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Superposition Quantification*

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Abstract *The principle of superposition is universal and lies at the heart of quantum theory. Although ever since the inception of quantum mechanics a century ago, superposition has occupied a central and pivotal place, rigorous and systematic studies of the quantification issue have attracted significant interests only in recent years, and many related problems remain to be investigated. In this work we introduce a figure of merit which quantifies superposition from an intuitive and direct perspective, investigate its fundamental properties, connect it to some coherence measures, illustrate it through several examples, and apply it to analyze wave-particle duality.*

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1 Introduction

The celebrated monograph of Dirac on quantum mechanics began with the principle of superposition,[1] which is the backbone and hallmark of quantum mechanics. Superposition stems from the linearity of quantum mechanics, exhibits simple and elegant mathematical structure as well as rich and profound physical contents (e.g., the Bohr complementarity principle and the wave-particle duality) with wide range applications. The linear structure of quantum mechanics is extremely rigid. Violation of linearity will lead to non-causality and other unphysical consequences.

From a fundamental point of view, superposition incorporates coherently the sum of pure quantum states, in radical contrast to the incoherent mixing of density operators. Many quantum phenomena have their origins in superposition. Coherence and interference spring from superposition, while decoherence may be interpreted as breaking of superposition. Entanglement arises from the interplay of superposition and tensor product. Quantum correlations have their underpinning in superposition. Quantum no-cloning is also a consequence of the restriction imposed by superposition. Modern quantum information science exploits extensively superposition, which is a necessary ingredient in many quantum substrates. Superpositions of quantum states are ubiquitously used to create weird material states in order to exploit quantum technologies.[2] Among the celebrated examples of superposition of quantum states are the Schrödinger cat state, the Bell states, the GHZ state, the W state, the NOON state, etc. All these states are important examples of quantum entanglement. We may wonder what are the quantitative and qualitative differences between them in terms of superposition. When one talks about superposition, one is usually concerned with pure states, however, even for mixed states, it still seems that there is certain degree of superposition therein, and it is desirable to quantify the superposition in mixed states. Another important feature of superposition is the fragility, but the issue of how fragile it is certainly requires a quantitative description. In constructing robust and macroscopic superposition, a quantitative theory is also necessary to assess the outcomes.

Given the basic and prominent nature of superposition, it is curious that quantitative studies of superposition and related issues of coherence quantification, in particular from the information-theoretic perspective, have only attracted attention quite recently,[3−25] although the quantitative investigations of wave-particle duality, from both theoretical and experimental perspectives, have made great progress in the last decades.[26−37] Explicit quantitative studies of superposition are quite few.[3] Quantification of superposition is an elusive and subtle subject. Inspired by the investigation of superposition in terms of relative entropy initiated by Åberg,[3] in this work we take a more direct and intuitive approach to superposition quantification, introduce an intrinsic measure of superpo-

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sition, and apply it to the analysis of wave-particle duality. The measure of superposition may also be interpreted as a bona fide coherence measure, which is intimately related to, but different from, the conventional ones.[4]

The work is arranged as follows. In Sec. 2, we introduce a measure of superposition, investigate its fundamental properties, and illustrate it by several important examples. We utilize the superposition measure to present some quantitative analysis of the wave-particle duality. We conclude with discussions in Sec. 3.

2 Quantifying Superposition

Inspired by the work of Åberg,[3] but with a different approach, we first introduce a general measure of superposition of a quantum state ρ with respect to an orthogonal decomposition of the system Hilbert space

$$H = H_1 \oplus H_2 \oplus \cdots \oplus H_m \tag{1}$$

of finite dimension n =dim$H$, where H_j may be of different dimensions. The decomposition is usually induced by the spectral resolution of some observable such as the Hamiltonian or the number operator with H_j the corresponding eigenspaces. A general element in the superposition of the subspaces $\{H_j\}$ is $|\Phi\rangle = \sum_{j=1}^m c_j|\phi_j\rangle$ with pure states $|\phi_j\rangle \in H_j$. We understand the superposition with equal absolute weight, i.e., $|c_j| = 1/\sqrt{m}$ for all j, as a standard superposition. In this setting, by comparing any state ρ (in general mixed) on H with these standard superpositions, we may define a natural measure of superposition of ρ as

$$V(\rho|\{H_j\}) := \max_{|\Phi\rangle}\langle\Phi|\rho|\Phi\rangle - \frac{1}{n}\,, \tag{2}$$

with the maximization being over

$$|\Phi\rangle = \frac{1}{\sqrt{m}}\sum_{j=1}^m |\phi_j\rangle\,, \quad |\phi_j\rangle \in H_j\,, \quad \langle\phi_j|\phi_j\rangle = 1\,.$$

Here the normalization of the various component states $|\phi_j\rangle$ is crucial. The substraction of $1/n$ is for the convention so that for the maximally mixed state $\rho = \mathbf{1}/n$, we have $V(\mathbf{1}/n|\{H_j\}) = 0$. In particular, when $\rho = |\Psi\rangle\langle\Psi|$ is a pure state, we have $V(|\Psi\rangle|\{H_j\}) := \max_{|\Phi\rangle} |\langle\Phi|\Psi\rangle|^2 - 1/n$. Note that under the above substraction convention, the superposition achieves its maximal value $1 - 1/n$ for any maximally superposed state

$$|\Psi\rangle = \frac{1}{\sqrt{m}}\sum_j |\phi_j\rangle\,, \quad |\phi_j\rangle \in H_j\,, \quad \langle\phi_j|\phi_j\rangle = 1\,.$$

Thus it seems reasonable to further normalize the superposition measure by multiplying it with the factor $n/(n-1)$ so that the superposition of the maximally superposed state takes the value of unity, however we will not take this convention in order to maintain the simplicity of the definition. It should be emphasized that superposition here is always understood with respect to an orthogonal sum decomposition of the total system Hilbert space (1), though non-orthogonal decomposition can also be treated.

Although the general cases with some H_i multidimensional are important, the most interesting and simplest case is that when all H_j are one-dimensional. In this scenario, there exists an orthonormal base $\{|j\rangle\}$ of the Hilbert space H such that $H_j = \{c|j\rangle : c \in C\}$ is spanned by a single vector $|j\rangle$. Usually, such an orthonormal base arises from the spectral decomposition of an observable $A = \sum_j a_j|j\rangle\langle j|$ as the eigen-states (e.g., energy eigenstates of the Hamiltonian), then we talk about superposition with respect to A. A superposition of this family of states takes the form $|\Psi\rangle = \sum_{j=1}^n c_j|j\rangle$ with c_j complex numbers satisfying the normalization condition $\sum_j |c_j|^2 = 1$. It is intuitive and reasonable to take the states satisfying $|c_j|^2 = 1/n$ for all j (i.e., with equal weight of magnitude) as a benchmark of superposition. Thus all benchmark superpositions of states with respect to $\{|j\rangle\}$ read

$$|\theta\rangle := \frac{1}{\sqrt{n}}\sum_{j=1}^n \mathrm{e}^{\mathrm{i}\theta_j}|j\rangle\,, \tag{3}$$

with $\theta = (\theta_1, \theta_2, \ldots, \theta_n) \in R^n$ essentially playing the role of phase factors, which are key ingredients in interferometry. In this context, we write $V(\rho|\{H_j\})$ as $V(\rho)$ with the understanding that the quantity is always defined with respect to a base $\{|j\rangle\}$, and the maximization in the measure of superposition defined by Eq. (2) takes the explicit form

$$\begin{aligned} V(\rho) &= \max_\theta\langle\theta|\rho|\theta\rangle - \frac{1}{n} = \frac{1}{n}\max_\theta \sum_{j\neq k} c_{jk}\,\mathrm{e}^{\mathrm{i}(\theta_j-\theta_k)} \\ &= \frac{2}{n}\max_\theta \mathrm{Re}\Big(\sum_{j<k} c_{jk}\,\mathrm{e}^{\mathrm{i}(\theta_j-\theta_k)}\Big)\,, \end{aligned} \tag{4}$$

where $c_{jk} = \langle k|\rho|j\rangle$, and thus ρ has the matrix representation $\rho = (c_{jk})$ (with respect to the canonical base). Clearly for any pure state, $V(|\Phi\rangle) = \max_\theta |\langle\theta|\Phi\rangle|^2 - 1/n$. This measure is different from the coherence measure[4]

$$C(\rho) = \frac{1}{n}\sum_{j\neq k} |c_{jk}| \tag{5}$$

defined via the l_1-norm, although they indeed coincide for pure states, which will be made explicit shortly. We emphasize that Eq. (4) is essentially a quadratic programming problem, and the maximization cannot be carried out analytically in general. However, various numerical methods are available.

Some fundamental properties of the superposition are as follows.

Theorem 1

(i) For an n-dimensional system, $0 \le V(\rho) \le 1 - 1/n$, and $V(\rho) = 0$ if and only if $\rho = \sum_j p_j|j\rangle\langle j|$ for some p_j, $p_j \ge 0$, $\sum_j p_j = 1$, i.e., diagonal in the base $\{|j\rangle\}$, while

$V(\rho)=1-1/n$ if and only if ρ is a pure state of the form given by Eq. (3).

(ii) The superposition vanishes after the quantum measurement $\Pi=\{\Pi_j:=|j\rangle\langle j|\}$ along the base: $V(\Pi(\rho))=0$, where $\Pi(\rho)=\sum_j \Pi_j\rho\Pi_j$.

(iii) The superposition measure is convex in the sense that

$$V\Big(\sum_i p_i\rho_i\Big)\le\sum_i p_iV(\rho_i)\,,$$

where ρ_i are density operators, $p_i\ge 0$, $\sum_i p_i=1$.

(iv) If $|\Psi\rangle=\sum_j c_j|j\rangle$ with $\sum_j|c_j|^2=1$, then

$$V(|\Psi\rangle)=\frac{1}{n}\sum_{j\neq k}|c_jc_k|\,.$$

(v) Let $\sum_{i=1}^m|c_i|^2=1$, then

$$V\Big(\sum_{i=1}^m c_i|\Phi_i\rangle\Big)\le\sum_{i=1}^m V(|\Phi_i\rangle)+\frac{m-1}{n}\,.$$

We proceed to the proof of the above results.

For (i), we first show that $V(\rho)\ge 0$, i.e., $\max_\theta\langle\theta|\rho|\theta\rangle\ge 1/n$. Suppose in the contrary that for all θ, it held that $\langle\theta|\rho|\theta\rangle<1/n$, then

$$\int_0^{2\pi}\cdots\int_0^{2\pi}\langle\theta|\rho|\theta\rangle\frac{\mathrm{d}\theta}{(2\pi)^n}<\frac{1}{n}\,,\tag{6}$$

where $\mathrm{d}\theta=\mathrm{d}\theta_1\mathrm{d}\theta_2\cdots\mathrm{d}\theta_n$. On the other hand, from Eq. (3) we have

$$|\theta\rangle\langle\theta|=\frac{1}{n}\sum_{jk}|j\rangle\langle k|\,\mathrm{e}^{\mathrm{i}(\theta_j-\theta_k)}\,,$$

and consequently by direct evaluation of the integral, we have

$$\int_0^{2\pi}\cdots\int_0^{2\pi}|\theta\rangle\langle\theta|\frac{\mathrm{d}\theta}{(2\pi)^n}=\frac{1}{n}\sum_j|j\rangle\langle j|=\frac{\mathbf{1}}{n}\,,$$

where $\mathbf{1}$ stands for the identity operator on H. This implies that

$$\begin{aligned}&\int_0^{2\pi}\cdots\int_0^{2\pi}\langle\theta|\rho|\theta\rangle\frac{\mathrm{d}\theta}{(2\pi)^n}\\&=\int_0^{2\pi}\cdots\int_0^{2\pi}\mathrm{tr}(\rho|\theta\rangle\langle\theta|)\frac{\mathrm{d}\theta}{(2\pi)^n}\\&=\mathrm{tr}\Big(\rho\int_0^{2\pi}\cdots\int_0^{2\pi}|\theta\rangle\langle\theta|\frac{\mathrm{d}\theta}{(2\pi)^n}\Big)=\frac{1}{n}\,,\end{aligned}\tag{7}$$

which contradicts inequality (6). Consequently, there exists θ such that $\langle\theta|\rho|\theta\rangle\ge 1/n$, i.e., $V(\rho)\ge 0$.

Alternatively (as suggested by the referee), the property $V(\rho)\ge 0$ can also be proved more easily as follows: by recognizing $|\theta\rangle$ as one of the basis vectors, the maximum of $\langle\theta|\rho|\theta\rangle$ (which is in fact the maximum diagonal element of the matrix representation of ρ in a reference basis containing $|\theta\rangle$) over all $|\theta\rangle$ is obviously larger than $1/n$ since $\mathrm{tr}\rho=1$.

The upper bound for $V(\rho)$ follows from the defining Eq. (4) since $\langle\theta|\rho|\theta\rangle=\mathrm{tr}\rho|\theta\rangle\langle\theta|\le\mathrm{tr}\rho=1$ for any θ.

It is clear from the last equality in Eq. (4) that $V(\rho)=0$ for any $\rho=\sum_j p_j|j\rangle\langle j|$ since the cross terms c_{jk}, $j\neq k$, of the matrix representation of ρ with respect to the base $\{|j\rangle\}$ all vanish. Next, we show that $V(\rho)=0$ implies that ρ is of the diagonal form $\rho=\sum_j p_j|j\rangle\langle j|$. From $V(\rho)=0$ it follows that $\max_\theta\langle\theta|\rho|\theta\rangle-1/n=0$. We claim that in this case actually $\langle\theta|\rho|\theta\rangle-1/n=0$ for any θ, i.e., $(1/n)\sum_{j\neq k}c_{jk}\,\mathrm{e}^{\mathrm{i}(\theta_j-\theta_k)}=0$ for any $\theta=(\theta_1,\theta_2,\ldots,\theta_n)$, which implies that $c_{jk}=0$ for $j\neq k$. Suppose in the contrary that there existed θ such that $\langle\theta|\rho|\theta\rangle-1/n<0$, then by the continuity of $\langle\theta|\rho|\theta\rangle$ with respect to θ, we would have

$$\int_0^{2\pi}\cdots\int_0^{2\pi}\langle\theta|\rho|\theta\rangle\frac{\mathrm{d}\theta}{(2\pi)^n}-\frac{1}{n}<0\,.$$

This contradicts Eq. (7).

The last statement in item (i) is clear from the defining Eq. (4).

To establish (ii), noting that $\Pi(\rho)=\sum_j\Pi_j\rho\Pi_j=\sum_j p_j|j\rangle\langle j|$ with $p_j=\mathrm{tr}\Pi_j\rho\Pi_j$, we have $\langle\theta|\pi(\rho)|\theta\rangle=\sum_j p_j/n=1/n$, and the desired result follows.

Item (iii) follows from

$$\begin{aligned}V\Big(\sum_i p_i\rho_i\Big)&=\max_\theta\Big\langle\theta\Big|\sum_i p_i\rho_i\Big|\theta\Big\rangle-\frac{1}{n}\\&=\max_\theta\sum_i p_i\langle\theta|\rho_i|\theta\rangle-\frac{1}{n}\\&\le\sum_i p_i\max_\theta\langle\theta|\rho_i|\theta\rangle-\frac{1}{n}\\&=\sum_i p_iV(\rho_i)\,.\end{aligned}$$

Item (iv) follows from the defining Eq. (4) by noting that if $\rho=(c_{jk})=|\Psi\rangle\langle\Psi|$ is pure, then $c_{jk}=c_j\bar{c}_k$, and the maximum can be directly evaluated.

To establish (v), noting that by the Cauchy–Schwarz inequality,

$$\begin{aligned}V\Big(\sum_{i=1}^m c_i|\Phi_i\rangle\Big)&=\max_\theta\Big|\langle\theta|\sum_{i=1}^m c_i|\Phi_i\rangle\Big|^2-\frac{1}{n}\\&=\max_\theta\Big|\sum_{i=1}^m c_i\langle\theta|\Phi_i\rangle\Big|^2-\frac{1}{n}\\&\le\max_\theta\Big(\sum_{i=1}^m|c_i|^2\Big)\Big(\sum_{i=1}^m|\langle\theta|\Phi_i\rangle|^2\Big)-\frac{1}{n}\\&\le\sum_{i=1}^m\max_\theta|\langle\theta|\Phi_i\rangle|^2-\frac{1}{n}\\&=\sum_{i=1}^m V(|\Phi_i\rangle)+\frac{m-1}{n}\,.\end{aligned}$$

Before applying the superposition measure to characterize wave-particle duality in the next section, we work out several examples to gain a more intuitive glimpse of this measure.

Example 1 Consider a qubit system with the canonical base $\{|0\rangle, |1\rangle\}$. For any mixed state $\rho = (c_{jk})$ represented in the matrix form relative to the canonical base, the superposition can be evaluated as $V(\rho) = |c_{12}|$, which coincides with the coherence measure $C(\rho)$.[4] In particular, for any pure state $|\Phi\rangle = a|0\rangle + b|1\rangle$, where a, $b \in C$, $|a|^2 + |b|^2 = 1$, we have $V(|\Phi\rangle) = |ab|$. We see that in the qubit case, the superposition indeed quantifies precisely the coherence (or interference), and coincides with the conventional measure of coherence.

Example 2 Recall item (iv) of Theorem 1 and Eq. (5), for an n-dimensional system with canonical base $\{|j\rangle\}$, any pure state $|\Psi\rangle = \sum_j c_j|j\rangle$ has the amount of superposition $V(|\Psi\rangle) = (1/n)\sum_{j\neq k}|c_jc_k|$. If $\rho = (c_{jk})$ (with respect to the canonical base) is a mixed state, then

$$V(\rho) = \frac{1}{n}\max_{\theta}\sum_{j\neq k} c_{jk}\,\mathrm{e}^{\mathrm{i}(\theta_j-\theta_k)}$$

is upper dominated by the widely used coherence measure defined by Eq. (5) in the sense that

$$V(\rho) \leq C(\rho)\,. \tag{8}$$

Noting the strict inequality may hold for some mixed states, as shown by a simple analysis of degrees of freedom: There are formally n freedoms to choose the numbers θ_j, but there are $n(n-1)/2$ freedoms to choose the signs of c_{jk}. An explicit example illustrating the difference between $V(\rho)$ and $C(\rho)$ is the state

$$\rho = \frac{1}{9}\begin{pmatrix} 3 & 1 & 1 \\ 1 & 3 & -1 \\ 1 & -1 & 3 \end{pmatrix}$$

expressed in the canonical base $\{|j\rangle\}$ for which $V(\rho) = 1/9 < C(\rho) = 2/9$.

Example 3 For a two-qubit system with the canonical base $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, consider the Bell-diagonal state

$$\rho = \frac{1}{4}\Big(\mathbf{1} + \sum_{j=1}^{3} c_j\sigma_j\otimes\sigma_j\Big) = \frac{1}{4}\begin{pmatrix} 1+c_3 & 0 & 0 & c_1-c_2 \\ 0 & 1-c_3 & c_1+c_2 & 0 \\ 0 & c_1+c_2 & 1-c_3 & 0 \\ c_1-c_2 & 0 & 0 & 1+c_3 \end{pmatrix},$$

with σ_j being the Pauli spin matrices, then

$$V(\rho) = \frac{1}{8}(|c_1-c_2| + |c_1+c_2|)\,.$$

In particular, for the Werner state $\rho = p|\Psi^-\rangle\langle\Psi^-| + (1-p)(\mathbf{1}/4)$ with $|\Psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$, $0 \leq p \leq 1$, we have $V(\rho) = p/4$.

Example 4 In a 3-qubit system, two prominent examples of superpositions of states are the GHZ state $|\mathrm{GHZ}\rangle = (1/\sqrt{2})(|000\rangle + |111\rangle)$ and the W state $|W\rangle = (1/\sqrt{3})(|001\rangle + |010\rangle + |100\rangle)$, we have

$$V(|\mathrm{GHZ}\rangle) = \frac{1}{8}\,,\quad V(|W\rangle) = \frac{2}{8}\,.$$

We see that from the superposition point of view, the W state exhibits higher degree of superposition as is intuitively clear, although the GHZ state is more entangled.

In terms of the measure of superposition, the notion of mutually unbiased bases may be simply formulated as that the amount of superposition of each state in a base achieves its maximal value with respect to the other base: If the base $\{|\alpha\rangle\}$ is mutually unbiased relative to $\{|j\rangle\}$, i.e., $|\langle j|\alpha\rangle| = 1/\sqrt{n}$ for all j and α, then $V(|\alpha\rangle) = 1 - 1/n$. It is an interesting problem to explore the relations of superposition with two mutually unbiased bases, and one expects some complementary relations.

Superposition is intimately related to coherence, and indeed, coherence usually follows from superposition. Thus a measure of superposition is naturally in the same time a measure of coherence. Our measure captures superposition directly, in contrast to the coherence measures, which are usually defined via distance to incoherent states. We emphasize that just like superposition, whenever we talk about coherence, we are referring to coherence with respect to a particular base. That is, superposition and coherence are contextual phenomena.

Now we discuss wave-particle duality in terms of superposition. Quantitative characterizations of wave-particle duality have been studied by many authors.[26–37] The amount of superposition $V(\rho)$ may be used to quantify the interference of an n-path interferometer. To extract and quantify the path information, one needs to couple the system with a measurement apparatus. Following the measurement scheme of von Neumann,[38] consider a system state $|\Psi^a\rangle = \sum_j c_j|j\rangle$ and a measurement coupling the state to an apparatus, which yields the combined system

$$|\Psi^{ab}\rangle = \sum_j c_j|j\rangle\otimes|d_j\rangle\,, \tag{9}$$

where $|d_j\rangle$ are detector states, in general not necessary orthogonal, which are used to extract information about the path $|j\rangle$. Here the system and the measurement apparatus are indicated by a and b, respectively. Since any coupling will lead to information leakage (superposition loss, decoherence), by intuition it is reasonable to expect the following result.

Theorem 2 It holds that

$$V(\rho^a) \leq V(|\Psi^a\rangle)\,, \tag{10}$$

where $\rho^a := \mathrm{tr}_b|\Psi^{ab}\rangle\langle\Psi^{ab}| = \sum_{jk} c_j\bar{c}_k\langle d_k|d_j\rangle|j\rangle\langle k|$ is the reduced state of the system a.

This follows from

$$V(\rho^a) = \frac{1}{n}\max_{\theta}\sum_{j\neq k} c_j\bar{c}_k\langle d_k|d_j\rangle\,\mathrm{e}^{\mathrm{i}(\theta_j-\theta_k)}$$

$$\leq \frac{1}{n}\sum_{j\neq k}|c_j\bar{c}_k|\cdot|\langle d_k|d_j\rangle|$$
$$\leq \frac{1}{n}\sum_{j\neq k}|c_j\bar{c}_k| = V(\Psi^a)$$

by noting that $|\langle d_k|d_j\rangle|\leq 1$.

Two extreme cases are of particular significance: On one hand, if $\{|d_j\rangle\}$ is an orthonormal base, i.e., we get the complete path information, then the superposition vanishes completely, i.e., $V(\rho^a)=0$. On the other hand, if all $|d_j\rangle$ are equal, we get no path information at all, and the superposition is preserved, i.e., $V(\rho^a)=V(|\Psi^a\rangle)$. Consequently, the superposition measure already nicely captures the extreme cases of the wave-particle duality. The difference $D(\rho^a):=V(|\Psi^a\rangle)-V(\rho^a)$ may be interpreted as the de-superposition (decoherence, path information, information leakage) due to the measurement. In this context, we have a mathematically trivial yet physically significant wave-particle duality relation $V(\rho^a)+D(\rho^a)=V(|\Psi^a\rangle)$.

In the following, we present an alternative and intuitive characterization of wave-particle duality based on our superposition measure and the Gram matrix (encoding the identity information in a quantum ensemble), which also constitutes a reinterpretation of the wave-particle duality in the spirit of Ref. [36].

A natural way to quantify the path information is to pursue the ability to discriminate the states in the quantum ensemble $\{|c_j|^2,|d_j\rangle\langle d_j|\}$, or equivalently, the subnormalized vectors $\{|c_j|\cdot|d_j\rangle\}$ of the measurement apparatus, arising from the detector state

$$\rho^b := \mathrm{tr}_a|\Psi^{ab}\rangle\langle\Psi^{ab}| = \sum_j |c_j|^2|d_j\rangle\langle d_j|$$

with each state $|d_j\rangle$ encoding the path information of $|j\rangle$. The Gram matrix of the ensemble $\{|c_j|\cdot|d_j\rangle\}$ is defined as[39–40]

$$G=(g_{jk}),\quad g_{jk}=|c_jc_k|\langle d_j|d_k\rangle\,,$$

whose absolute norm

$$Q(\rho^b):=\frac{1}{n}\sum_{j\neq k}|c_jc_k|\cdot|\langle d_j|d_k\rangle|$$

summarizes the difficulty (ambiguity) in discriminating the involved states. Noting that the maximum value of $Q(\rho^b)$ is $1-1/n$, thus

$$\Lambda(\rho^b):=1-\frac{1}{n}-Q(\rho^b)$$

may be interpreted as a measure for the path information. It is remarkable that this quantity actually serves as an upper bound to the minimal error probability for unambiguous discrimination of quantum states,[36,41–42] and has been used in quantifying wave-particle duality:[36]

$$C(\rho^a)+\Lambda(\rho^b)\leq 1-\frac{1}{n}\,, \qquad (11)$$

where the coherence measure $C(\rho)$ is different from our superposition measure $V(\rho)$ in general. Now the wave-particle duality in terms of the superposition measure $V(\rho)$ may be derived from inequalities (8) and (11) as

$$V(\rho^a)+\Lambda(\rho^b)\leq 1-\frac{1}{n}\,,$$

where $\rho^a=\mathrm{tr}_b|\Psi^{ab}\rangle\langle\Psi^{ab}|$, $\rho^b=\mathrm{tr}_a|\Psi^{ab}\rangle\langle\Psi^{ab}|$, with $|\Psi^{ab}\rangle$ being defined by Eq. (9). The physical meaning lies in that $V(\rho^a)$ quantifies the wave (superposition) property of the system a, while $\Lambda(\rho^b)$ quantifies the particle (which-path) information (also of system a with the path information encoded in the measurement apparatus b).

As a remark, here we would like to emphasize that Gram matrix plays a significant role in quantum information theory, which needs further exploration. Noting that in quantum chemistry, the Gram matrix of a set of base states is also called the overlap matrix. The relations between the states in an ensemble are encoded in the Gram (correlation) matrix. The Gram matrix of any orthonormal base is the identity matrix. Deviation from the identity matrix represents nonorhogonality, and thus quantumness or the difficulty for discriminating the states. The entropy of the Gram matrix equals the entropy of the reduced state ρ^b, which is also called exchange entropy.

3 Discussions

We have introduced a measure for superposition of quantum states, and have revealed some basic properties of this figure of merit. Applications to quantifying the wave-particle duality are illustrated. Superposition, as a basic principle of the mathematical structure of quantum mechanics, lies at the roots of coherence and interference, and consequently the superposition measure can naturally be regarded as a measure of coherence, which turns out to be intimately related to, but different from, the significant coherence measure defined via the l_1 norm.[3] They coincide for any (pure or mixed) qubit states, as well as for pure states in any dimension. However, they differ in general for mixed states in high dimensional systems. Many properties, such as the monotonicity under incoherent mappings, of the superposition measure remain to be further investigated. It will also be interesting to adopt the present method to the entropic approach, and to quantify superposition in terms of information-disturbance tradeoff and information conservation.[43–45]

In recent years, mesoscopic and macroscopic superpositions are attracting increasing interests,[46–55] the superpose measure may be useful for these issues. It is desirable to investigate the interplay between superposition and quantumness, in particular their relation in the context of quantum correlations, and to pursue a unified view of related issues from the perspective of symmetry breaking.

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