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Maximum Entanglement

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Abstract—We discuss a novel variational principle in quantum mechanics defining maximum entangled states in terms of quantum fluctuations of observables specifying these states.

There are a few reasons to study maximum entangled states (MES)specifically. First of all, a number of important quantum communication and computing protocols, such as quantum teleportation [1], are based on the use of MES. Then, if MES of a given system are known, all other entangled (but not maximum entangled) states of this system can be constructed from the MES by means of stochastic local transformations assisted by classical communications (SLOCC) [2, 3]. Finally, MES can be described in the succinct and elegant form of a new variational principle [4] and thereby illuminate the physical nature of the phenomenon.

The main objective of this note is to discuss the variational principle for MES [4] and to demonstrate how this principle can be employed to determine MES in different physical systems.

It should be stressed that the various definitions of entanglement are mostly intuitive and contain accidental together with essential. An example is provided by the definition elaborated by the NSF Workshop on Quantum Information Science [5]:

{Quantum entanglement is a subtle nonlocal correlation among the parts of a quantum system that has no classical analog. Thus, entanglement is best characterized and quantified as a feature of the system that cannot be created through local operations that act on the different parts separately, or by means of classical communication.}

This definition contains an *a priori* assumption of nonlocality that leads to a loss of generality. In particular, it leaves aside the single-particle entanglement [6], as well as entanglement in the Bose–Einstein condensate of atoms, where the requirement of nonlocality is meaningless because of the strong overlap of wavefunctions of different atoms [7].

The absence of a classical analog is a common feature of almost all definitions of entanglement. In the best way, this is expressed in the figurative definition, which is ascribed to Aser Peres (for reference, see [8]):

{Entanglement is a trick that quantum magicians use to produce phenomena that cannot be imitated by classical magicians.}

Probably, the characteristic feature of MES that most experts agree with is their maximal remoteness from what is called "classical reality" [4].

Note that this is a question of remoteness from the classical reality and not of its violation, described by Bell's type of inequalities and Greenberger–Horne–Zeilinger (GHZ) conditions, which can be manifested by unentangled states [9, 10].

The main difference between the quantum and classical levels of understanding of physical systems ("physical reality") is the existence of quantum fluctuations (uncertainties) that vanish for classical states. The reason for the existence of quantum fluctuations lies in the very heart of quantum mechanics, in interpreting physical observables as operators with specific algebraic properties (commutation relations) [11]. Thus, the remoteness of a quantum state from classical reality can be specified by the maximum of the total variance describing the range of quantum fluctuations of all essential measurements [4].

Consider a physical system S defined in the Hilbert space $\mathbb{H}(S)$. Let $\{M_i\}$ be the set of all essential measurements completely specifying the state ψ of the system in $\mathbb{H}(S)$. The choice of the essential observables depends on the physical measurements we are going to perform over the system, or on the Hamiltonians, which are accessible for manipulations with states $\psi \in \mathbb{H}(S)$.

The set of essential measurements is usually associated with the dynamic symmetry group of the Hilbert space [9, 10]. For example, in the case of an N-qubit system defined in the space

$$\mathbb{H}(S) = \mathbb{H}_{2,N} = \bigotimes_{l=1}^{N} \mathbb{H}_2, \tag{1}$$

where $\mathbb{H}_2$ is the two-dimensional Hilbert space of states of spin $\frac{1}{2}$, the dynamic symmetry group is

$$G = SU(2) \times SU(2) \times \ldots \times SU(2) = \prod_{l=1}^{N} SU(2). \tag{2}$$

In each $\mathbb{H}_2$, the local measurements $\{M_i\}$ are given by the Pauli operators $\sigma_\alpha^{(i)}$ ($\alpha = 1, 2, 3$) [12] forming a representation of infinitesimal generators of the Lie algebra $\mathcal{L}^c = SU(2, \mathbb{C})$. The corresponding dynamic symmetry group

$$G^c = \prod_{l=1}^{N} \exp \mathcal{L}^c = \prod_{l=1}^{N} SU(2, \mathbb{C}) \tag{3}$$

is the complexification of G (2). Thus, in space (1), there are 3^N essential measurements provided by the Pauli operators $\sigma_\alpha^{(i)}$ ($i = 1, \ldots, N$, $\alpha = 1, 2, 3$).

The result of a quantum measurement is provided by the mean value

$$\langle M_i \rangle = \begin{cases} \langle \psi | M_i | \psi \rangle, \\ \mathrm{Tr}(\rho M_i) \end{cases} \tag{4}$$

and by the variance

$$V_i(M_i) = \begin{cases} \langle \psi | (\Delta M_i)^2 | \psi \rangle, \\ \mathrm{Tr}[\rho (\Delta M_i)^2] \end{cases} \tag{5}$$

in the case of pure and mixed states, respectively. Here,

$$(\Delta M_i)^2 \equiv (M_i - \langle M_i \rangle)^2$$

Then, the total variance describing the remoteness of a quantum state in $\mathbb{H}(S)$ from the classical reality takes the form

$$\mathbb{V} = \sum V_i(M_i). \tag{6}$$

According to our definition [4], the maximum of the total variance (6) corresponds to the averaging in the right-hand side of (6) over MES:

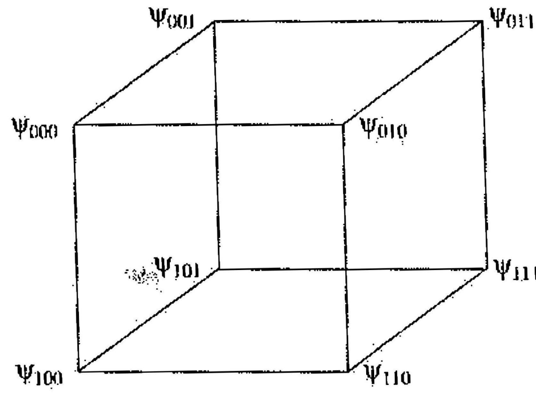
$$\max \mathbb{V} = \sum \begin{cases} \langle \psi_{\mathrm{MES}} | (\Delta M_i)^2 | \psi_{\mathrm{MES}} \rangle, \\ \mathrm{Tr}[\rho_{\mathrm{MES}} (\Delta M_i)^2]. \end{cases} \tag{7}$$

Here, ψ_{MES} and ρ_{MES} denote the pure and mixed MES, respectively.

This equation (7) represents a new variational principle for MES [4], which specifies MES as the manifestation of quantum fluctuations at their extreme.

By this definition, MES represent an exact antithesis to coherent states, which manifest the minimum scale of quantum fluctuations and, therefore, are maximally close to the classical reality [13, 14].

This definition (7) can be expressed in a different way in the important case when the enveloping algebra



Structure of the three-dimensional matrix $[\psi]$ in the case of three qubits. Vertices of the cube are associated with the coefficients $\psi_{l_1 l_2 l_3}$ in Eq. (11) at $N = 3$.

of the Lie algebra $L(M_i)$ of all essential measurements contains a uniquely defined Casimir operator (scalar),

$$\hat{\mathbf{C}} = \sum M_i^2 = \mathbf{C} \times \mathbb{I}, \tag{8}$$

where $\mathbb{I}$ is the unit operator in $\mathbb{H}(S)$. Since $V_i(M_i) \geq 0$ always, it follows from (5) and (6) that the maximum in (7) is achieved if

$$\forall i \quad \langle M_i \rangle = 0. \tag{9}$$

This property of MES was noticed in [15]. It immediately follows from (5)–(7) and (9) that the maximum total variance has the form

$$\mathbb{V}_{\max} = \mathbf{C}. \tag{10}$$

As an illustrative example of considerable interest, we examine the system of N qubits. Hereafter, we consider pure states. The obtained results can be easily generalized to the case of mixed states through the use of the result from [16] that the mixed states can be treated as pure states of a certain doublet consisting of the system and its "mirror image."

Denote the base vectors in $\mathbb{H}_2$ in (1) by $\mathbf{e}_l = |l\rangle$, where $l = 0, 1$. Then, an arbitrary pure state in (1) takes the form

$$|\psi\rangle = \sum \psi_{l_1 l_2 \ldots l_N} \mathbf{e}_{l_1} \otimes \mathbf{e}_{l_2} \otimes \ldots \otimes \mathbf{e}_{l_N}. \tag{11}$$

The coefficients $\psi_{l_1 l_2 \ldots l_N}$ form a multidimensional matrix $[\psi]$ (concerning multidimensional matrix and determinants, see [17]). In the case of $N = 3$ qubits, for example, $[\psi]$ is a cube, as shown in the figure.

The local measurements, provided in the case of qubits by the Pauli matrices, have the form

$$\begin{cases} \sigma_1^{(j)} = (\mathbf{e}_{0_j} \mathbf{e}_{1_j}^+ + \mathrm{H.c.}) \\ \sigma_2^{(j)} = i(\mathbf{e}_{1_j} \mathbf{e}_{0_j}^+ - \mathrm{H.c.}) \\ \sigma_3^{(j)} = \mathbf{e}_{0_j} \mathbf{e}_{0_j}^+ - \mathbf{e}_{1_j} \mathbf{e}_{1_j}^+, \end{cases} \tag{12}$$

where $j = 1, \ldots, N$. Since

$$\forall \alpha, j \quad [\sigma_\alpha^{(j)}]^2 = \mathbb{1},$$

the maximum total variance in the system of N qubits takes the value

$$\mathbb{V}_{\max}(S_{2,N}) = 3N. \tag{13}$$

For example, GHZ states of three qubits

$$|GHZ_3\rangle = \frac{1}{\sqrt{2}}(\mathbf{e}_{0_1}\mathbf{e}_{0_2}\mathbf{e}_{0_3} \pm \mathbf{e}_{1_1}\mathbf{e}_{1_2}\mathbf{e}_{1_3}) \tag{14}$$

obey condition (9) and have $\mathbb{V}(GHZ_3) = \mathbb{V}_{\max}(S_{2,3}) = 9$. Hence, (14) is MES. At the same time, the simple separable state, say $\mathbf{e}_{0_1}\mathbf{e}_{0_2}\mathbf{e}_{0_3}$, has the minimum total variance $\mathbb{V}_{\min}(S_{2,3}) = 6$ and, hence, belongs to the class of coherent states of three qubits.

To stress the fact that the variational principle (7) defines MES by the extreme of quantum fluctuations, we consider the so-called W state of three qubits [2]

$$|W_3\rangle = \frac{1}{\sqrt{3}}(\mathbf{e}_{0_1}\mathbf{e}_{1_2}\mathbf{e}_{1_3} + \mathbf{e}_{1_1}\mathbf{e}_{0_2}\mathbf{e}_{1_3} + \mathbf{e}_{1_1}\mathbf{e}_{1_2}\mathbf{e}_{0_3}). \tag{15}$$

Definitely, this is not MES because

$$\mathbb{V}(W_3) = 8 + 2/3 < \mathbb{V}_{\max}(S_{2,3}) = 9.$$

At the same time, this state manifests quite a high level of quantum fluctuations, which strongly exceeds that of coherent states with $\mathbb{V}_{\min}(S_{2,3}) = 6$. Nevertheless, the W state (15) does not manifest entanglement at all, because the only entanglement monotone for three qubits, which is the 3-tangle [18], has zero value in this case [19].

This means that the remoteness of states from classical reality provided by the total variance (6) cannot be used as a measure of entanglement.

Before we begin to discuss the possible choice of a universal measure of entanglement, it should be noted that condition (9) can also be expressed in terms of the properties of the matrix $[\psi]$ in (11). Namely, state (11) obeys condition (9) iff the parallel slices of the matrix $[\psi]$ are mutually orthogonal and have the same norm [4, 9, 10].

In the case of two qubits, the parallel slices are provided by the rows and columns of the (2×2) matrix $[\psi]$. In the case of three qubits, these are the parallel faces of the cube shown in Fig. 1, and so on.

As regards the quantifying entanglement, there have been numerous attempts to define a proper measure of entangled states. The main requirements are as follows.

(1) The measure should be zero in the case of unentangled states and achieve the maximum for MES.

2 The measure should be an entanglement monotone [20], i.e., a function which does not increase under the set of local transformations.

These conditions, together with the definition of MES and the possibility to construct any entangled state from MES by means of SLOCC [2, 3], make it possible to discuss the measure of entanglement within the geometric invariant theory [9]. Concerning geometric invariant theory, see [21]. Physical applications of this theory are discussed in [22]. In particular, a new universal measure of entanglement based on the notions of geometric invariant theory can be introduced [4, 9]. This is the length of minimal vector in complex orbit of the state $\psi \in \mathbb{H}(S)$:

$$\mu(\psi) = \min_{g \in G^c} |g\psi|^2. \tag{16}$$

Here, g denotes a transformation from the complexified dynamic symmetry group G^c in $\mathbb{H}(S)$. This measure (16) obeys the above requirements. In particular, in the case of the two-qubit state (state (11) with $N = 2$), (16) is defined to be the determinant of $[\psi]$, which is just the concurrence [23]. In the case of three qubits ($N = 3$ in (11)), measure (16) gives Cayley's hyperdeterminant [17]

$$\begin{aligned} D[\psi] &= \psi_{000}^2\psi_{111}^2 + \psi_{001}^2\psi_{110}^2 + \psi_{010}^2\psi_{101}^2 \\ &+ \psi_{011}^2\psi_{100}^2 - 2[\psi_{000}(\psi_{001}\psi_{110} + \psi_{010}\psi_{101} \\ &+ \psi_{011}\psi_{110})\psi_{111} + \psi_{001}\psi_{010}\psi_{101}\psi_{110} \\ &+ \psi_{001}\psi_{011}\psi_{110}\psi_{100} + \psi_{010}\psi_{011}\psi_{101}\psi_{100}] \\ &+ 4(\psi_{000}\psi_{011}\psi_{101}\psi_{110} + \psi_{001}\psi_{010}\psi_{100}\psi_{111}), \end{aligned} \tag{17}$$

which is the only entanglement monotone of this system. It should be noted that (17) coincides with the square root of the 3-tangle [19]. Measure (16) can also be calculated in the case of four qubits (all geometric invariants of four qubits have been calculated recently [24]).

Although the variational principle (7) has a general meaning, our consideration so far has applied to systems of qubits. Consider now a more complicated case of qutrit systems defined in the Hilbert space

$$\mathbb{H}_{3,N} = \bigotimes_{l=1}^{N} \mathbb{H}_3, \tag{18}$$

where $\mathbb{H}_3$ is the three-dimensional state spanned by the vectors $\mathbf{e}_l = |l\rangle$, where $l = 0, 1, 2$. An example is provided by the spin-1 systems.

For qutrit systems, a single-particle MES is allowed [4, 10]. Choosing the measurements as the infinitesimal generators of the $SL(2, \mathbb{C})$ algebra in three dimensions

$$\begin{cases} M_x = \dfrac{1}{\sqrt{2}}[(\mathbf{e}_0 + \mathbf{e}_2)\mathbf{e}_1^+ + \text{H.c.}] \\ M_y = \dfrac{-i}{\sqrt{2}}[(\mathbf{e}_0 - \mathbf{e}_2)\mathbf{e}_1^+ - \text{H.c.}] \\ M_z = \mathbf{e}_0\mathbf{e}_0^+ - \mathbf{e}_2\mathbf{e}_2^+, \end{cases} \tag{19}$$

we can easily see that the variational principle (7) expressed in the form of condition (9) defines the single-qutrit states

$$|\psi_{3,1}\rangle = \begin{cases} \frac{1}{\sqrt{2}}(\mathbf{e}_0 + e^{i\varphi_2}\mathbf{e}_2) \\ \mathbf{e}_1 \\ |\psi_0|(e^{i\varphi_0}\mathbf{e}_0 + e^{i\varphi_2}\mathbf{e}_2) \pm i|\psi_1|e^{i(\varphi_0+\varphi_2)/2}\mathbf{e}_1, \end{cases} \quad (20)$$

where ψ_l denotes the coefficients in

$$|\psi_{3,1}\rangle = \sum_{l=1}^{3} \psi_l \mathbf{e}_l \quad (21)$$

and $\varphi_{0,2}$ are arbitrary phases of the corresponding complex coefficients ψ_l. In the last state in (20),

$$2|\psi_0|^2 + |\psi_1|^2 = 1.$$

All the states in (21) have a maximum total variance $\max \mathbb{V}_{3,1} = 2$, while the coherent single-qutrit state has a minimum total variance $\min \mathbb{V}_{3,1} = 1$. Thus, a single qutrit has infinitely many MES with respect to measurements (19).

From the physical point of view, the subscript l in (21) should correspond to the internal degrees of freedom of a particle. As a possible realization, the states of $\pi^{\pm}$ and π^0 mesons with respect to up and down quarks should be mentioned here [4]. Namely, the quark states of $\pi^{\pm}$ mesons are coherent, while the quarks in π^0 are in MES. The extreme of quantum fluctuations, which is the basis of the variational principle for MES (7), sheds light on the fact that a π^0 meson is much less stable than $\pi^{\pm}$ mesons.

Generally, the variational principle (7) allows the existence of single-particle MES if the number of internal degrees of freedom exceeds two. It also follows from (7) and (9) that a single qubit is not able to manifest MES.

Consider now the two-qutrit system defined in the nine-dimensional Hilbert space

$$\mathbb{H}_{3,2} = \mathbb{H}_3 \otimes \mathbb{H}_3. \quad (22)$$

A pure state in (22) has the form

$$|\psi_{3,2}\rangle = \sum \psi_{l_1 l_2} \mathbf{e}_{l_1} \otimes \mathbf{e}_{l_2}. \quad (23)$$

We now note that the increase in the number of degrees of freedom per party also enlarges the possible choice of measurements [10]. In the case of qutrits, in addition to (19), one can choose the measurements corresponding to the local symmetry $SU(3)$ and provided by the eight independent operators out of the nine operators of the form

$$\{M\} = \left\{ \begin{array}{c} \mathbf{e}_l\mathbf{e}_l^+ - \mathbf{e}_{l+1}\mathbf{e}_{l+1}^+ \\ \frac{1}{2}(\mathbf{e}_l\mathbf{e}_{l+1}^+ + \text{H.c.}) \\ \frac{1}{2i}(\mathbf{e}_l\mathbf{e}_{l+1}^+ - \text{H.c.}) \end{array} \right\}. \quad (24)$$

Here, the cyclic permutations of subscripts are assumed, so that $l + 1 = 0$ if $l = 2$. It is clear that measurements (24) also include (19).

Using (9), it is a straightforward matter to see that there are infinitely many MES of the type of (23) with respect to (24) in the space (22). An important example is provided by the states

$$|\psi_q\rangle = \frac{1}{\sqrt{3}}(\mathbf{e}_{0_1}\mathbf{e}_{0_2} + e^{iq\phi_q}\mathbf{e}_{1_1}\mathbf{e}_{1_2} + e^{2iq\phi_q}\mathbf{e}_{2_1}\mathbf{e}_{2_2}), \quad (25)$$

where

$$\phi_q = \frac{2q\pi}{3}, \quad q = 0, 1, 2.$$

These states were introduced in the context of the quantum phase of the angular momentum of photons in [25] and as the states of "biphotons" [26]. These states were also discussed in connection with three-state quantum cryptography [27].

It is easy to construct a basis of MES in the Hilbert space (22) beginning with states (25) and using the local cyclic permutation operator [4] of the form

$$\mathscr{C} = \mathbf{e}_0\mathbf{e}_1^+ + \mathbf{e}_1\mathbf{e}_2^+ + \mathbf{e}_2\mathbf{e}_0^+. \quad (26)$$

Acting by (26) on the state of the first party in (25) once, we get

$$|\chi_q\rangle = \frac{1}{\sqrt{3}}(\mathbf{e}_{1_1}\mathbf{e}_{0_2} + e^{iq\phi_q}\mathbf{e}_{2_1}\mathbf{e}_{1_2} + e^{2iq\phi_q}\mathbf{e}_{0_1}\mathbf{e}_{2_2}). \quad (27)$$

Acting by (26) on the state of the first party once more, we obtain

$$|\eta_q\rangle = \frac{1}{\sqrt{3}}(\mathbf{e}_{2_1}\mathbf{e}_{0_2} + e^{iq\phi_q}\mathbf{e}_{0_1}\mathbf{e}_{1_2} + e^{2iq\phi_q}\mathbf{e}_{1_1}\mathbf{e}_{2_2}). \quad (28)$$

It is easily seen that states (27) and (28) obey conditions (9) and that states (25), (27), and (28) are mutually orthogonal. Thus, they form a basis of MES in space (22) of two qutrits.

In the case of a two-qutrit system, measure (16) coincides with the det[ψ] of the (3×3) matrix of coefficients in (23).

The local cyclic permutation operator (26) can be used to create MES from a certain generic MES in other cases as well [4]. For example, in the case of qubits,

(26) coincides with σ_1 in (12), while the generic MES can be chosen in GHZ form,

$$\frac{1}{\sqrt{2}}(\mathbf{e}_{0_1}\mathbf{e}_{0_2} \pm \mathbf{e}_{1_1}\mathbf{e}_{1_2}).$$

In the general case of qudits (d degrees of freedom per party), the local cyclic permutation operator can be represented as the $(d \times d)$ matrix of the form

$$\mathscr{C} = \begin{pmatrix} 0 & 1 & 0 & & 0 \\ 0 & 0 & 1 & & 0 \\ & & & & \\ 0 & 0 & 0 & & 1 \\ 1 & 0 & 0 & & 0 \end{pmatrix},$$

which obeys the condition $\mathscr{C}^d = \mathbb{I}$.

In summary, we have analyzed the new variational principle (16) in quantum mechanics defining MES of physical systems in terms of the extreme of quantum fluctuations of all essential measurements specifying either the pure or mixed state of the system. In a sense, this principle is similar to the maximum entropy principle in statistical mechanics.

It should be stressed that the definition in terms of the variational principle has a number of heuristic advantages. First of all, it defines quantum entanglement as a physical phenomenon irrespective of information processing and other possible applications of entanglement. This, in turn, makes it possible to separate the essential from accidental and discard the inessential requirements, such as the nonlocality, nonseparability, and violation of classical realism.

This also leads to an expansion of the notion of entanglement to the branches of quantum physics that are not directly connected with the information processing and quantum computation. The above considered example of entangled quark states in π^0 mesons should be mentioned here.

The revelation of the physical nature of maximum entanglement provided by the maximum scale of quantum fluctuations of the corresponding states gives a clue in the problem of stabilization of entanglement. Namely, to make a persistent MES of a given system, we should first exert influence upon the system to achieve the state with the maximum scale of quantum fluctuations. Then, we should decrease the energy of the system up to a (local) minimum under the condition of retention of the fluctuation scale. The possible realizations of this approach were discussed in [28, 29] for atomic entanglement.

Finally, the mathematical structure hidden behind the variational principle for maximum entanglement establishes contacts between the notion of entanglement and geometric invariant theory. In particular, it opens a natural way of classifying entangled states in terms of the complex orbits of states [3, 9, 24], as well as of the quantification of entanglement through the use of measure (16).

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