## **Multipartite Entanglement Witnesses**

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We derive a set of algebraic equations, the so-called multipartite separability eigenvalue equations. Based on their solutions, we introduce a universal method for the construction of multipartite entanglement witnesses. We witness multipartite entanglement of  $10^3$  coupled quantum oscillators, by solving our basic equations analytically. This clearly demonstrates the feasibility of our method for studying ultrahigh orders of multipartite entanglement in complex quantum systems.

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Entanglement represents a fundamental quantum correlation between compound quantum systems. Since the early days of quantum physics, this property has been used to illustrate the surprising consequences of the quantum description of nature [1,2]. Moreover, entanglement plays a fundamental role in various applications and protocols in quantum information science [3–5].

In multipartite systems a separable state is a statistical mixture of product states [6]. A quantum state is entangled, whenever it cannot be represented in this form. Various forms of multipartite entanglement are known [7–10]. The most prominent and nonequivalent forms of entangled multipartite quantum states are the GHZ state [11] and the W state [12], which have been generalized to so-called cluster and graph states [13,14]. Another classification is given in terms of partial and full (or genuine) multipartite entanglement, for an introduction see, e.g., [4,5]. Beyond finite dimensional systems, multipartite quantum entanglement in continuous variable systems turns out to be a cumbersome problem. Even in the case of Gaussian states, there exist multipartite entangled states, which cannot be distilled [15].

High orders of multipartite entanglement are of great interest, for example, in quantum metrology. Multipartite entanglement has been shown to be essential to reach the maximal sensitivity in metrological tasks [16]. In this context, the quantum Fisher information has been used to characterize the entanglement [17–19].

The detection of entanglement is typically done via the construction of proper entanglement witnesses [20–22], being equivalent to the method of positive, but not completely positive maps. A witness is an observable, which is non-negative for separable states, and it can have a negative expectation value for entangled states. For different kinds of entanglement, different types of witnesses have been considered: bipartite witnesses [21,23], Schmidt number witnesses [24,25], and multipartite witnesses for partial and genuine entanglement [26–29]. A systematic approach for witnessing entanglement in complex quantum systems is missing yet.

Recently, we considered the construction of bipartite entanglement witnesses with the so-called separability eigenvalue equations [23]. We have shown that the same equations need to be solved to obtain entanglement quasiprobabilities, which are nonpositive distributions if and only if the corresponding quantum state is entangled [30]. Moreover, we have shown that the Schmidt number witnesses can be obtained by solving the related Schmidt number eigenvalue problem [25].

In the present Letter, we derive a set of algebraic equations, which yield the construction of arbitrary multipartite entanglement witnesses. For these so-called multipartite separability eigenvalue equations, we will study some fundamental properties, which uncover the structure of multipartite entanglement. Examples are given to witness partial and full entanglement in multipartite composed systems, for pure and mixed quantum states in discrete and continuous variable systems.

In the following, we consider a composed Hilbert space  $\mathcal{H} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N$ . It has been shown that, without loss of generality, we could assume that the individual subsystems are finite dimensional ones [31]. Let us consider a partition  $I_1 \cdots I_K$  of the index set  $I = \{1, \ldots, N\}$ . A quantum state  $\hat{\sigma}$  is separable for the given partition, if it can be written as a classical mixture of product states [6]

$$\hat{\sigma} = \int_{\mathcal{S}_{I_1}:\dots:I_K} dP(a_1,\dots,a_K) |a_1,\dots,a_K\rangle \langle a_1,\dots,a_K|, \qquad (1)$$

with *P* being a classical probability distribution and  $S_{I_1:\dots:I_K}$  being the set of pure and normalized separable states. If a quantum state  $\hat{\varrho}$  cannot be written in the form of Eq. (1), it is referred to as multipartite entangled.

A multipartite entanglement witness for the given partition is a Hermitian operator  $\hat{W}$ , with

$$\langle \hat{W} \rangle = \operatorname{tr}(\hat{\sigma} \ \hat{W}) \ge 0, \quad \text{for all } \hat{\sigma} \text{ separable,}$$
  
$$\langle \hat{W} \rangle = \operatorname{tr}(\hat{\varrho} \ \hat{W}) < 0, \quad \text{for at least one } \hat{\varrho}.$$
 (2)

Based on Refs. [23,32], it can readily be shown that any witness can be presented in the form

$$\hat{W} = f_{I_1:\dots:I_K}(\hat{L})\hat{1} - \hat{L},$$
(3)

where  $\hat{L}$  is a general Hermitian operator and the function  $f_{I_1:\dots:I_k}(\hat{L})$  denotes the maximally attainable expectation value for separable states

 $f_{I_1:\cdots:I_K}(\hat{L}) = \sup\{\langle a_1,\ldots,a_K | \hat{L} | a_1,\ldots,a_K \rangle\}.$ 

The supremum is taken over all  $|a_1, \ldots, a_K\rangle \in S_{I_1; \cdots; I_K}$ .

Hence, we can formulate a necessary and sufficient entanglement criterion being equivalent to the witness criterion: A quantum state  $\hat{\varrho}$  is entangled with respect to the partition  $I_1, \ldots I_K$ , if and only if there exists a Hermitian operator  $\hat{L}$  such that

$$\operatorname{tr}(\hat{\varrho}\,\hat{L}) > f_{I_1:\dots:I_{\kappa}}(\hat{L}). \tag{4}$$

This means that the mean value of  $\hat{L}$  exceeds the boundary of mean values for separable states. A replacement  $\hat{L} \mapsto -\hat{L}$  leads to a similar entanglement criterion, but with the greatest lower bound (inf) instead of the least upper bound (sup):

$$\operatorname{tr}(\hat{\varrho}\,\hat{L}) < \inf\{\langle a_1, \dots, a_K | \hat{L} | a_1, \dots, a_K \rangle\}.$$
(5)

For both entanglement criteria, we have to solve the following optimization problem for an observable  $\hat{L}$ 

$$G = \langle a_1, \dots, a_K | \hat{L} | a_1, \dots, a_K \rangle \to \text{optimum},$$
  

$$C = \langle a_1, \dots, a_K | a_1, \dots, a_K \rangle - 1 \equiv 0,$$
(6)

where G represents the function to be optimized, and C is the normalization condition. For such an optimization problem, we can apply the method of Lagrangian multipliers. In our case, the optimization condition is

$$0 = \frac{\partial G}{\partial \langle a_j|} - g \frac{\partial C}{\partial \langle a_j|}, \quad \text{for } j = 1, \dots, K, \quad (7)$$

where g is the Lagrangian multiplier and 0 is the null vector in the subspace given by the partition  $I_j$ . The partial derivatives of G can be computed as

$$\frac{\partial G}{\partial \langle a_j |} = \frac{\partial \langle a_1, \dots, a_N | \hat{L} | a_1, \dots, a_N \rangle}{\partial \langle a_j |}$$

$$= \frac{\partial [\operatorname{tr}_{I_1} \dots \operatorname{tr}_{I_K} (\hat{L} | a_1, \dots, a_K) \langle a_1, \dots, a_K |)]}{\partial \langle a_j |}$$

$$= \operatorname{tr}_{I_1} \dots \operatorname{tr}_{I_{j-1}} \operatorname{tr}_{I_{j+1}} \dots \operatorname{tr}_{I_K} (\hat{L} [| a_1, \dots, a_{j-1}) \rangle$$

$$\times \langle a_1, \dots, a_{j-1} | \otimes \hat{1}_{I_j} \otimes | a_{j+1}, \dots, a_K \rangle$$

$$\times \langle a_{j+1}, \dots, a_K |] | a_j \rangle$$

$$= \hat{L}_{a_1, \dots, a_{j-1}, a_{j+1}, \dots, a_K} |a_j \rangle.$$
(8)

The case  $\hat{L} = \hat{1}$  yields the derivatives of *C*. Let us also note that we assumed that the indices of the sets  $I_j$  are ordered in a form that all elements of  $I_j$  are larger then the elements of  $I_{j'}$  for j > j'. This assumption is justified by the fact that one can employ, without loss of generality, a

permutation of the Hilbert spaces  $\mathcal{H}_1 \dots \mathcal{H}_N$  to order them in the required form.

The Euler-Lagrangian optimization condition in Eq. (7) can be reformulated for all j = 1, ..., K as

$$0 = \hat{L}_{a_1, \dots, a_{j-1}, a_{j+1}, \dots, a_K} |a_j\rangle - g |a_j\rangle,$$
(9)

where all eigenstates are normalized ones,  $\langle a_j | a_j \rangle = 1$ . In addition, we may evaluate the value of g. We can do this by multiplying Eq. (9) with  $\langle a_j |$ . This yields

$$g = \langle a_j | \hat{L}_{a_1, \dots, a_{j-1}, a_{j+1}, \dots, a_K} | a_j \rangle$$
  
=  $\langle a_1, \dots, a_K | \hat{L} | a_1, \dots, a_K \rangle = G_{\text{optimum}}.$  (10)

Hence, the Lagrangian multiplier corresponds to an optimal expectation value of  $\hat{L}$  for separable states. In conclusion of this derivation, we get an algebraic problem whose solutions give all optimal expectation values.

Definition: MSE(value) equations.—The equations

$$\hat{L}_{a_1,...,a_{j-1},a_{j+1},...,a_K} |a_j\rangle = g |a_j\rangle$$
 for  $j = 1,...,K$ 

are defined as the first form of the multipartite separability eigenvalue, MSE(value), equations. The value g is denoted as the MSE(value) of  $\hat{L}$ , and the product vector  $|a_1, \ldots, a_K\rangle$  is the corresponding multipartite separability eigenvector, MSE(vector).

As a final conclusion from this derivation we get

$$f_{I_1:\dots:I_K}(\hat{L}) = \sup\{g:g \text{ is MSE value of } \hat{L}\},$$
 (11)

and condition (5) is given by the infimum of all MSE (values). This means that all multipartite entanglement witnesses can be constructed from the solutions of the MSE(value) equations,

$$\hat{W} = \sup\{g\}\hat{1} - \hat{L}.$$
 (12)

In case we consider finite Hilbert spaces (dim  $\mathcal{H} < \infty$ ), we can replace sup and inf by max and min, respectively.

The derived MSE(value) equations play a fundamental role for multipartite entanglement tests. They give the possibility to construct arbitrary entanglement witnesses on the basis of the solution of an algebraic eigenvalue problem of an observable  $\hat{L}$ . Numerical and analytical methods—originally developed to solve eigenvalue problems—can be applied to handle the multipartite entanglement problem in quantum physics in a systematic way. Before we apply our method, let us formulate some fundamental properties of the MSE(value) equations. The proofs are given in Secs. I–III of the Supplemental Material [33].

Proposition: Second form of MSE(value) equations.— The Hermitian operator  $\hat{L}$  has the MSE(value) g for the  $MSE(vector) |a_1, \ldots, a_K\rangle$ , if and only if it fulfills the second form of the MSE(value) equations

$$\hat{L}|a_1,\ldots,a_K\rangle = g|a_1,\ldots,a_K\rangle + |\chi\rangle,$$

with  $\langle a_1, \ldots, a_{j-1}, x, a_{j+1}, \ldots, a_K | \chi \rangle = 0$  for all  $|x\rangle \in \bigotimes_{i \in I_j} \mathcal{H}_i$  and  $j = 1, \ldots, K$ .

This proposition transforms the coupled system of eigenvalue equations, which has been defined in the first form of the MSE(value) equations, into a single, but perturbed eigenvalue problem. This second form yields several implications. For example, if an eigenvector is a product vector  $|a_1, \ldots, a_K\rangle$ , it is also an MSE(vector) with  $|\chi\rangle \equiv 0$ . In addition, we also conclude that the operator  $\hat{L}$  yields a true entanglement witness, cf. Eq. (2), if and only if the eigenspace of the largest eigenvalue, does not contain a product vector.

Proposition: Transformation properties.—A Hermitian operator  $\hat{L}$  has a MSE(value) g for the MSE(vector)  $|a_1, \ldots, a_K\rangle$ . Then, the operator

$$\hat{L}' = (\hat{U}_1 \otimes \cdots \otimes \hat{U}_K)^{\dagger} [\lambda_1 \hat{1} + \lambda_2 \hat{L}] (\hat{U}_1 \otimes \cdots \otimes \hat{U}_K),$$

with  $\lambda_1$ ,  $\lambda_2 \in \mathbb{R} \setminus \{0\}$  and  $\hat{U}_j$  being unitary operations acting locally on the partition  $I_j$ , has the MSE(value)  $g' = \lambda_1 + \lambda_2 g$  and the MSE(vectors)  $|a'_1, \dots, a'_K\rangle = \hat{U}_1^{\dagger} \otimes \cdots \otimes \hat{U}_K^{\dagger} |a_1, \dots, a_K\rangle$ .

This transformation allows us to consider a whole class of witnesses, by solving the MSE(value) equation for a particular operator  $\hat{L}$ . In addition, the shifting of  $\hat{L}$  to  $\hat{L}'$ allows us to consider positive semidefinite operators only. Note that the invariance of the MSE(values) under local unitaries is of particular interest for the quantification of multipartite entanglement, see, e.g., [4,5].

Proposition: Cascaded structure.—The nonzero solutions of an N + 1-partite operator  $\hat{L}' = |\psi\rangle\langle\psi|$  are identical to the solutions of an *N*-partite operator  $\hat{L} = \text{tr}_{N+1}\hat{L}'$ .

This property is quite surprising. It shows us that all possible entanglement witnesses—based on positive semidefinite operators  $\hat{L}$ —of an *N*-partite system can be constructed by a few simple entanglement witnesses in a N + 1-partite system,  $\hat{L}' = |\psi\rangle\langle\psi|$ . An arbitrary rank of  $\hat{L}$  can be achieved by choosing a state  $|\psi\rangle$  with the same Schmidt rank for the bipartition  $I_1 = \{1, \ldots, N\}$  and  $I_2 = \{N + 1\}$ , cf. Sec. III in [33].

In the following, we apply our method to analytically derive multipartite entanglement tests. First, we may consider witnesses for prominent examples of states in a three qubit systems. In a second step, we apply our method to get a multipartite entanglement test in a complex continuous variable system.

Let us consider a generalized tripartite W state

$$|\psi_W\rangle = \lambda_1 |1, 0, 0\rangle + \lambda_2 |0, 1, 0\rangle + \lambda_3 |0, 0, 1\rangle,$$
 (13)

with  $|\lambda_1|^2 + |\lambda_2|^2 + |\lambda_3|^2 = 1$ , which defines the observable  $\hat{L} = |\psi_W\rangle\langle\psi_W|$ . In Sec. IV of [33], we solve the MSE (value) equation of  $\hat{L}$ . This gives

$$f_{\{1\}:\{2,3\}}(\hat{L}) = \max\{|\lambda_1|^2, |\lambda_2|^2 + |\lambda_3|^2\},\$$

$$f_{\{2\}:\{1,3\}}(\hat{L}) = \max\{|\lambda_2|^2, |\lambda_1|^2 + |\lambda_3|^2\},\$$

$$f_{\{3\}:\{1,2\}}(\hat{L}) = \max\{|\lambda_3|^2, |\lambda_1|^2 + |\lambda_2|^2\},\$$

$$f_{\{1\}:\{2\}:\{3\}}(\hat{L}) = \max\{|\lambda_1|^2, |\lambda_2|^2, |\lambda_3|^2, g_0\},\$$
(14)

with

$$g_0 = \frac{4|\lambda_1|^2|\lambda_2|^2|\lambda_3|^2}{(|\lambda_1|^2 + |\lambda_2|^2 + |\lambda_3|^2)^2 - 2(|\lambda_1|^4 + |\lambda_2|^4 + |\lambda_3|^4)}.$$

Hence, we can formulate the following multipartite entanglement conditions: A quantum state  $\hat{\rho}$  is partially entangled, if  $\langle \psi_W | \hat{\rho} | \psi_W \rangle > f_{\{1\}:\{2\}:\{3\}}(\hat{L})$ . The corresponding entanglement witness is

$$\hat{W}_{\text{part}} = \max\{g_0, |\lambda_1|^2, |\lambda_2|^2, |\lambda_3|^2\}\hat{1} - |\psi_W\rangle\langle\psi_W|.$$
(15)

A quantum state  $\hat{\rho}$  is fully entangled, if  $\langle \psi_W | \hat{\rho} | \psi_W \rangle > \max\{f_{\{1\}:\{2,3\}}(\hat{L}), f_{\{2\}:\{1,3\}}(\hat{L}), f_{\{3\}:\{1,2\}}(\hat{L})\}$ . The corresponding entanglement witness is

$$\hat{W}_{\text{full}} = \max\{|\lambda_i|^2 + |\lambda_j|^2 : i \neq j\}\hat{1} - |\psi_W\rangle\langle\psi_W|.$$
(16)

In Fig. 1, we apply the considered witness to study the entanglement of a noisy W state.

In a second step, a generalized GHZ state is given,

$$|\psi_{\text{GHZ}}\rangle = \kappa_0 |0, 0, 0\rangle + \kappa_1 |1, 1, 1\rangle,$$
 (17)

together with  $|\kappa_0|^2 + |\kappa_1|^2 = 1$ , which yields an observable  $\hat{L} = |\psi_{\text{GHZ}}\rangle\langle\psi_{\text{GHZ}}|$ . From Sec. V of [33], we get the maximal MSE(values)

$$f_{\{1\}:\{2,3\}}(\hat{L}) = f_{\{2\}:\{1,3\}}(\hat{L}) = f_{\{3\}:\{1,2\}}(\hat{L}) = f_{\{1\}:\{2\}:\{3\}}(\hat{L})$$
$$= \max\{|\kappa_0|^2, |\kappa_1|^2\}.$$
(18)

Hence, a state  $\hat{\rho}$  is genuinely tripartite entangled, if  $\langle \psi_{\text{GHZ}} | \hat{\rho} | \psi_{\text{GHZ}} \rangle > \max\{|\kappa_0|^2, |\kappa_1|^2\}$ , see Fig. 2. Note that the corresponding witness



FIG. 1 (color online). The entanglement test in Eq. (4) for a W state mixed with white noise,  $\hat{\rho} = p(1/8)\hat{1} + (1-p)|\psi_W\rangle\langle\psi_W|$  $\lambda_1 = \lambda_2 = \lambda_3 = (1/\sqrt{3})$ , is plotted for  $0 \le p \le 1$ . The boundary for partial or full separability is 4/9 or 2/3, respectively. The expectation value  $\langle \hat{L} \rangle$  exceeds the boundary for full or partial separability as long as the mixing parameter is p < (40/63) or p < (8/21), respectively.



FIG. 2 (color online). The expectation value  $\langle \hat{L} \rangle$  for a GHZ state mixed with white noise,  $\hat{\rho} = p(1/8)\hat{1} + (1-p)|\psi_{\text{GHZ}}\rangle\langle\psi_{\text{GHZ}}|$ [ $\kappa_0 = \kappa_1 = (1/\sqrt{2})$ ], is plotted. The lower boundary for partial and full entanglement is 1/2. The expectation value  $\langle \hat{L} \rangle$  exceeds this boundary—which automatically implies genuine entanglement—as long as the mixing parameter is p < (8/14).

$$\hat{W} = \max\{|\kappa_0|^2, |\kappa_1|^2\}\hat{1} - |\psi_{\text{GHZ}}\rangle\langle\psi_{\text{GHZ}}|, \quad (19)$$

cannot discriminate between partially and fully entangled states, see Eq. (18), which is possible for the generalized *W*-state projection in the previous example.

As a proof of principle, we are going to test multipartite entanglement of a continuous variable system. Our considered example is a system of N coupled harmonic oscillators. The observable we are using to verify entanglement is the total energy of this system,  $\hat{L} = \hat{H}$ ,

$$\hat{H} = \sum_{j=1}^{N} \left( \frac{\vec{\hat{p}}_{j}^{2}}{2m} + \frac{m\omega^{2}\vec{\hat{r}}_{j}^{2}}{2} \right) + \frac{\gamma}{4} \sum_{j,j'=1}^{N} |\vec{\hat{r}}_{j} - \vec{\hat{r}}_{j'}|^{2}, \quad (20)$$

where  $\gamma$  denotes the coupling strength of the interaction,  $\vec{\hat{r}}_j$  the position and  $\vec{\hat{p}}_j$  the momentum operator. Let us note that we considered an even more general case in Sec. VI of [33]. For the partition  $I_1, \ldots, I_K$ , we get the smallest MSE (value) of the Hamiltonian as

$$E[I_{1}, ..., I_{K}] = \frac{3}{2} \hbar \omega \sum_{j=1}^{K} \left( [N_{j} - 1] \sqrt{1 + N \frac{\gamma}{m\omega^{2}}} + \sqrt{1 + [N - N_{j}] \frac{\gamma}{m\omega^{2}}} \right), \quad (21)$$

where  $N_j = |I_j|$  is the number of subsystems in  $I_j$ . The resulting witness reads as

$$\hat{W}_{I_1,\dots,I_K} = E[I_1,\dots,I_K]\hat{1} - \hat{H}.$$
 (22)

In the special case K = 1 ( $I_1 = I$ ), we get the true ground state energy of the system,

$$E[I] = \frac{3}{2}\hbar\omega \left( \sqrt{1 + N\frac{\gamma}{m\omega^2}} (N-1) + 1 \right).$$
(23)

In case of full separability, K = N ( $I_j = \{j\}$ ), we have a minimal energy of

$$E[\{1\}, \dots, \{N\}] = \frac{3}{2}\hbar\omega N\sqrt{1 + [N-1]\frac{\gamma}{m\omega^2}}.$$
 (24)



FIG. 3 (color online). The energy difference  $\Delta = (\langle \hat{H} \rangle - E[I])/((3/2)\hbar\omega)$  between quantum states and the ground state of the system is plotted depending on the interaction strength. The boundary  $\Delta_{1000}$  corresponds to the minimal attainable energy for fully separable states. All quantum states having an energy below  $\Delta_5$  ( $N_1 = \cdots = N_5 = 200$ ) reveal entanglement between more than 200 oscillators. The quantum states in the range below  $\Delta_2$  ( $N_1 = N_2 = 500$ ) exhibit entanglement distributed over more than 500 subsystems.

In Fig. 3, we plotted the corresponding entanglement test based on Eq. (5), for  $N = 10^3$  interacting oscillators. For the witnessing by the total energy  $\hat{H}$ , no information about the structure of the quantum states is needed.

In conclusion, we have derived an algebraic set of equations to construct arbitrary entanglement witnesses. We studied some fundamental properties of these equations. For example, they are invariant under local unitary transformations and have a cascaded structure. The latter allows us to deduce all entanglement witnesses from elementary projections. Our method enables us to use all known procedures for solving eigenvalue problems to construct entanglement witnesses. We applied our method to analytically identify full and partial entanglement of generalized, noisy GHZ and W states. Moreover, we witnessed multipartite entanglement for a system of 10<sup>3</sup> interacting oscillators, by analytical computation of the energetic boundaries of separable states. This demonstrates the feasibility of our method for studying ultrahigh orders of multipartite entanglement, which are of fundamental interest for understanding the transition from the microscopic to the macroscopic world.

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- [33] See Supplemental Material at http://link.aps.org/ supplemental/10.1103/PhysRevLett.111.110503 for the proofs of the propositions and analytical solutions of the MSE(value) equations.