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Nonlocal Parameters for Multiparticle Density Matrices

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As far as entanglement is concerned, two density matrices of n particles are completely equivalent if one can be transformed into the other by local unitary transformations. We present two methods to find whether or not two generic density matrices of arbitrary numbers of spin-$1/2$ particles are equivalent. Both methods describe density matrices in terms of a finite number of invariant parameters.

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Nonlocality is a fundamental characteristic of quantum mechanics. Its importance lies not only in philosophical considerations of the nature of quantum theory, but also in applications where it has emerged recently that nonlocality is the key ingredient in quantum computation [1] and communication [2] and plays an important role in cryptography [3,4]. It has become clear that entanglement is a resource which may be manipulated (for example, by concentration [5], dilution, or purification [6–8]).

From the point of view of nonlocality, two states are completely equivalent if one can be transformed into the other by means of local unitary transformations. How to determine whether or not two states are locally equivalent is still an open question. In this Letter we solve this problem for systems containing arbitrary numbers of spin-$1/2$ particles in generic mixed states.

As discussed in [9], the space of pure states of n spin-$1/2$ particles is $\mathbb{C}^{2^n} = \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2$; however, not all of the 2^n complex parameters have nonlocal significance: the group of local transformations, $U(2)^n$, acts on the space of states, and two states which may be reached from each other by local actions are equivalent as far as their nonlocal properties are concerned. Each equivalence class of locally equivalent density matrices is an *orbit* of this group. For many purposes, only parameters describing nonlocal properties are significant; an example is that any good measure of entanglement must be invariant under local transformations [6,10–13], and thus it should be a function of nonlocal parameters only. Here and henceforth we will refer to parameters which are invariant under local transformations as invariants. Invariants are also relevant in discussions of Bell inequalities [14,15] and teleportation, etc. [16]. A key question is to identify the invariants.

In this paper we will focus on density matrices and show that, for $n \geq 2$, of the $2^{2n} - 1$ real parameters describing density matrices of n spin-$1/2$ particles $2^{2n} - 3n - 1$ are invariant under local transformations, $U(2)^n$. For an arbitrary set of n particles, the number of nonlocal parameters is $\prod_r d_r^2 - \sum_r d_r^2 + n - 1$ where d_r is the dimension of the state space of the rth particle. For n spin-$\frac{1}{2}$ particles we also show how to characterize generic orbits, both by giving an explicit parametrization of the orbits and by finding a finite set of polynomial invariants which separate the orbits. Thus given two density matrices we can compute explicitly whether they are on the same orbit or not. Other authors have also discussed the use of invariants in discussing entanglement [17,18] and applied invariant theory to quantum codes [19].

In order to calculate the number of functionally independent invariants it will be convenient to find the dimension of the orbit of a generic density matrix under the group of local transformations. The dimension of the orbit is the number of parameters describing the location of a density matrix on the orbit. The total number of parameters ($2^{2n} - 1$ real parameters) describing the space of density

matrices minus the number of parameters describing a generic orbit (the dimension of the orbit) gives the number of parameters describing the location of the orbit in the space of orbits, i.e., the number of parameters describing the nonlocal properties of the density matrices.

To fix notation, it will be convenient to consider the case of a one-particle density matrix first. The space of pure states of a single spin-1/2 particle is $\mathbb{C}^2$, and thus a density matrix is a 2×2 complex matrix which is Hermitian, positive, and with trace one, and may therefore be described by three real parameters. A particularly convenient representation of such a matrix is $\rho = \frac{1}{2}(1_2 + \alpha_i \sigma_i)$, where α_i, $i = 1, 2, 3$ are real and σ_i are the Pauli matrices.

Under a local transformation by a unitary matrix U, ρ is transformed as

$$\rho \mapsto U \rho U^\dagger. \tag{1}$$

Every unitary matrix may be written as a product of an element of SU(2) and a phase transformation, represented by a unitary matrix $e^{i\phi} 1_2$. This latter element clearly leaves any density matrix invariant under the transformation (1) so that when considering the action (1) we may restrict attention to elements of SU(2). In order to find the number of invariants, it will be more convenient to find the dimension of a generic orbit under the action of SU(2). To do so one may work infinitesimally. Thus, associated with the action of the Lie algebra of the group of local transformations acting on the space of density matrices there is a vector field: if we take an element T of a basis for the Lie algebra, the action of the group element $k = \exp i\epsilon T$ on an element ρ induces an action on functions from ρ to $\mathbb{C}$; and the vector field, X_T, associated with the Lie algebra element T is found by differentiating

$$\begin{aligned} X_T f(\rho) &\stackrel{\text{def}}{=} \frac{\partial}{\partial \epsilon} f(e^{i\epsilon T}\rho)|_{\epsilon=0} \\ &= \frac{\partial}{\partial \epsilon} f(\rho + \delta\rho)|_{\epsilon=0}. \end{aligned} \tag{2}$$

The linear span of tangent vectors at the point ρ associated with the whole Lie algebra forms the tangent space to the orbit at the point ρ and so the number of linearly independent tangent vectors at this point gives the dimension of the orbit.

A general element of the Lie algebra in the spin-1/2 representation is given by $T = \eta_i \sigma_i$, and its action on the density matrix is to give an infinitesimal transformation $\delta\rho = i[T, \rho]$ where $[\,,\,]$ is the matrix commutator.

We may therefore calculate the three vector fields X_i associated with the Lie algebra elements σ_i as

$$X_i = -\epsilon_{ijk}\alpha_j \frac{\partial}{\partial \alpha_k}. \tag{3}$$

We note that at generic values of $\alpha_1, \alpha_2, \alpha_3$ only two of these tangent vectors are linearly independent since $\alpha_1 X_1 + \alpha_2 X_2 + \alpha_3 X_3 = 0$. Thus the dimension of the generic orbit is two and therefore of the three parameters describing a generic density matrix, two are noninvariant leaving only one invariant parameter, as one expects since only the single independent eigenvalue of ρ is invariant under local transformations.

We note that the effect of the transformations (1) is to act on the vector α by rotation by an orthogonal matrix, i.e., an element of SO(3)—this follows from the fact that $\alpha_i \sigma_i$ is the representative of a Lie algebra element and the conjugation action (1) is the adjoint action of the group on its Lie algebra. We may thus find a way of exhibiting the invariant under local transformations: $I = \alpha_i \alpha_j \delta_{ij} = |\alpha|^2$ where we have used the fact that SO(3) has an invariant tensor δ_{ij}. We note that this invariant may also be expressed as $I = \mathrm{Tr}(\rho^2) - \frac{1}{2}$.

We now turn to the case of two-particle density matrices. Such a density matrix has 15 real parameters, and the maximum dimension that a generic orbit could have is six [corresponding to two copies of SU(2)] if all the tangent vectors corresponding to a basis of the Lie algebra were independent. We will show that the tangent vectors do indeed span six dimensions, and thus that there are nine nonlocal parameters.

We may write a density matrix as

$$\begin{aligned} \rho = \frac{1}{4}(1_2 \otimes 1_2 + \alpha \cdot \sigma \otimes 1_2 + 1_2 \otimes \beta \cdot \sigma \\ + R_{ij}\sigma_i \otimes \sigma_j). \end{aligned} \tag{4}$$

The action of a Lie algebra element of the subgroup SU(2) acting on the first component of the tensor product is

$$\begin{aligned} \delta^{(1)}\rho = -\frac{1}{2}(\alpha_k \eta_m \epsilon_{mki} \sigma_i \otimes 1_2 \\ + R_{kj}\eta_m \epsilon_{mki} \sigma_i \otimes \sigma_j), \end{aligned} \tag{5}$$

with a similar expression coming from the action of a Lie algebra element of the subgroup SU(2) acting on the second component of the tensor product.

The vector fields corresponding to the six basis elements $\sigma_k \otimes 1_2$, $1_2 \otimes \sigma_k$ are

$$\begin{aligned} X_k &= -\frac{1}{2}\epsilon_{kim}\left(\alpha_i \frac{\partial}{\partial \alpha_m} + R_{ij}\frac{\partial}{\partial R_{mj}}\right), \\ Y_k &= -\frac{1}{2}\epsilon_{kim}\left(\beta_i \frac{\partial}{\partial \beta_m} + R_{ji}\frac{\partial}{\partial R_{jm}}\right). \end{aligned} \tag{6}$$

Consider the set X_k first: one can see that these three are linearly independent at generic points by considering the coefficients of $\partial/\partial\alpha_i$, since a linear relation would have to be of the form $\alpha_k X_k = 0$, but one can see that this relation will not hold for nonzero α's by looking at the coefficients of the partial derivatives with respect to R_{ij}. Similarly, by considering the coefficients of the partial derivatives with respect to $\beta_1, \beta_2, \beta_3$, one sees that Y_1, Y_2, Y_3 are linearly independent. Finally, we note that the coefficients of the partial derivatives with respect to $\beta_1, \beta_2, \beta_3$ are zero for

X_1, X_2, X_3 and the coefficients of the partial derivatives with respect to $\alpha_1, \alpha_2, \alpha_3$ are zero for Y_1, Y_2, Y_3 so that there can be no linear relation at all between the six vector fields $X_1, X_2, X_3, Y_1, Y_2, Y_3$. Thus the dimension of the orbit of a generic density matrix is 6 and thus the number of nonlocal parameters, $15 - 6 = 9$.

In general, we can consider a system of n particles with individual state spaces of dimensions $d_1, \ldots, d_n$. By finding the number of linearly independent tangent vectors, as above, it may be shown that out of the total number of parameters only $\prod_r d_r^2 - \sum_r d_r^2 + n - 1$ are nonlocal invariants.

Let us now return to the case of $n \geq 2$ spin-1/2 particles and explicitly identify a set of invariant parameters which characterize generic orbits. To be explicit, consider the case of three spin-1/2 particles with density matrix which may be written as

$$\rho = \frac{1}{8}(1_2 \otimes 1_2 \otimes 1_2 + \alpha_i \sigma_i \otimes 1_2 \otimes 1_2 + \beta_i 1_2 \otimes \sigma_i \otimes 1_2 + \gamma_i 1_2 \otimes 1_2 \otimes \sigma_i + R_{ij} \sigma_i \otimes \sigma_j \otimes 1_2 + S_{ij} \sigma_i \otimes 1_2 \otimes \sigma_j + T_{ij} 1_2 \otimes \sigma_i \otimes \sigma_j + Q_{ijk} \sigma_i \otimes \sigma_j \otimes \sigma_k). \quad (7)$$

The action by a local unitary transformation on the first component in the tensor product induces the following transformations on components of ρ: $\alpha_i \mapsto L_{ij}\alpha_j$; $R_{ij} \mapsto L_{ik}R_{kj}$; $S_{ij} \mapsto L_{ik}S_{kj}$; $Q_{ijk} \mapsto L_{im}Q_{mjk}$ where L_{ij} is an orthogonal matrix, and the other components of ρ do not change. Local actions on the second and third components of the tensor product induce similar transformations of β, R, T, Q and γ, S, T, Q, respectively, by orthogonal matrices M and N independent of L.

We may fix a canonical point on a generic orbit as follows: first let us define

$$X_{ii'} = Q_{ijk}Q_{i'jk}, \qquad Y_{jj'} = Q_{ijk}Q_{ij'k}, \qquad Z_{kk'} = Q_{ijk}Q_{ijk'}, \quad (8)$$

and perform unitary transformations on particles 1, 2, and 3 so as to move to a point on the orbit in which X, Y, and Z are diagonal; generically the diagonal entries are distinct and we can arrange them in decreasing order (X, Y, and Z are Hermitian, positive matrices). The only remaining transformations which leave X, Y, and Z in these forms are local unitary transformations which induce orthogonal transformations in which L_{ij}, M_{ij}, and N_{ij} are one of the matrices $\mathrm{diag}(1,-1,-1), \mathrm{diag}(-1,1,-1), \mathrm{diag}(-1,-1,1)$.

We may specify a canonical point on the generic orbit uniquely by specifying that all the components of α have the same sign, and similarly for β and γ. This method works as long as X, Y, and Z have distinct eigenvalues and the components of α, β, and γ are not zero at the canonical point on the orbit. The parameters which describe the generic orbits are the components of $\alpha, \beta, \gamma, R, S, T$, and Q at the canonical point on the orbit. We note that the number of parameters describing the canonical point are the $2^6 - 1 = 63$ components of $\alpha, \beta, \gamma, R, S, T$, and Q minus the $3 \times 3 = 9$ constraints that the nondiagonal elements of X, Y, and Z are zero; thus the number of nonlocal parameters is 54 as given by the general formula.

We note that the fact that the canonical point, as constructed, is unique means that all points on the same orbit will have the same canonical representative: conversely, if two density matrices ρ_1 and ρ_2 have the same canonical form, then $U_1\rho_1U_1^\dagger = \rho_{\mathrm{canonical}} = U_2\rho_2U_2^\dagger$ for some U_1 and U_2, so that $\rho_2 = (U_2^\dagger U_1)\rho_1(U_2^\dagger U_1)^\dagger$, and thus ρ_1 and ρ_2 are on the same orbit.

We now describe a *finite* set of polynomial invariants which separate generic orbits by finding a set which allows one to calculate the components of $\alpha, \beta, \gamma, R, S, T$, and Q at this canonical point. The complete infinite set of polynomial invariants is found by contracting the indices of $\alpha, \beta, \gamma, R, S, T$, and Q with the invariant tensors δ_{ij} and ϵ_{ijk}. However, we may find a finite set of invariants which separates generic orbits. First we note that $\mathrm{tr}(X), \mathrm{tr}(X^2)$, and $\mathrm{tr}(X^3)$ determine the diagonal elements λ_1^2, λ_2^2, and λ_3^2 of X, and similarly for Y and Z. Now consider the three invariants $A_{2n} = \alpha^T X^{n-1}\alpha$, $n = 1, 2, 3$. We may write these three invariants in the following way:

$$\begin{pmatrix} 1 & 1 & 1 \\ \lambda_1^2 & \lambda_2^2 & \lambda_3^2 \\ \lambda_1^4 & \lambda_2^4 & \lambda_3^4 \end{pmatrix} \begin{pmatrix} a_1^2 \\ a_2^2 \\ a_3^2 \end{pmatrix} = \begin{pmatrix} A_2 \\ A_4 \\ A_6 \end{pmatrix}, \quad (9)$$

where a_1, a_2, and a_3 are the components of α at the canonical point on the orbit. The Vandermonde matrix Λ on the left of Eq. (9) has determinant $(\lambda_1^2 - \lambda_2^2)(\lambda_2^2 - \lambda_3^2)(\lambda_3^2 - \lambda_1^2)$, and we may solve for a_1^2, a_2^2, and a_3^2 as long as $\det\Lambda$ is nonzero. Also if the invariant

$$A_9 = \epsilon_{ijk}\alpha_i(X\alpha)_j(X^2\alpha)_k = a_1a_2a_3 \det\Lambda \quad (10)$$

is nonzero, then we may determine the sign of the components of α; recall that, by definition, all the components of α have the same sign at the canonical point. The analogous expressions B_9, C_9 determine the values of β and γ at the canonical point. The values of the components of R at the canonical point may be calculated from the following nine invariants:

$$I_{r,s} = (X^{r-1}\alpha)_i(Y^{s-1}\beta)_j R_{ij}, \qquad r, s = 1, 2, 3. \quad (11)$$

These nine equations may be put together into a matrix form $I = ((\Lambda F) \otimes (MG))R$, where I and R are column vectors with nine components and the matrix Λ is the Vandermonde matrix in Eq. (9), M is the analogous matrix with λ_i^2 replaced by μ_i^2 (the diagonal elements of Y), and F and G are $\mathrm{diag}(a_1, a_2, a_3)$ and $\mathrm{diag}(b_1, b_2, b_3)$, respectively.

We note that $\det(\Lambda F) = A_9$ and $\det(MG) = B_9$, so since we are assuming that these are nonzero we may invert the matrix equation to find the components R_{ij}. The components of S and T may be found in a similar way. Finally, we may use the 27 invariants,

$$I_{r,s,t} = (X^{r-1}\alpha)_i (Y^{s-1}\beta)_j (Z^{t-1}\gamma)_k Q_{ijk}\,, \tag{12}$$

to find the components of Q at the canonical point on the orbit in terms of the $I_{r,s,t}$ (there will, of course, be some relations between these components due to the constraints that X, Y, and Z are diagonal).

Thus, by showing that the following set of polynomial invariants is sufficient to calculate the components of a generic density matrix at the canonical point we have demonstrated that they characterize generic orbits:

$$\begin{aligned}
&\mathrm{tr}\, X^r, \qquad \mathrm{tr}\, Y^r, \qquad \mathrm{tr}\, Z^r,\\
&\alpha^{\mathrm{T}} X^{r-1}\alpha, \qquad \beta^{\mathrm{T}} Y^{r-1}\beta, \qquad \gamma^{\mathrm{T}} Z^{r-1}\gamma\,,\\
&\alpha \cdot (X\alpha) \wedge (X^2\alpha), \qquad \beta \cdot (Y\beta) \wedge (Y^2\beta), \qquad \gamma \cdot (Z\gamma) \wedge (Z^2\gamma)\,,\\
&(X^{r-1}\alpha)_i (Y^{s-1}\beta)_j R_{ij}, \qquad (Y^{r-1}\beta)_i (Z^{s-1}\gamma)_j T_{ij}\,,\\
&(X^{s-1}\alpha)_i (Z^{r-1}\gamma)_j S_{ij}, \qquad (X^{r-1}\alpha)_i (Y^{s-1}\beta)_j (Z^{t-1}\gamma)_k Q_{ijk}\,;
\end{aligned} \tag{13}$$

the indices r, s, t range over the values $1, 2, 3$.

If two density matrices have different values of any of these invariants they are not on the same orbit; if they have the same value of all of these invariants, and if A_9, B_9, and C_9 are nonzero, then the density matrices are locally equivalent.

We note that the number of independent components of a generic density matrix at the canonical point is equal to the number of functionally independent parameters calculated at the beginning of this Letter. However, the number of polynomial invariants needed to characterize the generic orbit is greater than this; this is related to the fact that the ring of invariants is nonpolynomial, i.e., that the geometry of the space of orbits is nontrivial.

The procedure given above can be used for all $n \geq 2$: Use the tensors of highest rank and rank one in the expression for ρ to fix a canonical point on the orbit; the polynomials which separate the generic orbits are the analogs of those used in the case $n = 3$.

In the case of $n = 2$ this method can be used but there is some redundancy in the description we have given: the matrices $X_{ii'} = R_{ij}R_{i'j}$ and $Y_{jj'} = R_{ij}R_{ij'}$ [using the notation of (4)] have the same eigenvalues and the matrix R_{ij} is diagonal at the canonical point. In this case there are nine functionally independent invariants which specify the squares of the nonzero components of α, β, and R at the canonical point on a generic orbit: $\mathrm{tr}X^n$, $\alpha^T X^{m-1}\alpha$, and $\beta^T Y^{p-1}\beta$, where n, m, p take the values $1, 2, 3$. Additional invariants are needed to specify the signs of the nonzero components. The five invariants $\alpha \cdot (X\alpha) \wedge (X^2\alpha)$, $\beta \cdot (Y\beta) \wedge (Y^2\beta)$, and $\alpha X^{r-1} R\beta, r = 1, 2, 3$, are sufficient to determine these signs for generic orbits and hence separate these orbits. In fact, using slightly different arguments, one can show that, in this case, one can reduce the number of polynomial invariants to ten, namely, $\mathrm{tr}X$, $\mathrm{tr}X^2$, $\det R$, $\alpha^T X^{r-1}\alpha$, $\alpha^T X^{r-1} R\beta$, $r = 1, 2, 3$, and A_9, which are subject to a single relation expressing A_9^2 as a function of the other invariants.

The general idea of investigating canonical points on orbits in the way we have described is also appropriate for higher spins, but the situation is somewhat more complicated. Consider the example of two particles of spin one in which case the unitary group under which ρ transforms (by conjugation) is SU(3). However, the adjoint representation of SU(3) is not equivalent to SO(8) but to an eight dimensional subgroup of it; this means that we cannot use SU(3) transformations to bring 8×8 symmetric matrices to diagonal form. Thus the canonical form is rather more complicated than in the case of spin-$1/2$ particles.

The physical significance of the invariant parameters is that they encode the *entire* information about the nonlocal properties of the density matrices. However, the detailed meaning of each of the parameters individually (apart from α^2, β^2, and γ^2 which are essentially the local entropies of the individual particles when the others are traced over) is an important but open question.

In summary, we have shown how to calculate the number of functionally independent parameters needed to determine whether or not two density matrices are locally equivalent. We have also shown how to characterize the generic classes of locally equivalent density matrices of n spin-$1/2$ particles by two methods: (a) By finding an explicit set of nonpolynomial invariants (the components of the density matrices at the canonical points on the orbits) and (b) by finding an explicit finite set of polynomial invariants. These methods work for generic density matrices; in a future publication we intend to give a systematic method for characterizing classes of locally equivalent nongeneric density matrices. In particular, this will give a

basis for the ring of invariants. We note that the canonical point on certain types of nongeneric orbit has a nontrivial stability group; this is a signature that density matrices on this orbit have special types of entanglement [9].

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