$

(i) Noting that $\{a, b\}$ is linearly independent if and only if $T_{a,b}$ is invertible, it follows that $|\alpha a + \beta b|$ can be rewritten as $|\alpha a + \beta b| = \sqrt{\tilde{\alpha}^2 + \tilde{\beta}^2}$ with $(\tilde{\alpha}, \tilde{\beta})^{\mathsf{T}} = T_{a,b}^{\frac{1}{2}}(\alpha, \beta)^{\mathsf{T}}$. Let $(\tilde{r}, \tilde{s}) = (r, s)T_{a,b}^{-\frac{1}{2}}$, then $d\tilde{\alpha}d\tilde{\beta} = \sqrt{\det(T_{a,b})}d\alpha d\beta$, or equivalently, $d\alpha d\beta = \frac{1}{\sqrt{\det(T_{a,b})}}d\tilde{\alpha}d\tilde{\beta}$. By change of variables $(\alpha, \beta) \to (\tilde{\alpha}, \tilde{\beta})$, we have

$$f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle}(\boldsymbol{r}, \boldsymbol{s}) = \frac{3}{(2\pi)^2 \sqrt{\det(\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}})}} \int_{\mathbb{R}^2} d\tilde{\alpha} d\tilde{\beta} e^{i((\tilde{r} - \tilde{a}_0)\tilde{\alpha} + (\tilde{s} - \tilde{b}_0)\tilde{\beta})} \\ \frac{\sin\left(\sqrt{\tilde{\alpha}^2 + \tilde{\beta}^2}\right) - \sqrt{\tilde{\alpha}^2 + \tilde{\beta}^2} \cos\left(\sqrt{\tilde{\alpha}^2 + \tilde{\beta}^2}\right)}{\left(\sqrt{\tilde{\alpha}^2 + \tilde{\beta}^2}\right)^3}.$$

Furthermore, using the polar coordinate $\tilde{\alpha} = q \cos \theta$, $\tilde{\beta} = q \sin \theta$, $q \ge 0, \theta \in [0, 2\pi]$, then $\omega_{A,B}(r, s) = \sqrt{(\tilde{r} - \tilde{a}_0)^2 + (\tilde{s} - \tilde{b}_0)^2}$. Noting the fact that

$$\int_0^{2\pi} e^{i(u\cos\theta + v\sin\theta)} d\theta = 2\pi J_0(\sqrt{u^2 + v^2}) \quad (\forall u, v \in \mathbb{R})$$

where $J_0(z) = \frac{1}{\pi} \int_0^{\pi} \cos(z \cos \theta) d\theta$ is the Bessel function of first kind, we have

$$\begin{split} f_{\langle A \rangle, \langle B \rangle}(r,s) &= \frac{3}{(2\pi)^2 \sqrt{\det(T_{a,b})}} \int_0^\infty dq \frac{\sin q - q \cos q}{q^2} \\ &\int_0^{2\pi} d\theta e^{iq[(\tilde{r} - \tilde{a}_0) \cos \theta + (\tilde{s} - \tilde{b}_0) \sin \theta]} \\ &= \frac{3}{2\pi \sqrt{\det(T_{a,b})}} \int_0^\infty dq \frac{\sin q - q \cos q}{q^2} J_0 \\ &\left(q \sqrt{(\tilde{r} - \tilde{a}_0)^2 + (\tilde{s} - \tilde{b}_0)^2}\right) \\ &= \frac{3}{2\pi \sqrt{\det(T_{a,b})}} \int_0^\infty \frac{\sin q - q \cos q}{q^2} J_0 \left(q \cdot \omega_{A,B}(r,s)\right) dq \\ &= \frac{3}{2\pi \sqrt{\det(T_{a,b})}} \sqrt{1 - \omega_{A,B}^2(r,s)} H(1 - \omega_{A,B}(r,s)). \end{split}$$

Here in the last equality, we used Proposition 3.6.

(ii) If $\{a, b\}$ is linearly dependent, without loss of generality, we assume that $b = \kappa \cdot a$ for some $\kappa \neq 0$. Performing change of variables $(\alpha, \beta) \rightarrow (\alpha', \beta')$ where $\alpha' = \alpha + \kappa \beta$ and $\beta' = \beta$, the Jacobian is given by

$$\det\left(\frac{\partial(\alpha',\,\beta')}{\partial(\alpha,\,\beta)}\right) = \left|\begin{array}{c} 1 \ \kappa \\ 0 \ 1 \end{array}\right| = 1 \neq 0.$$

Now,

$$f_{\langle A \rangle, \langle B \rangle}(r, s) = \frac{3}{4\pi^2} \int_{\mathbb{R}^2} d\alpha' d\beta' e^{i((r-a_0)(\alpha'-\kappa\beta')+(s-b_0)\beta')} \\ \frac{\sin(|a||\alpha'|) - |a||\alpha'|\cos(|a||\alpha'|)}{|a|^3|\alpha'|^3} \\ = \frac{1}{2\pi} \int_{\mathbb{R}} e^{i((s-b_0)-\kappa(r-a_0))\beta'} d\beta' \times \frac{3}{2\pi} \int_{\mathbb{R}} d\alpha' e^{i(r-a_0)\alpha'} \\ \frac{\sin(|a||\alpha'|) - |a||\alpha'|\cos(|a||\alpha'|)}{|a|^3|\alpha'|^3} \\ = \delta \left((s-b_0) - \kappa(r-a_0) \right) \times \frac{3}{2\pi} \int_{\mathbb{R}} d\alpha' e^{i(r-a_0)\alpha'} \\ \frac{\sin(|a||\alpha'|) - |a||\alpha'|\cos(|a||\alpha'|)}{(|a||\alpha'|)^3}$$

where

$$\frac{3}{2\pi} \int_{\mathbb{R}} d\alpha' e^{i(r-a_0)\alpha'} \frac{\sin(|\mathbf{a}| | \alpha' |) - |\mathbf{a}| | \alpha' | \cos(|\mathbf{a}| | \alpha' |)}{(|\mathbf{a}| | \alpha' |)^3}$$

$$= \frac{3}{2\pi} \int_0^\infty d\alpha' \left(e^{i(r-a_0)\alpha'} + e^{-i(r-a_0)\alpha'} \right) \frac{\sin(|\mathbf{a}| | \alpha' |) - |\mathbf{a}| | \alpha' | \cos(|\mathbf{a}| | \alpha' |)}{(|\mathbf{a}| | \alpha' |)^3}$$

$$= \frac{3}{2\pi} \frac{1}{|\mathbf{a}|} \int_0^\infty \left(e^{i\frac{r-a_0}{|\mathbf{a}|}q} + e^{-i\frac{r-a_0}{|\mathbf{a}|}q} \right) \frac{\sin q - q \cos q}{q^3} dq$$

$$= \frac{6}{2\pi} \frac{1}{|\mathbf{a}|} \int_0^\infty dq \cos\left(\frac{r-a_0}{|\mathbf{a}|}q\right) \frac{\sin q - q \cos q}{q^3}$$

Due to the fact that

$$\int_0^\infty dq \cos(pq) \frac{\sin q - q \cos q}{q^3} = \begin{cases} \frac{\pi}{4}(1 - p^2), & \text{if } |p| \le 1\\ 0, & \text{if } |p| \ge 1 \end{cases}$$

we obtain

$$\frac{3}{2\pi} \int_{\mathbb{R}} \mathrm{d}\alpha' e^{\mathrm{i}(r-a_0)\alpha'} \frac{\sin(|\mathbf{a}| | \alpha' |) - |\mathbf{a}| | \alpha' | \cos(|\mathbf{a}| | \alpha' |)}{(|\mathbf{a}| | \alpha' |)^3}$$

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and use the fact that $|\mathbf{a}| = \frac{\lambda_2(A) - \lambda_1(A)}{2}$ and $a_0 = \frac{1}{2} \operatorname{Tr} (\mathbf{A}) = \frac{\lambda_1(A) + \lambda_2(A)}{2}$, we have

$$\frac{3}{2\pi} \int_{\mathbb{R}} d\alpha' e^{i(r-a_0)\alpha'} \frac{\sin(|\mathbf{a}| |\alpha'|) - |\mathbf{a}| |\alpha'| \cos(|\mathbf{a}| |\alpha'|)}{(|\mathbf{a}| |\alpha'|)^3} \\ = \frac{3!}{V^3(\lambda(\mathbf{A}))} (r - \lambda_1(\mathbf{A}))(\lambda_2(\mathbf{A}) - r)(H(r - \lambda_1(\mathbf{A})) - H(r - \lambda_2(\mathbf{A}))) = f_{(\mathbf{A})}(r).$$

Therefore,

$$f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle}(r, s) = \delta((s - b_0) - \kappa(r - a_0)) f_{\langle \boldsymbol{A} \rangle}(r),$$

where $f_{(A)}(r)$ is from Proposition 3.4, which is the desired result.

Proposition 3.8 The joint probability distribution density of the uncertainties $(\Delta_{\rho} A, \Delta_{\rho} B)$ for a pair of qubit observables $A = a_0 \mathbb{1} + a \cdot \sigma$, $B = b_0 \mathbb{1} + b \cdot \sigma$, $(a_0, a), (b_0, b) \in \mathbb{R}^4$, where $\{a, b\}$ is linearly independent, and ρ is resulted from partially tracing a subsystem over a Haar-distributed random pure state on $\mathbb{C}^2 \otimes \mathbb{C}^2$, is given by

$$f_{\Delta A,\Delta B}(x, y) = \frac{2xy \sum_{j \in \{\pm\}} f_{\langle A \rangle, \langle B \rangle}(r_+(x), s_j(y))}{\sqrt{(|a|^2 - x^2)(|b|^2 - y^2)}},$$

where $r_{\pm}(x) = a_0 \pm \sqrt{|a|^2 - x^2}$, $s_{\pm}(y) = b_0 \pm \sqrt{|b|^2 - y^2}$, and $f_{\langle A \rangle, \langle B \rangle}(\cdot, \cdot)$ is given in Proposition 3.7.

Proof Noting that

$$\delta(x^2 - (\Delta_\rho A)^2) = \delta(x^2 - (r - \lambda_1(A))(\lambda_2(A) - r))) = \delta(g_x(r)),$$

where $g_x(r) = x^2 - (r - \lambda_1(A))(\lambda_2(A) - r)$. Similarly, $\delta(y^2 - (\Delta_\rho B)^2) = \delta(h_y(s))$, where $h_y(s) = y^2 - (s - \lambda_1(B))(\lambda_2(B) - s)$. Consequently,

$$f_{\Delta A,\Delta B}(x, y) = 4xy \int_{\mathcal{D}(\mathbb{C}^2)} d\mu(\rho)\delta(x^2 - (\Delta_{\rho}A)^2)\delta(y^2 - (\Delta_{\rho}B)^2)$$
$$= 4xy \int_{\mathbb{R}^2} dr ds f_{\langle A \rangle, \langle B \rangle}(r, s)\delta(g_x(r))\delta(h_y(s)),$$

where $f_{\langle A \rangle, \langle B \rangle}(r, s)$ is determined by Proposition 3.7. Noting that

$$\delta(g_{x}(r)) = \frac{1}{|g'_{x}(r_{+}(x))|} \delta_{r_{+}(x)} + \frac{1}{|g'_{x}(r_{-}(x))|} \delta_{r_{-}(x)},$$

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$$\delta(h_{y}(s)) = \frac{1}{\left|h'_{y}(s_{+}(y))\right|} \delta_{s_{+}(y)} + \frac{1}{\left|h'_{y}(s_{-}(y))\right|} \delta_{s_{-}(y)},$$

we obtain

$$\delta(g_x(r))\delta(h_y(s)) = \frac{\delta_{(r_+,s_+)} + \delta_{(r_+,s_-)} + \delta_{(r_-,s_+)} + \delta_{(r_-,s_-)}}{4\sqrt{(|\boldsymbol{a}|^2 - x^2)(|\boldsymbol{b}|^2 - y^2)}}.$$

Based on this observation, we get

$$f_{\Delta A,\Delta B}(x, y) = \frac{xy}{\sqrt{(|a|^2 - x^2)(|b|^2 - y^2)}} \sum_{i,j \in \{\pm\}} f_{\langle A \rangle, \langle B \rangle}(r_i, s_j).$$

It is easily checked that $\omega_{A,B}(r_+, s_+) = \omega_{A,B}(r_-, s_-)$, $\omega_{A,B}(r_+, s_-) = \omega_{A,B}(r_-, s_+)$, therefore

$$\sum_{\substack{i,j\in\{\pm\}\\}} f_{\langle A\rangle,\langle B\rangle}(r_i,s_j)$$
$$= 2\sum_{j\in\{\pm\}} f_{\langle A\rangle,\langle B\rangle}(r_+,s_j),$$

and

$$f_{\Delta \boldsymbol{A},\Delta \boldsymbol{B}}(x,y) = \frac{2xy\sum_{j\in\{\pm\}}f_{\langle \boldsymbol{A}\rangle,\langle \boldsymbol{B}\rangle}(r_+,s_j)}{\sqrt{(|\boldsymbol{a}|^2 - x^2)(|\boldsymbol{b}|^2 - y^2)}},$$

which is the desired result.

Proof of Lemma 2.1 With Proposition 3.8, we now make an analysis of the support of $f_{\Delta A, \Delta B}$. In fact, due to the relation between $f_{\Delta A, \Delta B}$ and $f_{\langle A \rangle, \langle B \rangle}$, the support of $f_{\Delta A, \Delta B}$ can be identified by the support of $f_{\langle A \rangle, \langle B \rangle}$ which can be seen from Proposition 3.7 (i),

$$\operatorname{supp}(f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle}) = \left\{ (r, s) \in \mathbb{R}^2 : \omega_{\boldsymbol{A}, \boldsymbol{B}}(r, s) \leq 1 \right\}.$$

Note that $f_{\Delta A,\Delta B}(x, y)$ is defined on the first quadrant $\mathbb{R}^2_{\geq 0}$, if xy > 0, then $f_{\Delta A,\Delta B}(x, y) = 0$ if and only if

$$\sum_{i,j\in\{\pm\}} f_{\langle A\rangle,\langle B\rangle}(r_i(x),s_j(y)) = 0,$$

i.e., $f_{\langle A \rangle, \langle B \rangle}(r_i(x), s_j(y)) = 0$ because $f_{\langle A \rangle, \langle B \rangle}$ is a non-negative function. This means that all four points $(r_{\pm}(x), s_{\pm}(y))$ are not in the support of $f_{\langle A \rangle, \langle B \rangle}$. Therefore, the

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uncertainty region (i.e., the support of $f_{\Delta A, \Delta B}$) of A and B is given by the following set:

$$\mathcal{U}_{\Delta A,\Delta B} = \operatorname{supp}(f_{\Delta A,\Delta B}) = D_{a,b}^+ \cup D_{a,b}^-,$$

where, via $\boldsymbol{u}_{\epsilon}(x, y) = \left(\sqrt{|\boldsymbol{a}|^2 - x^2}, \epsilon \sqrt{|\boldsymbol{b}|^2 - y^2}\right),$
$$D_{a,b}^{\epsilon} := \left\{ (x, y) \in \mathbb{R}^2_{\geq 0} \cap ([0, |\boldsymbol{a}|] \times [0, |\boldsymbol{b}|]) : \boldsymbol{u}_{\epsilon}(x, y) \boldsymbol{T}_{a,b}^{-1} \boldsymbol{u}_{\epsilon}^{\mathsf{T}}(x, y) \leq 1 \right\}, \quad \epsilon \in \{\pm\}.$$

This is what we want. Furthermore, we have

$$D_{a,b}^{\epsilon} = \left\{ (x, y) \in \mathbb{R}^{2}_{\geq 0} \cap ([0, |a|] \times [0, |b|]) : |b|^{2} x^{2} + |a|^{2} y^{2} + 2\epsilon \langle a, b \rangle \sqrt{(|a|^{2} - x^{2})(|b|^{2} - y^{2})} \geq |a|^{2} |b|^{2} + \langle a, b \rangle^{2} \right\}.$$

Therefore, the uncertainty region $\mathcal{U}_{\Delta A, \Delta B} = \left\{ (\Delta_{\rho} A, \Delta_{\rho} B) \in \mathbb{R}^2_{\geq 0} : \rho \in D(\mathbb{C}^2) \right\}$ of *A* and *B* is determined by the following inequality:

$$|\mathbf{b}|^{2} x^{2} + |\mathbf{a}|^{2} y^{2} + 2 |\langle \mathbf{a}, \mathbf{b} \rangle |\sqrt{(|\mathbf{a}|^{2} - x^{2})(|\mathbf{b}|^{2} - y^{2})} \ge |\mathbf{a}|^{2} |\mathbf{b}|^{2} + \langle \mathbf{a}, \mathbf{b} \rangle^{2},$$

where $x \in [0, |a|]$ and $y \in [0, |b|]$.

3.2 Proof of formula (2.6)

Since the $\mathcal{U}(\theta)$ is defined by

$$\mathcal{U}(\theta) := \left\{ (x, y) \in [0, 1]^2 : x^2 + y^2 + 2 |\cos \theta| \sqrt{(1 - x^2)(1 - y^2)} \ge 1 + \cos^2 \theta \right\}.$$

The volume (i.e., the area for 2D domain) of the uncertainty region $\mathcal{U}(\theta)(\theta \in [0, \pi/2])$ is calculated as follows

$$\operatorname{vol}(\mathcal{U}(\theta)) = \frac{1}{2}(\pi - 3\theta)\sin\theta - \cos\theta + 1.$$

Indeed, if $\theta \in [0, \pi/4]$, then $\mathcal{U}(\theta)$ becomes

$$0 \leqslant x \leqslant \sin \theta, -x \cos \theta + \sin \theta \sqrt{1 - x^2} \leqslant y \leqslant x \cos \theta + \sin \theta \sqrt{1 - x^2};$$

$$\sin \theta \leqslant x \leqslant \cos \theta, x \cos \theta - \sin \theta \sqrt{1 - x^2} \leqslant y \leqslant x \cos \theta + \sin \theta \sqrt{1 - x^2};$$

$$\cos \theta \leqslant x \leqslant 1, x \cos \theta - \sin \theta \sqrt{1 - x^2} \leqslant y \leqslant 1.$$

Hence,

$$\operatorname{vol}(\mathcal{U}(\theta)) = \int_0^{\sin\theta} \mathrm{d}x \int_{\sqrt{1-x^2}\sin\theta - x\cos\theta}^{\sqrt{1-x^2}\sin\theta + x\cos\theta} \mathrm{d}y + \int_{\sin\theta}^{\cos\theta} \int_{x\cos\theta - \sqrt{1-x^2}\sin\theta}^{x\cos\theta + \sqrt{1-x^2}\sin\theta} \mathrm{d}y$$

$$+ \int_{\cos\theta}^{1} dx \int_{x\cos\theta - \sqrt{1 - x^2}\sin\theta}^{1} dy$$
$$= \frac{1}{2} (\pi - 3\theta) \sin\theta - \cos\theta + 1.$$

If $\theta \in [\pi/4, \pi/2]$, then $\mathcal{U}(\theta)$ becomes

$$0 \leq x \leq \cos\theta, -x\cos\theta + \sin\theta\sqrt{1 - x^2} \leq y \leq x\cos\theta + \sin\theta\sqrt{1 - x^2};$$

$$\cos\theta \leq x \leq \sin\theta, -x\cos\theta + \sin\theta\sqrt{1 - x^2} \leq y \leq 1;$$

$$\sin\theta \leq x \leq 1, x\cos\theta - \sin\theta\sqrt{1 - x^2} \leq y \leq 1,$$

implying that

$$\operatorname{vol}(\mathcal{U}(\theta)) = \int_0^{\cos\theta} dx \int_{\sqrt{1-x^2}\sin\theta + x\cos\theta}^{\sqrt{1-x^2}\sin\theta + x\cos\theta} dy + \int_{\cos\theta}^{\sin\theta} dx \int_{\sqrt{1-x^2}\sin\theta - x\cos\theta}^1 dy + \int_{\sin\theta}^1 dx \int_{x\cos\theta - \sqrt{1-x^2}\sin\theta}^1 dy = \frac{1}{2}(\pi - 3\theta)\sin\theta - \cos\theta + 1.$$

In summary, we get the desired result. We remark here that for general lengths |a| and |b|, we immediately get that $\operatorname{vol}(\mathcal{U}_{\Delta A,\Delta B}) = |a| |b| \operatorname{vol}(\mathcal{U}(\theta))$.

As some representatives, in Fig. 3, we plot the PDFs (probability density functions) over their respective uncertainty regions $\mathcal{U}(\theta)$ for $\theta \in \{\frac{\pi}{8}, \frac{\pi}{4}, \frac{3\pi}{8}\}$, and the probability density functions on $\mathcal{U}(\theta)$.

3.3 Proof of Theorem 2.2

Based on the proof of Lemma 2.1, we now present the proof of Theorem 2.2.

Proof of Theorem 2.2 Let $\sqrt{|a|^2 - x^2} = X$, $\sqrt{|b|^2 - y^2} = Y$ in Lemma 2.1, where $X \in [0, |a|], Y \in [0, |b|]$ due to the fact that $x \in [0, |a|], y \in [0, |b|]$. Thus, we get that

$$\min\left\{x^2 + y^2 : (x, y) \in \mathcal{U}_{\Delta A, \Delta B}\right\}$$

= Tr $(\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}})$ - max $\left\{X^2 + Y^2 : (X, \pm Y)\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}}^{-1}(X, \pm Y)^{\mathsf{T}} \leqslant 1\right\}$.

It is easily seen that the objection function $x^2 + y^2$, where $(x, y) \in \mathcal{U}_{\Delta A, \Delta B}$, attains its minimal value on the boundary curve $\partial \mathcal{U}_{\Delta A, \Delta B}$ of the uncertainty region $\mathcal{U}_{\Delta A, \Delta B}$; this also corresponds to the objection function $X^2 + Y^2$ attains its maximal value on the boundary curve $(X, \pm Y)T_{a,b}^{-1}(X, \pm Y)^{\mathsf{T}} = 1$.

Denote by $\lambda_k(T_{a,b})(k = 1, 2)$ the two eigenvalues of the matrix $T_{a,b}$. By Spectral Decomposition Theorem, we get that there exists orthogonal $O \in O(2)$ such that



Fig. 3 Plots of the uncertainty region $\mathcal{U}(\theta)$ and the pdf on it for a pair of qubit observables $\mathbf{A} = a_0 \mathbb{1} + \mathbf{a} \cdot \boldsymbol{\sigma}$ and $\mathbf{B} = b_0 \mathbb{1} + \mathbf{b} \cdot \boldsymbol{\sigma}$, where $|\mathbf{a}| = |\mathbf{b}| = 1$ and $\langle \mathbf{a}, \mathbf{b} \rangle = \cos(\theta)$

$$\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b}} = \boldsymbol{O} \operatorname{diag}(\lambda_1(\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b}}), \lambda_2(\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b}})) \boldsymbol{O}^{\mathsf{T}}.$$

Now, let $(X', Y')^{\mathsf{T}} = \boldsymbol{O}(X, \pm Y)^{\mathsf{T}}$. Then,

$$(X, \pm Y)T_{a,b}^{-1}(X, \pm Y)^{\mathsf{T}} = (X', Y')\operatorname{diag}(\lambda_1^{-1}(T_{a,b}), \lambda_2^{-1}(T_{a,b}))(X', Y')^{\mathsf{T}}$$
$$= \frac{X'^2}{\lambda_2(T_{a,b})} + \frac{Y'^2}{\lambda_2(T_{a,b})}.$$

Because these rotations do not change the length of vectors, we get that

$$\max\{X^{2} + Y^{2} : (X, \pm Y)T_{a,b}^{-1}(X, \pm Y)^{\mathsf{T}} = 1\}$$

= $\max\left\{X^{2} + (\pm Y)^{2} : (X, \pm Y)T_{a,b}^{-1}(X, \pm Y)^{\mathsf{T}} = 1\right\}$
= $\max\left\{X'^{2} + Y'^{2} : \frac{X'^{2}}{\lambda_{2}(T_{a,b})} + \frac{Y'^{2}}{\lambda_{2}(T_{a,b})} = 1\right\}.$

Again, the above optimization problem becomes

$$\min\left\{x^2 + y^2 : (x, y) \in \partial \mathcal{U}_{\Delta A, \Delta B}\right\} = \operatorname{Tr}\left(\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}}\right)$$
$$- \max\left\{X'^2 + Y'^2 : \frac{X'^2}{\lambda_2(\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}})} + \frac{Y'^2}{\lambda_2(\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}})} = 1\right\}.$$

Therefore,

$$\min\left\{x^2 + y^2 : (x, y) \in \mathcal{U}_{\Delta A, \Delta B}\right\} = \operatorname{Tr}\left(\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}}\right) - \lambda_{\max}(\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}})$$

implying that

$$(\Delta_{\rho} A)^{2} + (\Delta_{\rho} B)^{2} \ge \lambda_{\min}(T_{a,b}) = \frac{1}{2} \left(|a|^{2} + |b|^{2} - \sqrt{(|a|^{2} - |b|^{2})^{2} + 4\langle a, b \rangle^{2}} \right).$$

Next, we show the second inequality concerning standard deviations. We recall that the boundary curve of uncertainty region $\mathcal{U}_{\Delta A, \Delta B}$ is given by

$$|\mathbf{b}|^{2} x^{2} + |\mathbf{a}|^{2} y^{2} + 2 |\langle \mathbf{a}, \mathbf{b} \rangle | \sqrt{(|\mathbf{a}|^{2} - x^{2})(|\mathbf{b}|^{2} - y^{2})} = |\mathbf{a}|^{2} |\mathbf{b}|^{2} + \langle \mathbf{a}, \mathbf{b} \rangle^{2}.$$

Let θ be the angle between a and b. It is easily seen that such boundary curve intersects two points, respectively, with two axis, whose coordinates are $(|a| \sin \theta, 0)$ and $(0, |b| \sin \theta)$. It suffices to consider the part of such boundary curve over the interval $[0, |a| \sin \theta]$, whose equation is, indeed, given by

$$y = \frac{|\mathbf{b}|}{|\mathbf{a}|} \left(-\cos\theta x + \sin\theta \sqrt{|\mathbf{a}|^2 - x^2} \right).$$

Then, the optimization problem min $\{x + y : (x, y) \in \mathcal{U}_{\Delta A, \Delta B}\}$ is equivalent to that choosing minimal positive real number R such that the straight line, described by the equation x + y = R, and the part of the boundary curve over the closed interval **b** | $[0, |\mathbf{a}| \sin \theta],$ intersects only one point. Clearly, v a $\left(-\cos\theta x + \sin\theta\sqrt{|a|^2 - x^2}\right)$, where $x \in [0, |a|\sin\theta]$, is a concave function, which means the part of the boundary curve on $[0, |a| \sin \theta]$ should be above the straight line x + y = R. This situation appears if and only if the straight line x + y = R gets through one point whose horizontal or vertical coordinate is $\min(|\mathbf{a}| \sin \theta, |\mathbf{b}| \sin \theta) = \min(|\mathbf{a}|, |\mathbf{b}|) \sin \theta$. Therefore, R = $\min(|a|, |b|) \sin \theta$, which can be also rewritten as

$$R = \min(|a|, |b|) \sin \theta = \frac{\min(|a|, |b|) \max(|a|, |b|)}{\max(|a|, |b|)} \sin \theta = \frac{|a \times b|}{\max(|a|, |b|)}$$

Finally, we obtain that

$$\Delta_{\rho} \boldsymbol{A} + \Delta_{\rho} \boldsymbol{B} \ge \min \left\{ \boldsymbol{x} + \boldsymbol{y} : (\boldsymbol{x}, \boldsymbol{y}) \in \mathcal{U}_{\Delta \boldsymbol{A}, \Delta \boldsymbol{B}} \right\} = \frac{|\boldsymbol{a} \times \boldsymbol{b}|}{\max(|\boldsymbol{a}|, |\boldsymbol{b}|)},$$

This completes the proof.

3.4 Proof of Lemma 2.3

The proof of Lemma 2.3 will be also recognized as Propositions 3.9 and 3.10. In order to present the proof of Lemma 2.3, we next derive the joint probability distribution density

$$f_{\Delta A,\Delta B,\Delta C}(x, y, z) = \int_{\mathcal{D}(\mathbb{C}^2)} \mathrm{d}\mu(\rho)\delta(x - \Delta_{\rho}A)\delta(y - \Delta_{\rho}B)\delta(z - \Delta_{\rho}C)$$

of the uncertainties $(\Delta_{\rho} A, \Delta_{\rho} B, \Delta_{\rho} C)$ of the three qubit observables A, B, C. For this purpose, we first derive the joint probability distribution density

$$f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle, \langle \boldsymbol{C} \rangle}(\boldsymbol{r}, \boldsymbol{s}, t) = \int_{\mathcal{D}(\mathbb{C}^2)} \mathrm{d}\mu(\rho) \delta(\boldsymbol{r} - \langle \boldsymbol{A} \rangle_{\rho}) \delta(\boldsymbol{s} - \langle \boldsymbol{B} \rangle_{\rho}) \delta(\boldsymbol{t} - \langle \boldsymbol{C} \rangle_{\rho})$$

of the mean value $(\langle A \rangle_{\rho}, \langle B \rangle_{\rho}, \langle C \rangle_{\rho})$ of A, B, C, where ρ is resulted from partially tracing a subsystem over a Haar-distributed random pure state on $\mathbb{C}^2 \otimes \mathbb{C}^2$.

Proposition 3.9 For three qubit observables $\mathbf{A} = a_0 \mathbb{1} + \mathbf{a} \cdot \boldsymbol{\sigma}$, $\mathbf{B} = b_0 \mathbb{1} + \mathbf{b} \cdot \boldsymbol{\sigma}$, $\mathbf{C} = c_0 \mathbb{1} + \mathbf{c} \cdot \boldsymbol{\sigma}$ $(a_0, \mathbf{a}), (b_0, \mathbf{b}), (c_0, \mathbf{c}) \in \mathbb{R}^4$, let

$$T_{a,b,c} = \begin{pmatrix} \langle a, a \rangle \langle a, b \rangle \langle a, c \rangle \\ \langle b, a \rangle \langle b, b \rangle \langle b, c \rangle \\ \langle c, a \rangle \langle c, b \rangle \langle c, c \rangle \end{pmatrix}$$

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(i) If rank $(T_{a,b,c}) = 3$, i.e., $\{a, b, c\}$ is linearly independent, then

$$f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r, s, t) = \frac{3(1 + \operatorname{sign}(1 - \omega_{A,B,C}(r, s, t)))}{8\pi\sqrt{\det(T_{a,b,c})}}$$
$$= \begin{cases} \frac{3}{4\pi\sqrt{\det(T_{a,b,c})}}, & \text{if } \omega_{A,B,C}(r, s, t) < 1\\ \frac{3}{8\pi\sqrt{\det(T_{a,b,c})}}, & \text{if } \omega_{A,B,C}(r, s, t) = 1\\ 0, & \text{if } \omega_{A,B,C}(r, s, t) > 1 \end{cases}$$

where $\omega_{A,B,C}(r,s,t) = \sqrt{(r-a_0,s-b_0,t-c_0)T_{a,b,c}^{-1}(r-a_0,s-b_0,t-c_0)^{T}}$. (ii) If rank $(T_{a,b,c}) = 2$, without loss of generality, we assume that $\{a, b\}$ are linearly

independent and $c = \kappa_a \cdot a + \kappa_b \cdot b$ for some κ_a and κ_b with $\kappa_a \kappa_b \neq 0$, then

$$f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle, \langle \boldsymbol{C} \rangle}(r, s, t) = \delta((t - c_0) - \kappa_{\boldsymbol{a}}(r - a_0) - \kappa_{\boldsymbol{b}}(s - b_0))f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle}(r, s).$$

where $f_{\langle A \rangle, \langle B \rangle}(r, s)$ is from Proposition 3.7.

(iii) If rank $(T_{a,b,c}) = 1$, without loss of generality, we may assume that $b = \kappa_{ba} \cdot a$, $c = \kappa_{ca} \cdot a$ for some κ_{ba} and κ_{ca} with $\kappa_{ba}\kappa_{ca} \neq 0$, then

$$f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle, \langle \boldsymbol{C} \rangle}(r, s, t) = \delta((s - b_0) - \kappa_{\boldsymbol{b}\boldsymbol{a}}(r - a_0))\delta((t - c_0) - \kappa_{\boldsymbol{c}\boldsymbol{a}}(r - a_0))f_{\langle \boldsymbol{A} \rangle}(r),$$

where $f_{\langle A \rangle}(r)$ is from Proposition 3.4.

Proof (i) If rank $(T_{a,b,c}) = 3$, then $T_{a,b,c}$ is invertible. Using the integral representation of delta function, we have

$$f_{\langle \boldsymbol{A} \rangle, \langle \boldsymbol{B} \rangle, \langle \boldsymbol{C} \rangle}(\boldsymbol{r}, \boldsymbol{s}, t) = \frac{1}{8\pi^3} \int_{\mathbb{R}^3} d\alpha d\beta d\gamma e^{i(\boldsymbol{r}\alpha + \boldsymbol{s}\beta + t\gamma)} \int_{\mathcal{D}(\mathbb{C}^2)} d\mu(\rho) e^{-i\operatorname{Tr}\left(\boldsymbol{S}^{(\alpha, \beta, \gamma)}\rho\right)}.$$

where $d\alpha d\beta d\gamma$ is the Lebesgue volume element in \mathbb{R}^3 , $S^{(\alpha,\beta,\gamma)} = \alpha A + \beta B + \gamma C$. By Proposition 3.3, we have

$$\int_{\mathcal{D}(\mathbb{C}^2)} d\mu(\rho) e^{-i\operatorname{Tr}\left(S^{(\alpha,\beta,\gamma)}\rho\right)} = 3e^{-i(a_0\alpha+b_0\beta+c_0\gamma)}$$

$$\frac{\sin\left(|\alpha a + \beta b + \gamma c|\right) - |\alpha a + \beta b + \gamma c|\cos\left(|\alpha a + \beta b + \gamma c|\right)}{|\alpha a + \beta b + \gamma c|^3}$$

Consequently,

$$f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r, s, t) = \frac{3}{8\pi^3} \int_{\mathbb{R}^3} d\alpha d\beta d\gamma e^{i((r-a_0)\alpha + (s-b_0)\beta + (t-c_0)\gamma)} \frac{\sin(|\alpha a + \beta b + \gamma c|) - |\alpha a + \beta b + \gamma c|\cos(|\alpha a + \beta b + \gamma c|)}{|\alpha a + \beta b + \gamma c|^3}$$

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Let $(\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma})^{\mathsf{T}} = T_{a,b,c}^{\frac{1}{2}}(\alpha, \beta, \gamma)^{\mathsf{T}}$, then $d\alpha d\beta d\gamma = det^{-\frac{1}{2}} (T_{a,b,c}) d\tilde{\alpha} d\tilde{\beta} d\tilde{\gamma}$, and

$$\begin{split} &\int_{\mathrm{D}(\mathbb{C}^2)} \mathrm{d}\mu(\rho) e^{-\mathrm{i}\operatorname{Tr}\left(\boldsymbol{S}^{(\alpha,\beta,\gamma)}\rho\right)} \\ &= 3e^{-\mathrm{i}(\tilde{a}_0\tilde{\alpha} + \tilde{b}_0\tilde{\beta} + \tilde{c}_0\tilde{\gamma})} \\ & \frac{\sin\left(\sqrt{\tilde{\alpha}^2 + \tilde{\beta}^2 + \tilde{\gamma}^2}\right) - \sqrt{\tilde{\alpha}^2 + \tilde{\beta}^2 + \tilde{\gamma}^2}\cos\left(\sqrt{\tilde{\alpha}^2 + \tilde{\beta}^2 + \tilde{\gamma}^2}\right)}{\left(\tilde{\alpha}^2 + \tilde{\beta}^2 + \tilde{\gamma}^2\right)^{\frac{3}{2}}} \end{split}$$

Let $(\tilde{r}, \tilde{s}, \tilde{t}) = (r, s, t) T_{a,b,c}^{-\frac{1}{2}}$ and $(\tilde{a}_0, \tilde{b}_0, \tilde{c}_0) = (a_0, b_0, c_0) T_{a,b,c}^{-\frac{1}{2}}$, then

$$f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r, s, t) = \frac{3}{8\pi^3 \sqrt{\det(T_{a,b,c})}} \int_{\mathbb{R}^3} d\tilde{\alpha} d\tilde{\beta} d\tilde{\gamma} e^{i\left((\tilde{r} - \tilde{a}_0)\tilde{\alpha} + (\tilde{s} - \tilde{b}_0)\tilde{\beta} + (\tilde{t} - \tilde{c}_0)\tilde{\gamma}\right)} \\ \times \frac{\sin\left(\sqrt{\tilde{\alpha}^2 + \tilde{\beta}^2 + \tilde{\gamma}^2}\right) - \sqrt{\tilde{\alpha}^2 + \tilde{\beta}^2 + \tilde{\gamma}^2} \cos\left(\sqrt{\tilde{\alpha}^2 + \tilde{\beta}^2 + \tilde{\gamma}^2}\right)}{\left(\tilde{\alpha}^2 + \tilde{\beta}^2 + \tilde{\gamma}^2\right)^{\frac{3}{2}}}.$$

Denote $\tilde{z}_0 = (\tilde{r} - \tilde{a}_0, \tilde{s} - \tilde{b}_0, \tilde{t} - \tilde{c}_0)$ and $\tilde{z} = (\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma})$, the last integral can be rewritten as

$$\begin{split} &\int_{\mathbb{R}^3} \mathrm{d}\tilde{z} e^{\mathrm{i}\langle \tilde{z}_0, \tilde{z}\rangle} \frac{\sin|\tilde{z}| - |\tilde{z}|\cos|\tilde{z}|}{|\tilde{z}|^3} \\ &= \int_0^\infty \mathrm{d}q q^2 \int_{\mathbb{R}^3} \mathrm{d}\tilde{u} \delta(1 - |\tilde{u}|) e^{\mathrm{i}q\langle \tilde{z}_0, \tilde{u}\rangle} \frac{\sin q - q\cos q}{q^3} \\ &= \int_0^\infty \mathrm{d}q \frac{\sin q - q\cos q}{q} \int_{\mathbb{R}^3} \mathrm{d}\tilde{u} \delta(1 - |\tilde{u}|) e^{\mathrm{i}q\langle \tilde{z}_0, \tilde{u}\rangle}, \end{split}$$

where $d\tilde{z} = d\tilde{\alpha} d\tilde{\beta} d\tilde{\gamma}$ is the Lebesgue volume element in \mathbb{R}^3 . From

$$\begin{split} &\int_{\mathbb{R}^3} \mathrm{d}\tilde{\boldsymbol{u}} \delta(1 - |\,\tilde{\boldsymbol{u}}\,|) e^{\mathrm{i}q\langle \tilde{z}_0, \tilde{\boldsymbol{u}} \rangle} = 4\pi \, \int \mathrm{d}\mu_{\mathrm{Haar}}(\tilde{\boldsymbol{u}}) e^{\mathrm{i}q\langle \tilde{z}_0, \tilde{\boldsymbol{u}} \rangle} \\ &= 4\pi \, \times \frac{1}{2} \int_{-1}^1 \mathrm{d}\tau e^{\mathrm{i}q |\,\tilde{z}_0\,|\tau} = 4\pi \, \frac{\sin(q \,|\,\tilde{z}_0\,|)}{q \,|\,\tilde{z}_0\,|}, \end{split}$$

where, in the second equality, we used the probability density function of inner product of two random unit vectors, a result has been already obtained in [35], we obtain

$$\int_{\mathbb{R}^3} d\tilde{z} e^{i(\tilde{z}_0,\tilde{z})} \frac{\sin|\tilde{z}| - |\tilde{z}|\cos|\tilde{z}|}{|\tilde{z}|^3} = \frac{4\pi}{|\tilde{z}_0|} \int_0^\infty dq \frac{\sin(|\tilde{z}_0|q)(\sin q - q\cos q)}{q^2}$$
$$= \pi^2 \frac{|\tilde{z}_0| - ||\tilde{z}_0| - 1| - \operatorname{sign}(|\tilde{z}_0| - 1)}{|\tilde{z}_0|}.$$

Therefore,

$$f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r, s, t) = \frac{3 \left(|\tilde{z}_0| - ||\tilde{z}_0| - 1| - \text{sign}(|\tilde{z}_0| - 1) \right)}{8\pi \sqrt{\det(T_{a,b,c})} |\tilde{z}_0|}.$$

Noting that $|\tilde{z}_0| = \sqrt{(\tilde{r} - \tilde{a}_0)^2 + (\tilde{s} - \tilde{b}_0)^2 + (\tilde{t} - \tilde{c}_0)^2} = \omega_{A,B,C}(r,s,t)$, we finally get

$$f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r, s, t) = \frac{3(1 + \operatorname{sign}(1 - \omega_{A, B, C}(r, s, t)))}{8\pi \sqrt{\operatorname{det}(T_{a, b, c})}}.$$

(ii) In this case,

$$\begin{split} f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r, s, t) \\ &= \frac{3}{(2\pi)^3} \int_{\mathbb{R}^3} d\alpha d\beta d\gamma e^{i((r-a_0)\alpha + (s-b_0)\beta + (t-c_0)\gamma)} \\ &\times \left(\frac{\sin |(\alpha + \gamma \kappa_a)a + (\beta + \gamma \kappa_b)b|}{|(\alpha + \gamma \kappa_a)a + (\beta + \gamma \kappa_b)b|^3} \right. \\ &\left. - \frac{\cos |(\alpha + \gamma \kappa_a)a + (\beta + \gamma \kappa_b)b|}{|(\alpha + \gamma \kappa_a)a + (\beta + \gamma \kappa_b)b|^2} \right). \end{split}$$

Let $(\alpha', \beta', \gamma') = (\alpha + \gamma \kappa_a, \beta + \gamma \kappa_b, \gamma)$, then the Jacobian of $(\alpha, \beta, \gamma) \to (\alpha', \beta', \gamma')$ is given by

$$\det\left(\frac{\partial(\alpha',\,\beta',\,\gamma')}{\partial(\alpha,\,\beta,\,\gamma)}\right) = \begin{vmatrix} 1 & 0 & \kappa_{a} \\ 0 & 1 & \kappa_{b} \\ 0 & 0 & 1 \end{vmatrix} = 1 \neq 0.$$

Thus, we have

$$f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r, s, t) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{i\gamma'((t-c_0)-\kappa_a(r-a_0)-\kappa_b(s-b_0))} d\gamma'$$

$$\times \frac{3}{(2\pi)^2} \int_{\mathbb{R}^2} d\alpha' d\beta' e^{i((r-a_0)\alpha'+(s-b_0)\beta')}$$

$$\frac{\sin |\alpha' a + \beta' b| - |\alpha' a + \beta' b| \cos |\alpha' a + \beta' b|}{|\alpha' a + \beta' b|^3}$$

$$= \delta \left((t-c_0) - \kappa_a(r-a_0) - \kappa_b(s-b_0) \right) f_{\langle A \rangle, \langle B \rangle}(r, s),$$

where $f_{\langle A \rangle, \langle B \rangle}(r, s)$ is from Proposition 3.7.

(iii) In this case, we have

$$f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r, s, t) = \frac{3}{(2\pi)^3} \int_{\mathbb{R}^3} d\alpha d\beta d\gamma e^{i((r-a_0)\alpha + (s-b_0)\beta + (t-c_0)\gamma)} \times \frac{\sin(|\mathbf{a}||\alpha + \kappa_{ba}\beta + \kappa_{ca}\gamma|) - |\mathbf{a}||\alpha + \kappa_{ba}\beta + \kappa_{ca}\gamma|\cos(|\mathbf{a}||\alpha + \kappa_{ba}\beta + \kappa_{ca}\gamma|)}{|\mathbf{a}|^3|\alpha + \kappa_{ba}\beta + \kappa_{ca}\gamma|^3}.$$

Let $(\alpha', \beta', \gamma') = (\alpha + \kappa_{ba}\beta + \kappa_{ca}\gamma, \beta, \gamma)$, then the Jacobian of the transformation $(\alpha, \beta, \gamma) \rightarrow (\alpha', \beta', \gamma')$ is given by

$$\det\left(\frac{\partial(\alpha',\,\beta',\,\gamma')}{\partial(\alpha,\,\beta,\,\gamma)}\right) = \begin{vmatrix} 1 & \kappa_{ba} & \kappa_{ca} \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} = 1 \neq 0,$$

and we have

$$\begin{split} f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r, s, t) \\ &= \frac{3}{(2\pi)^3} \int_{\mathbb{R}^3} d\alpha' d\beta' d\gamma' e^{i((r-a_0)(\alpha'-\kappa_{ba}\beta'-\kappa_{ca}\gamma')+(s-b_0)\beta'+(t-c_0)\gamma')} \\ &\frac{\sin\left(|a||\alpha'|\right) - |a||\alpha'|\cos\left(|a||\alpha'|\right)}{|a|^3|\alpha'|^3} \\ &= \frac{1}{2\pi} \int_{\mathbb{R}} e^{i[(s-b_0)-\kappa_b(r-a_0)]\beta'} d\beta' \times \frac{1}{2\pi} \int_{\mathbb{R}} e^{i[(t-c_0)-\kappa_c(r-a_0)]\gamma'} d\gamma' \\ &\times \frac{3}{2\pi} \int_{\mathbb{R}} d\alpha' e^{i(r-a_0)\alpha'} \frac{\sin\left(|a||\alpha'|\right) - |a||\alpha'|\cos\left(|a||\alpha'|\right)}{|a|^3|\alpha'|^3} \\ &= \delta\left((s-b_0) - \kappa_{ba}(r-a_0)\right) \delta\left((t-c_0) - \kappa_{ca}(r-a_0)\right) f_{\langle A \rangle}(r), \end{split}$$

where $f_{\langle A \rangle}(r)$ is from Proposition 3.4.

Proposition 3.10 The joint probability distribution density of $(\Delta_{\rho} A, \Delta_{\rho} B, \Delta_{\rho} C)$ for a triple of qubit observables $A = a_0 \mathbb{1} + a \cdot \sigma$, $B = b_0 \mathbb{1} + b \cdot \sigma$, $C = c_0 \mathbb{1} + c \cdot \sigma$, $(a_0, a), (b_0, b), (c_0, c) \in \mathbb{R}^4$, where $\{a, b, c\}$ is linearly independent, and ρ is resulted from partially tracing a subsystem over a Haar-distributed random pure state on $\mathbb{C}^2 \otimes \mathbb{C}^2$, is given by

$$f_{\Delta \boldsymbol{A},\Delta \boldsymbol{B},\Delta \boldsymbol{C}}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{z}) = \frac{2xyz}{\sqrt{(a^2 - x^2)(b^2 - y^2)(c^2 - z^2)}} \sum_{j,k \in \{\pm\}} f_{\langle \boldsymbol{A} \rangle,\langle \boldsymbol{B} \rangle,\langle \boldsymbol{C} \rangle}(\boldsymbol{x}_+,y_j,z_k).$$

Here, $f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r, s, t)$ is the joint probability distribution density of the mean values $(\langle A \rangle_{\rho}, \langle B \rangle_{\rho}, \langle C \rangle_{\rho})$, determined by Proposition 3.9, and

$$x_{\pm} = a_0 \pm \sqrt{|\boldsymbol{a}|^2 - x^2}, \quad y_{\pm} = b_0 \pm \sqrt{|\boldsymbol{b}|^2 - y^2}, \quad z_{\pm} = c_0 \pm \sqrt{|\boldsymbol{c}|^2 - z^2}.$$

Proof Noting that

$$f_{\Delta A,\Delta B,\Delta C}(x, y, z) = \int_{S(\mathbb{C}^2)} d\mu(\rho)\delta(x - \Delta_{\rho}A)\delta(y - \Delta_{\rho}B)\delta(z - \Delta_{\rho}C)$$

= $8xyz \int_{S(\mathbb{C}^2)} d\mu(\rho)\delta\left(x^2 - (\Delta_{\rho}A)^2\right)\delta\left(y^2 - (\Delta_{\rho}B)^2\right)\delta\left(z^2 - (\Delta_{\rho}C)^2\right),$

and

$$\delta\left(x^2 - (\Delta_{\rho} \boldsymbol{A})^2\right)\delta\left(y^2 - (\Delta_{\rho} \boldsymbol{B})^2\right)\delta\left(z^2 - (\Delta_{\rho} \boldsymbol{C})^2\right) = \delta(g_x(r))\delta(h_y(s))\delta(l_z(t)),$$

where $g_x(r) = x^2 - (r - \lambda_1(A))(\lambda_2(A) - r), \ h_y(s) = y^2 - (s - \lambda_1(B))(\lambda_2(B) - s), \ l_z(t) = z^2 - (t - \lambda_1(C))(\lambda_2(C) - t)$, we have

$$\begin{split} f_{\Delta A,\Delta B,\Delta C}(x, y, z) &= 8xyz \int_{\mathbb{R}^3} \mathrm{d} r \mathrm{d} s \mathrm{d} t \, \delta(g_x(r)) \delta(h_y(s)) \delta(l_z(t)) f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r, s, t) \\ &= \frac{xyz}{\sqrt{(|a|^2 - x^2)(|b|^2 - y^2)(|c|^2 - z^2)}} \\ &\sum_{i,j,k \in \{\pm\}} \left\langle \delta_{(r_i(x), s_j(y), t_k(z))}, f_{\langle A \rangle, \langle B \rangle, \langle C \rangle} \right\rangle \\ &= \frac{xyz \sum_{i,j,k \in \{\pm\}} f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r_i(x), s_j(y), t_k(z))}{\sqrt{(|a|^2 - x^2)(|b|^2 - y^2)(|c|^2 - z^2)}} \\ &= \frac{2xyz \sum_{j,k \in \{\pm\}} f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r_+, s_j, t_k)}{\sqrt{(|a|^2 - x^2)(|b|^2 - y^2)(|c|^2 - z^2)}}, \end{split}$$

where we have used the fact that

$$\begin{aligned} f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r_+, s_+, t_+) &= f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r_-, s_-, t_-), \\ f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r_+, s_+, t_-) &= f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r_-, s_-, t_+), \\ f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r_+, s_-, t_+) &= f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r_-, s_+, t_-), \\ f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r_+, s_-, t_-) &= f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r_-, s_+, t_+). \end{aligned}$$

This completes the proof.

We now turn to the uncertainty region for a triple (A, B, C) of qubit observables $A = a_0 \mathbb{1} + a \cdot \sigma$, $B = b_0 \mathbb{1} + b \cdot \sigma$ and $C = c_0 \mathbb{1} + c \cdot \sigma$ with (a_0, a) , (b_0, b) , $(c_0, c) \in \mathbb{R}^4$, and $\{a, b, c\}$ being linearly independent. Denote $u_{\epsilon_b, \epsilon_c}(x, y, z) = ((|a|^2 - x^2)^{1/2}, \epsilon_b (|b|^2 - y^2)^{1/2}, \epsilon_c (|c|^2 - z^2)^{1/2})$, where $\epsilon_b, \epsilon_c \in \{\pm 1\}$, and

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$$T_{a,b,c} = \begin{pmatrix} \langle a, a \rangle \langle a, b \rangle \langle a, c \rangle \\ \langle b, a \rangle \langle b, b \rangle \langle b, c \rangle \\ \langle c, a \rangle \langle c, b \rangle \langle c, c \rangle \end{pmatrix}.$$

Let γ , β and α be the angles between a and b, a and c, b and c, respectively, where α , β , $\gamma \in (0, \pi)$. Set $\phi(t_1, t_2, t_3) = \cos(t_1) - \cos(t_2)\cos(t_3)$.

Proof of Lemma 2.3 In fact, due to the relation between $f_{\Delta A, \Delta B, \Delta C}$ and $f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}$, in Proposition 3.10, the support of $f_{\Delta A, \Delta B, \Delta C}$ can be identified by the support of $f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}$ which can be seen from Proposition 3.9 (i),

$$\operatorname{supp}(f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}) = \left\{ (r, s, t) \in \mathbb{R}^2 : \omega_{A, B, C}(r, s, t) \leq 1 \right\}.$$

With the support of $f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}$, now we can make an analysis of the support of $f_{\Delta A, \Delta B, \Delta C}$. Note that $f_{\Delta A, \Delta B, \Delta C}(x, y, z)$ is defined on the first quadrant $\mathbb{R}^3_{\geq 0}$, if xyz > 0, then $f_{\Delta A, \Delta B, \Delta C}(x, y, z) = 0$ if and only if

$$\sum_{i,j,k\in\{\pm\}} f_{\langle \boldsymbol{A}\rangle,\langle \boldsymbol{B}\rangle,\langle \boldsymbol{C}\rangle}(r_i(x),s_j(y),t_k(z)) = 0,$$

i.e., $f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}(r_i(x), s_j(y), t_k(z)) = 0$ because $f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}$ is a non-negative function. This means that all eight points $(r_{\pm}(x), s_{\pm}(y), t_{\pm}(z))$ are not in the support of $f_{\langle A \rangle, \langle B \rangle, \langle C \rangle}$. Therefore, the uncertainty region (i.e., the support of $f_{\Delta A, \Delta B, \Delta C}$) of A, B, and C is given by the following set:

$$\mathcal{U}_{\Delta A,\Delta B,\Delta C} = \operatorname{supp}(f_{\Delta A,\Delta B,\Delta C}) = D_{a,b,c}^{++} \cup D_{a,b,c}^{+-} \cup D_{a,b,c}^{-+} \cup D_{a,b,c}^{--},$$

ere, via $\boldsymbol{u}_{\epsilon_{b},\epsilon_{c}}(x, y, z) = \left(\sqrt{|\boldsymbol{a}|^{2} - x^{2}}, \epsilon_{b}\sqrt{|\boldsymbol{b}|^{2} - y^{2}}, \epsilon_{c}\sqrt{|\boldsymbol{c}|^{2} - z^{2}}\right),$
 $D_{\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}}^{\epsilon_{b}\epsilon_{c}} = \left\{(x, y, z) \in \mathbb{R}^{3}_{\geq 0} : \boldsymbol{u}_{\epsilon_{b},\epsilon_{c}}(x, y, z) T_{\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}}^{-1}\boldsymbol{u}_{\epsilon_{b},\epsilon_{c}}^{\mathsf{T}}(x, y, z) \leqslant 1\right\}$

for $\epsilon_b, \epsilon_c \in \{\pm\}$. Now, the inequality

$$\boldsymbol{u}_{\epsilon_b,\epsilon_c}(x, y, z) \boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}}^{-1} \boldsymbol{u}_{\epsilon_b,\epsilon_c}^{\mathsf{T}}(x, y, z) \leqslant 1$$

is reduced into the following:

$$\begin{bmatrix} \det(\boldsymbol{T}_{\boldsymbol{b},\boldsymbol{c}})x^{2} + \det(\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{c}})y^{2} + \det(\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b}})z^{2} \\ +2(\langle \boldsymbol{a},\boldsymbol{b}\rangle\langle \boldsymbol{a},\boldsymbol{c}\rangle\langle \boldsymbol{b},\boldsymbol{c}\rangle - |\boldsymbol{a}|^{2} |\boldsymbol{b}|^{2} |\boldsymbol{c}|^{2}) \\ +2\epsilon_{\boldsymbol{b}}(|\boldsymbol{c}|^{2}\langle \boldsymbol{a},\boldsymbol{b}\rangle - \langle \boldsymbol{a},\boldsymbol{c}\rangle\langle \boldsymbol{b},\boldsymbol{c}\rangle)\sqrt{(|\boldsymbol{a}|^{2} - x^{2})(|\boldsymbol{b}|^{2} - y^{2})} \\ +2\epsilon_{\boldsymbol{b}}\epsilon_{\boldsymbol{c}}(|\boldsymbol{a}|^{2}\langle \boldsymbol{b},\boldsymbol{c}\rangle - \langle \boldsymbol{a},\boldsymbol{b}\rangle\langle \boldsymbol{a},\boldsymbol{c}\rangle)\sqrt{(|\boldsymbol{b}|^{2} - y^{2})(|\boldsymbol{c}|^{2} - z^{2})} \end{bmatrix}$$

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$$+2\epsilon_{c}(|\boldsymbol{b}|^{2}\langle\boldsymbol{a},\boldsymbol{c}\rangle-\langle\boldsymbol{a},\boldsymbol{b}\rangle\langle\boldsymbol{b},\boldsymbol{c}\rangle)\sqrt{(|\boldsymbol{c}|^{2}-z^{2})(|\boldsymbol{a}|^{2}-x^{2})}\Big]$$

$$\times \operatorname{sign}\left(|\boldsymbol{a}|^{2}\langle\boldsymbol{b},\boldsymbol{c}\rangle^{2}+|\boldsymbol{b}|^{2}\langle\boldsymbol{a},\boldsymbol{c}\rangle^{2}+c^{2}\langle\boldsymbol{a},\boldsymbol{b}\rangle^{2}-|\boldsymbol{a}|^{2}|\boldsymbol{b}|^{2}|\boldsymbol{c}|^{2}\right)$$

$$-2\langle\boldsymbol{a},\boldsymbol{b}\rangle\langle\boldsymbol{a},\boldsymbol{c}\rangle\langle\boldsymbol{b},\boldsymbol{c}\rangle)$$

$$\leqslant 0.$$

Denote the angle between a and b by γ ; the angle between a and c by β ; the angle between b and c by α . Thus,

$$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = |\boldsymbol{a}| |\boldsymbol{b}| \cos(\gamma), \quad \langle \boldsymbol{a}, \boldsymbol{c} \rangle = |\boldsymbol{a}| |\boldsymbol{c}| \cos(\beta), \quad \langle \boldsymbol{b}, \boldsymbol{c} \rangle = |\boldsymbol{b}| |\boldsymbol{c}| \cos(\alpha).$$

We also write $\phi(t_1, t_2, t_3) := \cos(t_1) - \cos(t_2)\cos(t_3)$. By scaling transformations:

$$(x, y, z) \longmapsto (ax, by, cz)$$

without loss of generality, we assume |a| = |b| = |c| = 1, then the above inequalities is equivalent to:

$$\begin{bmatrix} \sin^{2}(\alpha)x^{2} + \sin^{2}(\beta)y^{2} + \sin^{2}(\gamma)z^{2} \\ +2\epsilon_{b}\phi(\gamma, \alpha, \beta)\sqrt{(1-x^{2})(1-y^{2})} + 2\epsilon_{b}\epsilon_{c}\phi(\alpha, \beta, \gamma)\sqrt{(1-y^{2})(1-z^{2})} \\ +2\epsilon_{c}\phi(\beta, \gamma, \alpha)\sqrt{(1-z^{2})(1-x^{2})} + 2(\cos(\alpha)\cos(\beta)\cos(\gamma)-1) \end{bmatrix} \\ \times \operatorname{sign}\left(\cos^{2}(\alpha) + \cos^{2}(\beta) + \cos^{2}(\gamma) - 2\cos(\alpha)\cos(\beta)\cos(\gamma) - 1\right) \\ \leqslant 0.$$

Note that three angles $\alpha, \beta, \gamma \in (0, \pi)$ should be such that

$$\det(\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}}) = 1 - \cos^2(\alpha) - \cos^2(\beta) - \cos^2(\gamma) + 2\cos(\alpha)\cos(\beta)\cos(\gamma) > 0$$

due to the fact that $\{a, b, c\}$ is linearly independent. Because

$$-\det(\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}}) = \cos^2(\alpha) + \cos^2(\beta) + \cos^2(\gamma) - 2\cos(\alpha)\cos(\beta)\cos(\gamma) - 1 = 0$$

if and only if $\cos(\gamma) = \cos(\alpha + \beta)$ or $\cos(\gamma) = \cos(\alpha - \beta)$; if and only if $\cos(\beta) = \cos(\alpha + \gamma)$ or $\cos(\beta) = \cos(\alpha - \gamma)$; if and only if $\cos(\alpha) = \cos(\beta + \gamma)$ or $\cos(\alpha) = \cos(\beta - \gamma)$. Thus, the necessary and sufficient condition of $\det(T_{a,b,c}) = 0$ is either one of the following statements:

(i) $\alpha = \beta + \gamma$; (ii) $\beta = \gamma + \beta$; (iii) $\gamma = \alpha + \beta$; (iv) $\alpha + \beta + \gamma = 2\pi$. In other words, $det(T_{a,b,c}) > 0$ if and only if the following four inequalities should be satisfied

$$\alpha,\beta,\gamma\in(0,\pi):\ \alpha<\beta+\gamma,\ \beta<\gamma+\alpha,\ \gamma<\alpha+\beta,\ \alpha+\beta+\gamma<2\pi.$$

Under these conditions, the above inequalities are reduced to

$$\begin{aligned} &2\epsilon_b\phi(\gamma,\alpha,\beta)\sqrt{(1-x^2)(1-y^2)}+2\epsilon_b\epsilon_c\phi(\alpha,\beta,\gamma)\sqrt{(1-y^2)(1-z^2)}\\ &+2\epsilon_c\phi(\beta,\gamma,\alpha)\sqrt{(1-z^2)(1-x^2)}\\ &+\sin^2(\alpha)x^2+\sin^2(\beta)y^2+\sin^2(\gamma)z^2 \geqslant 2(1-\cos(\alpha)\cos(\beta)\cos(\gamma)). \end{aligned}$$

In order to get a more compact form of the above formula, we find that we can use the absolute function to get rid of ϵ_b with keeping $\epsilon_c \equiv \epsilon \in \{\pm 1\}$ due to the independence of ϵ_b and ϵ_c . Thus, they can also be rewritten as the following form by multiplying $\frac{1}{2}$ on both sides:

$$\begin{split} \left| \phi(\gamma, \alpha, \beta) \sqrt{1 - x^2} + \epsilon \phi(\alpha, \beta, \gamma) \sqrt{1 - z^2} \right| \sqrt{1 - y^2} \\ + \epsilon \phi(\beta, \gamma, \alpha) \sqrt{(1 - z^2)(1 - x^2)} \\ + \frac{1}{2} \left[\sin^2(\alpha) x^2 + \sin^2(\beta) y^2 + \sin^2(\gamma) z^2 \right] \geqslant 1 \\ - \cos(\alpha) \cos(\beta) \cos(\gamma) \quad (\epsilon \in \{\pm 1\}), \end{split}$$

where $x, y, z \in [0, 1]$.

3.5 Proof of Theorem 2.4

Based on the proof of Lemma 2.3, we present the proof of Theorem 2.4 as follows.

Proof of Theorem 2.4 Let $\sqrt{|a|^2 - x^2} = X$, $\sqrt{|b|^2 - y^2} = Y$, and $\sqrt{|c|^2 - z^2} = Z$ in Lemma 2.3, where $X \in [0, |a|]$, $Y \in [0, |b|]$, and $Z \in [0, |c|]$ due to the fact that $x \in [0, |a|]$, $y \in [0, |b|]$, and $z \in [0, |c|]$. Thus, we get that

$$\min\left\{x^2 + y^2 + z^2 : (x, y, z) \in \mathcal{U}_{\Delta A, \Delta B, \Delta C}\right\}$$

= Tr $(T_{a,b,c})$ - max $\left\{X^2 + Y^2 + Z^2 : (X, \epsilon_b Y, \epsilon_c Z)T_{a,b,c}^{-1}(X, \epsilon_b Y, \epsilon_c Z)^{\mathsf{T}} \leqslant 1\right\}$
 $(\epsilon_b, \epsilon_c \in \{\pm 1\}).$

It is easily seen that the objection function $x^2 + y^2 + z^2$, where $(x, y, z) \in \mathcal{U}_{\Delta A, \Delta B, \Delta C}$, attains its minimal value on the boundary surface $\partial \mathcal{U}_{\Delta A, \Delta B, \Delta C}$ of the uncertainty region $\mathcal{U}_{\Delta A, \Delta B, \Delta C}$; this also corresponds to the objection function $X^2 + Y^2 + Z^2$ attains its maximal value on the boundary surface

$$(X, \epsilon_b Y, \epsilon_c Z) \boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}}^{-1} (X, \epsilon_b Y, \epsilon_c Z)^{\mathsf{T}} = 1.$$

Denote by $\lambda_k(T_{a,b,c})(k = 1, 2, 3)$ the three eigenvalues of the matrix $T_{a,b,c}$. By Spectral Decomposition Theorem, we get that there exists orthogonal $O \in O(3)$ such that

$$\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}} = \boldsymbol{O} \operatorname{diag}(\lambda_1(\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}}), \lambda_2(\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}}), \lambda_3(\boldsymbol{T}_{\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}})) \boldsymbol{O}^{\mathsf{T}}$$

Now, let $(X', Y', Z')^{\mathsf{T}} = \boldsymbol{O}(X, \epsilon_b Y, \epsilon_c Z)^{\mathsf{T}}$. Then,

$$(X, \epsilon_b Y, \epsilon_c Z) T_{a,b,c}^{-1} (X, \epsilon_b Y, \epsilon_c Z)^{\mathsf{T}} = (X', Y', Z') \operatorname{diag}(\lambda_1^{-1} (T_{a,b,c}), \lambda_2^{-1} (T_{a,b,c}), \lambda_3^{-1} (T_{a,b,c})) (X', Y', Z')^{\mathsf{T}} = \frac{X'^2}{\lambda_2 (T_{a,b,c})} + \frac{Y'^2}{\lambda_2 (T_{a,b,c})} + \frac{Z'^2}{\lambda_3 (T_{a,b,c})}.$$

Because these rotations do not change the length of vectors, we get that

$$\max\{X^{2} + Y^{2} + Z^{2} : (X, \epsilon_{b}Y, \epsilon_{c}Z)T_{a,b,c}^{-1}(X, \epsilon_{b}Y, \epsilon_{c}Z)^{\mathsf{T}} = 1\}$$

=
$$\max\{X^{2} + (\epsilon_{b}Y)^{2} + (\epsilon_{c}Z)^{2} : (X, \epsilon_{b}Y, \epsilon_{c}Z)T_{a,b,c}^{-1}(X, \epsilon_{b}Y, \epsilon_{c}Z)^{\mathsf{T}} = 1\}$$

=
$$\max\{X'^{2} + Y'^{2} + Z'^{2} : \frac{X'^{2}}{\lambda_{2}(T_{a,b,c})} + \frac{Y'^{2}}{\lambda_{2}(T_{a,b,c})} + \frac{Z'^{2}}{\lambda_{3}(T_{a,b,c})} = 1\}.$$

Again, the above optimization problem becomes

$$\min\left\{x^{2} + y^{2} + z^{2} : (x, y, z) \in \partial \mathcal{U}_{\Delta A, \Delta B, \Delta C}\right\}$$

= Tr $(\mathbf{T}_{a,b,c})$ - max $\left\{X'^{2} + Y'^{2} + Z'^{2} : \frac{X'^{2}}{\lambda_{2}(\mathbf{T}_{a,b,c})} + \frac{Y'^{2}}{\lambda_{2}(\mathbf{T}_{a,b,c})} + \frac{Z'^{2}}{\lambda_{3}(\mathbf{T}_{a,b,c})} = 1\right\}$.

Therefore,

$$\min\left\{x^2 + y^2 + z^2 : (x, y, z) \in \mathcal{U}_{\Delta A, \Delta B, \Delta C}\right\} = \operatorname{Tr}\left(\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}}\right) - \lambda_{\max}(\boldsymbol{T}_{\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}})$$

implying that

$$(\Delta_{\rho} A)^{2} + (\Delta_{\rho} B)^{2} + (\Delta_{\rho} C)^{2} \ge \operatorname{Tr} \left(T_{a,b,c} \right) - \lambda_{\max} (T_{a,b,c}).$$

We are done.

3.6 Proof of Lemma 2.5

The proof of Lemma 2.5 is based on Propositions 3.11 and 3.12, which are described as follows.

For an *n*-tuple of qubit observables (A_1, \ldots, A_n) where

$$A_k = a_0^{(k)} \mathbb{1} + a_k \cdot \sigma, \qquad (a_0^{(k)}, a_k) \in \mathbb{R}^4, \quad k = 1, 2, \cdots, n,$$

the eigenvalues of A_k are given, respectively, by

$$\lambda_i(\mathbf{A}_k) = a_0^{(k)} + (-1)^i | \mathbf{a}_k |, \quad i = 1, 2; k = 1, \dots, n$$

By the assumption that $\lambda_2(A_k) > \lambda_1(A_k)$ for all k = 1, ..., n, we see that $|a_k| > 0, k = 1, 2, ..., n$. Let

$$f_{\langle A_1 \rangle, \cdots, \langle A_n \rangle}(r_1, \ldots, r_n) = \int_{\mathcal{D}(\mathbb{C}^2)} \mathrm{d}\mu(\rho) \prod_{k=1}^n \delta(r_k - \langle A_k \rangle_\rho)$$

be the joint probability density of the mean values of $(\langle A_1 \rangle_{\rho}, \cdots, \langle A_n \rangle_{\rho})$. Denote

$$T_{a_1,\ldots,a_n} = \begin{pmatrix} \langle a_1, a_1 \rangle & \langle a_1, a_2 \rangle & \cdots & \langle a_1, a_n \rangle \\ \langle a_2, a_1 \rangle & \langle a_2, a_2 \rangle & \cdots & \langle a_2, a_n \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle a_n, a_1 \rangle & \langle a_n, a_2 \rangle & \cdots & \langle a_n, a_n \rangle \end{pmatrix}$$

Proposition 3.11 Let (A_1, \ldots, A_n) be an n-tuple of qubit observables given by $A_k = a_0^{(k)} \mathbb{1} + a_k \cdot \sigma$, $(a_0^{(k)}, a_k) \in \mathbb{R}^4$, $k = 1, \cdots, n$, and let $f_{\langle A_1 \rangle, \cdots, \langle A_n \rangle}(r_1, \ldots, r_n)$ be the joint probability distribution density of the mean values $(\langle A_1 \rangle_{\rho}, \ldots, \langle A_n \rangle_{\rho})$, where ρ is resulted from partially tracing a subsystem over a Haar-distributed random pure state on $\mathbb{C}^2 \otimes \mathbb{C}^2$.

(i) If rank $(\mathbf{T}_{a_1,...,a_n}) = 3$, then without loss of generality, we can take nonzero coefficients κ_{lj} , $l = 4, \dots, n$, j = 1, 2, 3, such that $\mathbf{a}_l = \kappa_{l1}\mathbf{a}_1 + \kappa_{l2}\mathbf{a}_2 + \kappa_{l3}\mathbf{a}_3$. In this case,

$$f_{\langle A_1 \rangle, \dots, \langle A_n \rangle}(r_1, \dots, r_n) = f_{\langle A_1 \rangle, \langle A_2 \rangle, \langle A_3 \rangle}(r_1, r_2, r_3) \prod_{l=4}^n \delta\Big((r_l - a_0^{(l)}) - \sum_{j=1}^3 \kappa_{lj}(r_j - a_0^{(j)})\Big),$$

where $f_{\langle A_1 \rangle, \langle A_2 \rangle, \langle A_3 \rangle}$ is determined similarly by Proposition 3.9.

(ii) If rank($T_{a_1,...,a_n}$) = 2, then without loss of generality, we take nonzero coefficients $\eta_{li}, l = 2, \dots, n, i = 1, 2$, such that $a_l = \eta_{l1}a_1 + \eta_{l2}a_2$. In this case,

$$f_{\langle A_1 \rangle, \cdots, \langle A_n \rangle}(r_1, \dots, r_n) = f_{\langle A_1 \rangle, \langle A_2 \rangle}(r_1, r_2) \prod_{l=3}^n \delta\Big((r_l - a_0^{(l)}) - \sum_{i=1}^2 \eta_{li}(r_i - a_0^{(i)})\Big),$$

where $f_{\langle A_1 \rangle, \langle A_2 \rangle}$ is determined similarly by Proposition 3.7.

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$$f_{\langle A_1 \rangle, \cdots, \langle A_n \rangle}(r_1, \dots, r_n) = f_{\langle A_1 \rangle}(r_1) \prod_{l=2}^n \delta\left((r_l - a_0^{(l)}) - \kappa_l (r_1 - a_0^{(1)}) \right),$$

where $f_{(A_1)}$ is determined similarly by Proposition 3.4.

Proof By using integral representation of delta function *n* times in $f_{\langle A_1 \rangle,...,\langle A_n \rangle}$ and Proposition 3.3, we get

$$f_{\langle A_1 \rangle, ..., \langle A_n \rangle}(r_1, ..., r_n) = \frac{3}{(2\pi)^n} \int_{\mathbb{R}^n} \prod_{k=1}^n d\alpha_k e^{i \left(\sum_{k=1}^n (r_k - a_0^{(k)}) \alpha_k \right)} \\ \times \frac{\sin\left(\left| \sum_{k=1}^n \alpha_k a_k \right| \right) - \left| \sum_{k=1}^n \alpha_k a_k \right| \cos\left(\left| \sum_{k=1}^n \alpha_k a_k \right| \right)}{\left| \sum_{k=1}^n \alpha_k a_k \right|^3}.$$

(i) We have

$$\sum_{k=1}^{n} \alpha_k a_k = (\alpha_1 a_1 + \alpha_2 a_2 + \alpha_3 a_3) + \sum_{l=4}^{n} \alpha_l (\kappa_{l1} a_1 + \kappa_{l2} a_2 + \kappa_{l3} a_3)$$
$$= \left(\alpha_1 + \sum_{l=4}^{n} \kappa_{l1} \alpha_l\right) a_1 + \left(\alpha_2 + \sum_{l=4}^{n} \kappa_{l2} \alpha_l\right) a_2 + \left(\alpha_3 + \sum_{l=4}^{n} \kappa_{l3} \alpha_l\right) a_3.$$

Let

$$(\alpha'_1, \alpha'_2, \alpha'_3) = \left(\alpha_1 + \sum_{l=4}^n \kappa_{l1}\alpha_l, \alpha_2 + \sum_{l=4}^n \kappa_{l2}\alpha_l, \alpha_3 + \sum_{l=4}^n \kappa_{l3}\alpha_l\right),$$

$$(\alpha'_4, \dots, \alpha'_n) = (\alpha_4, \dots, \alpha_n),$$

then the Jacobian of the transformation $(\alpha_1, \ldots, \alpha_n) \rightarrow (\alpha'_1, \ldots, \alpha'_n)$ is given by

$$\det\left(\frac{\partial(\alpha'_1,\ldots,\alpha'_n)}{\partial(\alpha_1,\ldots,\alpha_n)}\right) = 1 \neq 0.$$

Noting that

$$\sum_{j=1}^{n} (r_j - a_0^{(j)}) \alpha_j = \sum_{j=1}^{3} (r_j - a_0^{(j)}) \left(\alpha'_j - \sum_{l=4}^{n} \kappa_{lj} \alpha'_l \right) + \sum_{l=4}^{n} (r_l - a_0^{(l)}) \alpha'_l$$
$$= \sum_{j=1}^{3} (r_j - a_0^{(j)}) \alpha'_j - \sum_{l=4}^{n} \left(\sum_{j=1}^{3} \kappa_{lj} (r_j - a_0^{(j)}) \right) \alpha'_l + \sum_{l=4}^{n} (r_l - a_0^{(l)}) \alpha'_l$$

$$=\sum_{l=1}^{3}(r_{l}-a_{0}^{(l)})\alpha_{l}'+\sum_{l=4}^{n}\left((r_{l}-a_{0}^{(l)})-\sum_{j=1}^{3}\kappa_{lj}(r_{j}-a_{0}^{(j)})\right)\alpha_{l}',$$

we have

$$f_{\langle A_1 \rangle, ..., \langle A_n \rangle}(r_1, ..., r_n) \\= \frac{3}{(2\pi)^3} \int_{\mathbb{R}^3} \prod_{l=1}^3 d\alpha'_l e^{i\left(\sum_{l=1}^3 (r_l - a_0^{(l)})\alpha'_l\right)} \\\frac{\sin\left(\left|\sum_{l=1}^3 \alpha'_l a_l\right|\right) - \left|\sum_{l=1}^3 \alpha'_l a_l\right| \cos\left(\left|\sum_{l=1}^3 \alpha'_l a_l\right|\right)}{\left|\sum_{l=1}^3 \alpha'_l a_l\right|^3} \\\times \prod_{l=4}^n \left(\frac{1}{2\pi} \int_{\mathbb{R}} d\alpha'_l e^{i\left((r_l - a_0^{(l)}) - \sum_{j=1}^3 \kappa_{lj}(r_j - a_0^{(j)})\right)\alpha'_l}\right),$$

therefore

$$f_{\langle A_1 \rangle, \dots, \langle A_n \rangle}(r_1, \dots, r_n) = f_{\langle A_1 \rangle, \langle A_2 \rangle, \langle A_3 \rangle}(r_1, r_2, r_3)$$
$$\prod_{l=4}^n \delta\Big((r_l - a_0^{(l)}) - \sum_{j=1}^3 \kappa_{lj}(r_j - a_0^{(j)})\Big).$$

Items (ii) and (iii) follow similarly.

Proposition 3.12 The joint probability distribution density of $(\Delta_{\rho} A_1, \ldots, \Delta_{\rho} A_n)$ for an *n*-triple of qubit observables defined by Eq. (3.1), where ρ is resulted from partialtracing a subsystem over a Haar-distributed random pure state on $\mathbb{C}^2 \otimes \mathbb{C}^2$, is given by

$$f_{\Delta A_1,...,\Delta A_n}(x_1,...,x_n) = \left(2\prod_{j=1}^n \frac{x_j}{\sqrt{|a_j|^2 - x_j^2}}\right) \sum_{\substack{j_2,...,j_n \in \{\pm\}}} f_{\langle A_1 \rangle,...,\langle A_n \rangle}(r_+^{(1)}(x_1), r_{j_2}^{(2)}(x_2), \ldots, r_{j_n}^{(n)}(x_n)),$$

where $f_{\langle A_1 \rangle, \dots, \langle A_n \rangle}(\cdot, \dots, \cdot)$ is determined by Proposition 3.11, and

$$r_{\pm}^{(k)}(x_k) := a_0^{(k)} \pm \sqrt{|a_k|^2 - x_k^2} \quad (k = 1, \dots, n).$$

Proof The proof goes similarly for Propositions 3.5, 3.8, and 3.10. We omitted here.

Proof of Lemma 2.5 From Proposition 3.11, we get the support of $f_{\langle A_1 \rangle,...,\langle A_n \rangle}$ which is given by, via

$$\begin{split} &\omega_{A_1,A_2,A_3}(r_1,r_2,r_3) \\ &= \sqrt{\left(r_1 - a_0^{(1)}, r_2 - a_0^{(2)}, r_3 - a_0^{(3)}\right) T_{a_1,a_2,a_3}^{-1} \left(r_1 - a_0^{(1)}, r_2 - a_0^{(2)}, r_3 - a_0^{(3)}\right)^{\mathsf{T}}}, \\ & \text{supp}(f_{\langle A_1 \rangle, \dots, \langle A_n \rangle}) \\ &= \left\{ (r_1, \dots, r_n) \in \mathbb{R}^n : \omega_{A_1,A_2,A_3}(r_1, r_2, r_3) \leqslant 1, r_l - a_0^{(l)} = \sum_{j=1}^3 \kappa_{lj}(r_j - a_0^{(j)}) (\forall l = 4, \dots, n) \right\}. \end{split}$$

By similar analysis as in the proofs of Propositions 3.4, 3.7, and 3.9, we obtain the support of $f_{\Delta A_1,...,\Delta A_n}$, i.e., the uncertainty region $\mathcal{U}_{\Delta A_1,...,\Delta A_n} = \operatorname{supp}(f_{\Delta A_1,...,\Delta A_n})$,

$$\sup (f_{\Delta A_1,...,\Delta A_n}) = \left\{ (x_1,...,x_n) \in \mathbb{R}^n_{\geqslant 0} : \begin{cases} \boldsymbol{u}_{\epsilon_1,\epsilon_2,\epsilon_3}(x_1,x_2,x_3) \boldsymbol{T}_{\boldsymbol{a}_1,\boldsymbol{a}_2,\boldsymbol{a}_3}^{-1} \boldsymbol{u}_{\epsilon_1,\epsilon_2,\epsilon_3}^{\mathsf{T}}(x_1,x_2,x_3) \leqslant 1 \\ \epsilon_l \sqrt{|\boldsymbol{a}_l|^2 - x_l^2} = \sum_{j=1}^3 \kappa_{lj} \epsilon_j \sqrt{|\boldsymbol{a}_j|^2 - x_j^2} (\forall l = 4,...,n) \end{cases} \right\}.$$

Here, $\epsilon_k \in \{\pm 1\}$ and $x_k \in [0, |a_k|]$, where $k = 1, \dots, n$.

3.7 Proof of Theorem 2.6

We consider now the uncertainty regions for multiple qubit observables. For an *n*-tuple of qubit observables (A_1, \ldots, A_n) , where $A_k = a_0^{(k)} \mathbb{1} + a_k \cdot \sigma$ with $(a_0^{(k)}, a_k) \in \mathbb{R}^4$, $k = 1, \ldots, n$, denote $T_{a_1,\ldots,a_n} = (\langle a_i, a_j \rangle)$. Note that $\{a_1, a_2, \ldots, a_n\}$ has at most three vectors that are linearly independent. Without loss of generality, we assume $\{a_1, a_2, a_3\}$ is linearly independent. The rest vectors can be linearly expressed by $\{a_1, a_2, a_3\}$, $a_l = \kappa_{l1}a_1 + \kappa_{l2}a_2 + \kappa_{l3}a_3$, for some coefficients κ_{lj} , $l = 4, \cdots, n$, j = 1, 2, 3. Set $u_{\epsilon_1, \epsilon_2, \epsilon_3}(x_1, x_2, x_3) = (\epsilon_1 \sqrt{|a_1|^2 - x_1^2}, \epsilon_2 \sqrt{|a_2|^2 - x_2^2}, \epsilon_3 \sqrt{|a_3|^2 - x_3^2})$, where $\epsilon_k \in \{\pm 1\}(k = 1, 2, 3)$.

Based on the proof of Lemma 2.5, we give the proof of Theorem 2.6.

Proof of Theorem 2.6 In Lemma 2.5, let $\sqrt{|a_k|^2 - x_k^2} := X_k \in [0, |a_k|](k = 1, ..., n)$ due to the fact that $x_k \in [0, |a_k|]$. This implies that

$$\begin{aligned} \min_{(x_1,\dots,x_n)\in\mathcal{U}_{\Delta A_1,\dots,\Delta A_n}} \sum_{k=1}^n x_k^2 \\ &= \operatorname{Tr}\left(\boldsymbol{T}_{a_1,\dots,a_n}\right) - \max\left\{\sum_{k=1}^n X_k^2 : \begin{cases} (\epsilon_1 X_1, \epsilon_2 X_2, \epsilon_3 X_3) \boldsymbol{T}_{a_1,a_2,a_3}^{-1}(\epsilon_1 X_1, \epsilon_2 X_2, \epsilon_3 X_3) \leqslant 1 \\ \epsilon_l X_l = \sum_{j=1}^3 \kappa_{lj} \epsilon_j X_j (\forall l = 4, \dots, n) \end{cases} \right] \\ &= \operatorname{Tr}\left(\boldsymbol{T}_{a_1,\dots,a_n}\right) - \max\left\{\sum_{k=1}^n Y_k^2 : \begin{cases} (Y_1, Y_2, Y_3) \boldsymbol{T}_{a_1,a_2,a_3}^{-1}(Y_1, Y_2, Y_3)^{\mathsf{T}} \leqslant 1 \\ Y_l = \sum_{j=1}^3 \kappa_{lj} Y_j (\forall l = 4, \dots, n) \end{cases} \right\}. \end{aligned}$$

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Next, we show that

$$\max\left\{\sum_{k=1}^{n} Y_{k}^{2} : \left\{ (Y_{1}, Y_{2}, Y_{3}) \boldsymbol{T}_{\boldsymbol{a}_{1}, \boldsymbol{a}_{2}, \boldsymbol{a}_{3}}^{-1} (Y_{1}, Y_{2}, Y_{3})^{\mathsf{T}} \leqslant 1 \\ Y_{l} = \sum_{j=1}^{3} \kappa_{lj} Y_{j} (\forall l = 4, \dots, n) \right\} = \lambda_{\max}(\boldsymbol{T}_{\boldsymbol{a}_{1}, \dots, \boldsymbol{a}_{n}}).$$

Indeed, let $P = (a_1, a_2, a_3)$, where each a_j is a column vector in \mathbb{R}^3 . Due to the fact that $a_l = \sum_{j=1}^3 \kappa_{lj} a_j (\forall l = 4, ..., n)$, we see that

$$(\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3) \begin{pmatrix} \kappa_{l1} \\ \kappa_{l2} \\ \kappa_{l3} \end{pmatrix} = \boldsymbol{P} \begin{pmatrix} \kappa_{l1} \\ \kappa_{l2} \\ \kappa_{l3} \end{pmatrix} = \boldsymbol{a}_l \iff \begin{pmatrix} \kappa_{l1} \\ \kappa_{l2} \\ \kappa_{l3} \end{pmatrix} = \boldsymbol{P}^{-1} \boldsymbol{a}_l.$$

Denote by $y := (Y_1, Y_2, Y_3)^T$. Then, $Y_l = \sum_{j=1}^3 \kappa_{lj} Y_j (l = 4, ..., n)$ can be rewritten as

$$Y_l = \left\langle \begin{pmatrix} \kappa_{l1} \\ \kappa_{l2} \\ \kappa_{l3} \end{pmatrix}, \begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \end{pmatrix} \right\rangle = \left\langle \boldsymbol{P}^{-1} \boldsymbol{a}_l, \, \boldsymbol{y} \right\rangle.$$

Based on the above observation, we have immediately that

$$\sum_{j=1}^{n} Y_{j}^{2} = \sum_{j=1}^{3} Y_{j}^{2} + \sum_{l=4}^{n} Y_{l}^{2} = \langle \mathbf{y}, \mathbf{y} \rangle + \sum_{l=4}^{n} \langle \mathbf{y}, \mathbf{P}^{-1} \mathbf{a}_{l} \rangle \langle \mathbf{P}^{-1} \mathbf{a}_{l}, \mathbf{y} \rangle$$
$$= \langle \mathbf{y} | \mathbb{1} | \mathbf{y} \rangle + \left\langle \mathbf{y} \left| \sum_{l=4}^{n} \left(\mathbf{P}^{-1} \mathbf{a}_{l} \right) \left(\mathbf{P}^{-1} \mathbf{a}_{l} \right)^{\mathsf{T}} \right| \mathbf{y} \right\rangle$$
$$= \left\langle \mathbf{y} \left| \mathbb{1} + \sum_{l=4}^{n} \left(\mathbf{P}^{-1} \mathbf{a}_{l} \right) \left(\mathbf{P}^{-1} \mathbf{a}_{l} \right)^{\mathsf{T}} \right| \mathbf{y} \right\rangle,$$

where, via $Q := P^{-1}$,

$$\mathbb{1} + \sum_{l=4}^{n} \left(\boldsymbol{P}^{-1} \boldsymbol{a}_{l} \right) \left(\boldsymbol{P}^{-1} \boldsymbol{a}_{l} \right)^{\mathsf{T}} = \boldsymbol{\mathcal{Q}} \left(\sum_{j=1}^{n} \boldsymbol{a}_{j} \boldsymbol{a}_{j}^{\mathsf{T}} \right) \boldsymbol{\mathcal{Q}}^{\mathsf{T}}$$

implying that

$$\sum_{j=1}^{n} Y_{j}^{2} = \left\langle \mathbf{y} \left| \boldsymbol{\mathcal{Q}} \left(\sum_{j=1}^{n} \boldsymbol{a}_{j} \boldsymbol{a}_{j}^{\mathsf{T}} \right) \boldsymbol{\mathcal{Q}}^{\mathsf{T}} \right| \mathbf{y} \right\rangle.$$

$$\max\left\{\sum_{k=1}^{n} Y_{k}^{2} : \left\{ (Y_{1}, Y_{2}, Y_{3}) \boldsymbol{T}_{a_{1}, a_{2}, a_{3}}^{-1} (Y_{1}, Y_{2}, Y_{3})^{\mathsf{T}} \leqslant 1 \\ Y_{l} = \sum_{j=1}^{3} \kappa_{lj} Y_{j} (\forall l = 4, \dots, n) \right\}$$
$$= \max_{\langle \boldsymbol{v}, \boldsymbol{v} \rangle \leqslant 1} \left\langle \boldsymbol{v} \left| \sum_{j=1}^{n} a_{j} a_{j}^{\mathsf{T}} \right| \boldsymbol{v} \right\rangle = \lambda_{\max} \left(\sum_{j=1}^{n} a_{j} a_{j}^{\mathsf{T}} \right)$$
$$= \lambda_{\max} (\boldsymbol{T}_{a_{1}, \dots, a_{n}}).$$

Here, the last equality is true since both MM^{T} and $M^{\mathsf{T}}M$ have the same spectrum when ignoring the zero eigenvalues for real matrix M. Hence, the same maximal eigenvalues $\lambda_{\max}(MM^{\mathsf{T}}) = \lambda_{\max}(M^{\mathsf{T}}M)$. Let $M = (a_1, \ldots, a_n)$. Then,

$$\sum_{j=1}^{n} a_j a_j^{\mathsf{T}} = M M^{\mathsf{T}}, \quad T_{a_1,\ldots,a_n} = M^{\mathsf{T}} M$$

These can give our desired result.

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