Nonlocal properties of two-qubit gates and mixed states
and optimization of quantum computations

Yuriy Makhlin

Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany
Landau Institute for Theoretical Physics, Kosygin st. 2, 117940 Moscow, Russia

Entanglement of two parts of a quantum system is a nonlocal property unaffected by local manipulations of these parts. It is described by quantities invariant under local unitary transformations. Here we present, for a system of two qubits, a set of invariants which provides a complete description of nonlocal properties. The set contains 18 real polynomials of the entries of the density matrix. We prove that one of two mixed states can be transformed into the other by single-bit operations if and only if these states have equal values of all 18 invariants. Corresponding local operations can be found efficiently. Without any of these 18 invariants the set is incomplete.

Similarly, nonlocal, entangling properties of two-qubit unitary gates are invariant under single-bit operations. We present a complete set of 3 real polynomial invariants of unitary gates. Our results are useful for optimization of quantum computations since they provide an effective tool to verify if and how a given two-qubit operation can be performed using exactly one elementary two-qubit gate, implemented by a basic physical manipulation (and arbitrarily many single-bit gates).

Introduction. Nonlocality is an important ingredient in quantum information processing, e.g. in quantum computation and quantum communication. Nonlocal correlations in quantum systems reflect entanglement between its parts. Genuine nonlocal properties should be described in a form invariant under local unitary operations. In this paper we discuss such locally invariant properties of (i) unitary transformations and (ii) mixed states of a two-qubit system.

Two unitary transformations (logic gates), and are called locally equivalent if they differ only by local operations: \( L = U_1MU_2 \), where \( U_1, U_2 \in SU(2)^{\otimes 2} \) are combinations of single-bit gates on two qubits. A property of a two-qubit operation can be considered non-local only if it has the same value for locally equivalent gates. We present a complete set of local invariants of a two-qubit gate: two gates are equivalent if and only if they have equal values of all these invariants. The set contains three real polynomials of the entries of the gate’s matrix. This set is minimal: the group \( SU(4) \) of two-qubit gates is 15-dimensional and local operations eliminate 2 \( \text{dim}[SU(2)^{\otimes 2}] = 12 \) degrees of freedom; hence any set should contain at least \( 15 - 12 = 3 \) invariants.

This result can be used to optimize quantum computations. Quantum algorithms are built out of elementary quantum logic gates. Any many-qubit quantum logic circuit can be constructed out of single-bit and two-bit operations. The ability to perform 1-bit and 2-bit operations is a requirement to any physical realization of quantum computers. Barenco et al. showed that the controlled-not (CNOT) gate together with single-bit gates is sufficient for quantum computations. Furthermore, it is easy to prove that any two-qubit gate \( M \) forms a universal set with single-bit gates, if \( M \) itself is not a combination of single-bit operations and the SWAP-gate, which interchanges the states of two qubits. The efficiency of such a universal set, that is the number of operations from the set needed to build a certain quantum algorithm, depends on \( M \).

For a particular realization of quantum computers, a certain two-qubit operation \( M \) (or a set \( \text{exp}[i\mathcal{H}t] \) of operations generated by a certain hamiltonian) is usually considered elementary. It can be performed by a basic physical manipulation (switching of one parameter or application of a pulse). Then the question of optimization arises: what is the most economical way to perform a particular computation, i.e. what is the minimal number of elementary steps? In many situations two-qubit gates are more costly than single-bit gates (e.g., they can take a longer time, involve complicated manipulations or stronger additional decoherence), and then only the number of two-bit gates counts.

The simplest and important version of this question is how a given two-bit gate \( L \) can be performed using the minimal number of elementary two-bit gates \( M \). In particular, when is it sufficient to employ \( M \) only once? This is the case when the two gates are locally equivalent, and computation of invariants gives an effective tool to verify this. Moreover, if \( M \) and \( L \) are equivalent, a procedure presented below allows to find efficiently single-bit gates \( U_1, U_2 \), which in combination with \( M \) produce \( L \). If one elementary two-bit step is not sufficient, one can ask how many are needed. Counting of dimensions suggests that two steps always suffice. However, this is not true for some gates \( M \) (bad entanglers).

A related problem is that of local invariants of quantum states. A mixed state is described by a density matrix \( \rho \). Two states are called locally equivalent if one can be transformed into the other by local operations: \( \rho \rightarrow U\rho U^\dagger \), where \( U \) is a local gate. Apparently, the coefficients of the characteristic polynomials of \( \rho \) and of the reduced density matrices of two qubits are locally invariant. The method developed in Refs., in principle, allows to compute all invariants. For a two-qubit system counting of dimensions shows that there should be 9 functionally independent invariants of density matrices.
with unit trace, but additional invariants may be needed to resolve a remaining finite number of states. A set of 20 invariants was presented in Ref. 8. However it was not clear if this set was complete, i.e. two states with the same invariants are bound by det \( M \) and the spectra of \( 1 \) and are bound by det \( M \). Indeed, a single-bit gate \( W \) is expressed in terms of a 6-dimensional, and hence coincides with the group. Thus local operations form a subgroup of the group.

The transformation of a matrix \( M \) from the standard basis of states \([00], [01], [10], [11]\) into the Bell basis is described as \( M \rightarrow M_B = Q^T MQ \), where

\[
Q = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 0 & 0 & i \\
0 & i & 1 & 0 \\
0 & i & -1 & 0 \\
1 & 0 & 0 & -i
\end{pmatrix}.
\]

Proof. We introduce a measure of entanglement in a pure 2-qubit state \( \psi_{\alpha\beta} \), a quadratic form \( \text{Ent} \psi \), which in the standard basis is defined as \( \text{Ent} \psi = \det \psi = \psi_{00} \psi_{11} - \psi_{01} \psi_{10} \). This quantity is locally invariant. Indeed, a single-bit gate \( W_1 \otimes W_2 \) transforms \( \psi \) into \( W_1 \psi W_2^* \), preserving the determinant.

Under a unitary operation \( V \) the matrix of this form transforms as \( \text{Ent} \rightarrow V^T \text{Ent} V \). In the Bell basis it is proportional to the identity matrix. Since local gates preserve this form, they are given by orthogonal matrices in this basis. As unitary and orthogonal they are also real. Thus local operations form a subgroup of the group \( SO(4, \mathbb{R}) \) of real orthogonal matrices. This subgroup is 6-dimensional, and hence coincides with the group.

Classification of two-qubit gates. Our result for unitary gates is expressed in terms of \( M_B \).

Theorem 2. The complete set of local invariants of a two-qubit gate \( M \), with det \( M = 1 \), is given by the set of eigenvalues of the matrix \( M_B^T M_B \).

In other words, two 2-bit gates with unit determinants, \( M \) and \( L \), are equivalent up to single-bit operations iff the spectra of \( M_B^T M_B \) and \( L_B^T L_B \) coincide. Since \( m \equiv M_B^T M_B \) is unitary, its eigenvalues have absolute value 1 and are bound by det \( m = 1 \). For such matrices the spectrum is completely described by a complex number tr \( m \) and a real number tr \( m^2 - \text{tr} m^2 \).

The matrix \( m \) is unitary and symmetric. The following statement is used in the proof of Theorem 2:

Lemma. Any unitary symmetric matrix \( m \) has a real orthogonal eigenbasis.

Proof. Any eigenbasis of \( m \) can be converted into a real orthogonal one, as seen from the following observation: If \( \psi \) is an eigenvector of \( m \) with eigenvalue \( \lambda \) then \( \psi^* \) is also an eigenvector with the same eigenvalue (conjugation of \( m^* \psi = m^{-1} \psi = \lambda^{-1} \psi = \lambda^* \psi \) gives this result). Hence, \( \psi^* \) are also eigenvectors.

Proof of Theorem 2. In the Bell basis local operations transform a unitary gate \( \hat{M}_B \) into \( O_1 \hat{M}_B O_2 \), where \( O_1, O_2 \in SO(4, \mathbb{R}) \) are orthogonal matrices. Therefore \( \hat{M}_B^T O_2^T O_1^T \hat{M}_B \) is transformed to \( O_2^T \hat{M}_B O_1 \). Obviously, the spectrum of \( m \) is invariant under this transformation.

To prove completeness of the set of invariants, we notice that the lemma above implies that \( m \) can be diagonalized by an orthogonal rotation \( O_M \), i.e. \( m = O_M^T d_M O_M \) where \( d_M \) is a diagonal matrix. Suppose that another gate \( L \) is given, and \( l = L_B^T L_B \) has the same spectrum as \( m \). Then the entries of \( d_M \) and \( d_L \) are related by a permutation. Hence \( d_M = P \hat{d}_L P \), where \( P \) is an orthogonal matrix, which permutes the basis vectors. Using the relation of \( m \) to \( d_M \) and of \( l \) to \( d_L \), we conclude that \( l = O^T m O \) where \( O \in SO(4, \mathbb{R}) \).

Single-bit operations \( O \) and \( \hat{O}' = L_B O^T L_B^T \) transform one gate into the other: \( \hat{L}_B = \hat{O}' M_B \hat{O} \). The gate \( \hat{O}' \) is a single-bit operation since it is real and orthogonal. Indeed, \( \hat{O}' O = (M_B^{-1})^T O L_B^T L_B O M_B^{-1} = (M^{-1})^T O L_B^T L_B O M_B^{-1} = 1 \). On the other hand, \( \hat{O}' \) is unitary as a product of unitary matrices. This implicates its reality.

So far we have discussed equivalence up to single-bit transformations with unit determinant. However, physically unitary gates are defined only up to an overall phase factor. The condition \( \det M = 1 \) fixes this phase factor but not completely: multiplication by \( \pm i \) preserves the determinant. With this in mind, we describe a procedure to verify if two two-qubit unitary gates with arbitrary determinants are equivalent up to local transformations and an overall phase factor:

We calculate \( m = M_B^T M_B \) for each of them and compare the pairs \( \{ \text{tr}^2 m \det M^1; \text{tr}^2 m \det M^2 \} \). If they coincide, the gates are equivalent and the proof of Theorem 2 allows to express explicitly one gate via the other and single-bit gates, \( O \) and \( \hat{O}' \).

Classification of two-qubit states. In this section we discuss equivalence and invariants of two-qubit states up to local operations. Let us express a 2-bit density matrix in terms of Pauli matrices acting on the first and the second qubit: \( \hat{\rho} = \frac{1}{2} \mathbb{1} + \sum_i s_i \sigma_i^1 + \sum_i p_i \sigma_i^2 + \beta_{ij} \sigma_i^1 \sigma_j^2 \). If the qubits are considered as spin-1/2 particles, then \( s \) and \( p \) are their average spins in the state \( \hat{\rho} \), while \( \beta \) is the spin-
spin correlator: $\beta_{ij} = (S_i^1 S_j^2)$. Any single-bit operation is represented by two corresponding $3 \times 3$ orthogonal real matrices of ‘spin rotations’, $O, P \in SO(3, \mathbb{R})$. Such an operation, $O \otimes P$, transforms $\hat{\beta}$ according to the rules: $s \rightarrow Os$, $p \rightarrow Pp$, and $\hat{\beta} \rightarrow O\hat{\beta}PT$. We find a set of invariants which completely characterize $\hat{\beta}$ up to local gates.

The density matrix is specified by 15 real parameters, while local gates form a 6-dimensional group. Thus we expect $15 - 6 = 9$ functionally independent invariants $(I_1-I_9$ in Table $I)$. However, these invariants fix a state only up to a finite symmetry group, and additional invariants are needed. In Table I we present a set of 18 polynomial invariants and prove that the set is complete.

\[ I_{1,2,3} \quad \det \hat{\beta}, \quad \text{tr}(\hat{\beta}^T \hat{\beta}), \quad \text{tr}(\hat{\beta}^2)^2 \]
\[ I_{4,5,6} \quad s^2, \quad |s|^2, \quad s \hat{\beta}^2 \]
\[ I_{7,8,9} \quad p^2, \quad |\hat{\beta}^2|^2, \quad s^2 (\hat{\beta}^2)^2 \]
\[ I_{10} \quad (s, \hat{\beta}^T s, \hat{\beta}^2 p) \]
\[ I_{11} \quad (p, \hat{\beta}^T p, \hat{\beta}^2 p) \]
\[ I_{12} \quad s \bar{p} (1; \pm b_1; 0) (\pm b_2; 1; 0) \]
\[ I_{13} \quad s \hat{\beta}^2 \hat{\beta} p (1; \pm b_1; 0) (\pm b_2; 1; 0) \]
\[ I_{14} \quad c_{ijk} e_{l mn} s_i \hat{\beta}_j p_l \bar{\beta}_m \bar{\beta}_n \]
\[ I_{15} \quad (s, \hat{\beta}^T s, \hat{\beta} p) \]
\[ I_{16} \quad (s, \hat{\beta}, \hat{\beta}^2 p) \]
\[ I_{17} \quad (s, \hat{\beta}^2, \hat{\beta}^2 p) \]
\[ I_{18} \quad (s, \hat{\beta} p, \hat{\beta}^2 p) \]

TABLE I. The complete set of invariants of a two-qubit state. Here $(a, b, c)$ stands for the triple scalar product $a \cdot (b \times c)$, and $e_{ijk}$ is the Levi-Cevita symbol; $s \hat{\beta}$ is a 3-vector with components $s_j \hat{\beta}_j$, etc. The last two columns present, for each invariant, $s, p$ in a situation when only this invariant distinguishes between two nonequivalent states. In these examples we assume a nondegenerate $\hat{\beta}$, with $b_3 = 0$ for $I_{12-18}$.

**Theorem 3.** Two states are locally equivalent exactly when the invariants $I_1-I_{18}$ have equal values for these states. (Only signs of $I_{10}, I_{11}, I_{15-18}$ are needed.)

None of the invariants can be removed from the set without affecting completeness, as demonstrated by examples in the table.

The proof below gives an explicit procedure to find single-bit gates which transform one of two equivalent states into the other.

**Proof.** It is clear that all $I_i$ in the table are invariant under independent orthogonal rotations $O, P$, i.e. under single-bit gates. To prove that they form a complete set, we show that for given values of the invariants one can be achieved by proper rotations $O, P$ (singular value decomposition). The invariants $I_1-I_3$ determine the diagonal entries of $\hat{\beta}$ up to a simultaneous sign change for any two of them. Using single-bit operations $R^i \otimes 1$ (where $R^i$ is the $\pi$-rotation about the axis $i = 1, 2, 3$) we can fix these signs: all three eigenvalues, $b_1, b_2, b_3$, can be made nonnegative, if $I_1 = \det \hat{\beta} \geq 0$, or negative, if $\det \hat{\beta} < 0$. Further transformations, with $O = P$ representing permutations of basis vectors, place them in any needed order.

From now on we consider only states with a fixed diagonal $\hat{\beta}$. Hence, only such single-bit gates, $O \otimes P$, are allowed which preserve $\hat{\beta}$. The group of such operations depends on $b_1, b_2, b_3$. We examine all possibilities below, showing that the invariants $I_{4-18}$ fix the state completely.

(A) $\hat{\beta}$ is nondegenerate: all $b_i$ are different. Then the only $\hat{\beta}$-preserving local gates are $r^i \equiv R^i \otimes R^i$.

The invariants $I_{4-6}$ and $I_{7-9}$ set absolute values of six components $s_i, p_i$, but not their signs. The signs are bound by other invariants. In particular, $I_{10}$ and $I_{11}$ fix the values of $s_1s_2s_3$ and $p_1p_2p_3$. Furthermore, $I_{12-14}$ give three linear constraints on three quantities $s,p_i$. When $\hat{\beta}$ is not degenerate, one can solve them for $s,p_i$. Let us consider several cases:

i) $s$ has at least two nonzero components, say $s_1, s_2$. These two can be made positive by single-bit gates $r^i$, $r^j$. After that, the signs of $p_{i=1,2}$ are fixed by values of $s_ip_i$, while $I_{10}$ fixes the sign of $s_3$. The sign of $p_3$ can be determined from $s_3p_3$, if $s_3 \neq 0$; if $s_3 = 0$ then $p_3$ is fixed by $I_{15} = p_3s_1s_2b_3(b_2^2 - b_1^2)$ or $I_{17} = p_3s_1s_2b_1b_2(b_2^2 - b_1^2)$.

If $p$ has at least two nonzero components, a similar argument applies, with $I_{11,16,18}$ instead of $I_{10,15,17}$. If both $s$ and $p$ have at most one nonzero component, $s_i$ and $p_j$, then either ii) $i = j$, and the signs are specified by $s_ip_i$ up to $\hat{\beta}$-preserving gates $r^k$; or iii) $i \neq j$, and one can use $r^i, r^j$ to make both components nonnegative.

(B) $\hat{\beta}$ has two equal nonzero eigenvalues: $b_3 \neq b_1 = b_2 \neq 0$. We define horizontal components $s_{\perp} = (s_1, s_2, 0), p_{\perp} = (p_1, p_2, 0)$. Then $\hat{\beta}$-preserving operations are generated by simultaneous, coinciding rotations of $s_{\perp}$ and $p_{\perp}$ [i.e. $s_{\perp} \rightarrow Os_{\perp}, p_{\perp} \rightarrow Op_{\perp}$, where $O \in SO(3,2)$ is a 2D-rotation], as well as $r^i$.

The invariants $I_{4-9}$ fix $s_{\perp}^2, s_{\perp}^3, p_{\perp}^2$ and $p_{\perp}^3$. To specify $s$ and $p$ completely the angle between $s_{\perp}$ and $p_{\perp}$, as well as the signs of $s_3$ and $p_3$ should be determined. These are bound by the remaining invariants. In particular, $I_{12-14}$ fix $s_3p_3$ and $s_{\perp}p_{\perp}$. The latter sets the angle between $s_{\perp}$ and $p_{\perp}$ up to a sign.

There are two possibilities: i) $s_3 = p_3 = 0$. The states with opposite angles are related by $r^1$ and hence equivalent. ii) $s_3 \neq 0$ (the case $p_3 \neq 0$ is analogous). Applying $r^1$, if needed, we can assume that $s_3$ is positive. Then, $p_3$ is specified by the value of $s_3p_3$. Apart from that, $I_{15}$ sets $(s_{\perp} \times p_{\perp})_3s_3$, and hence the sign of the cross product $s_{\perp} \times p_{\perp}$. This fixes the density matrix completely.

(C) $b_1 = b_2 = 0, b_3 \neq 0$. In this case $\hat{\beta}$-preserving operations are independent rotations of $s_{\perp} \times p_{\perp}$ [which
form $SO_1(2)^{\otimes 2}$ and $r^i$. The invariants $I_{1-9}$ fix $s_1^2, s_2^2,$ $p_1^2$, and $p_2^2$, while $I_{12}$ (or $I_{13}$) sets $s_3p_3$. It is easy to see that they specify the state completely.

(D) $b_1 = b_2 = b_3 \neq 0$. All transformations $O \otimes O$, where $O \in SO(3)$, preserve $\hat{\beta}$. The invariants $I_1, I_7$ and $I_{12}$ fix $s_2^2, p_2^2$ and $sp$, and this information is sufficient to determine $s$ and $p$ up to a rotation.

(E) $\beta = 0$. In this case all local transformations preserve $\hat{\beta}$; hence, $s$ and $p$ can rotate independently. The only nonzero invariants, $I_1$ and $I_7$, fix $s^2$ and $p^2$. □

**Discussion.** In this section we demonstrate applications of our results. We calculate the invariants for several two-qubit gates to find out which of them are locally equivalent. These gates include CNOT, SWAP and its square root, as well as several gates $\exp(i\mathcal{H}t)$.

Analyzing the invariants we see that to achieve CNOT one needs to perform a two-qubit gate at least twice if the latter is triggered by the Heisenberg Hamiltonian $\hat{\sigma}\hat{\sigma}$. At the same time SWAP and $\sqrt{\text{SWAP}}$ can be performed with one elementary two-bit gate $\hat{\sigma}$. The interaction $\sigma_y\sigma_y$ allows to perform CNOT in one step, while $\sigma_\perp\sigma_\perp$ requires at least two steps for all three gates.

In Josephson qubits [1] elementary two-bit gates are generated by the interaction $\mathcal{H} = -\frac{1}{2}E_1(\hat{\sigma}_x^1 + \hat{\sigma}_x^2) + (E_2/E_L)\hat{\sigma}_y^1\hat{\sigma}_y^2$. Investigation of the invariants shows that CNOT can be performed if $E_2$ is tuned to $\alpha E_L$ for a finite time $t = \frac{\alpha^2}{2}(n + 1)/4E_L$, where $n$ is an integer and $\alpha$ satisfies $\alpha^2 \cos^2\left(n + \frac{1}{2}\right) \sqrt{1 + \alpha^{-2}} = -1$.

For creation of entanglement between qubits a useful property of a two-qubit gate is its ability to produce a maximally entangled state (with $|\text{Ent }\psi\rangle = 1/2$) from an unentangled one $\hat{\rho}$. This property is locally invariant and one can show that a gate $M$ is a perfect entangler exactly when the convex hull of the eigenvalues of the corresponding matrix $m$ contains zero. In terms of the invariants, introduced in Table II, this condition reads: $\sin^2 \gamma \leq 4|G_1| \leq 1$ and $\cos \gamma (\cos \gamma - G_2) \geq 0$, where $G_1 = |G_1|e^{\gamma}$. Among the gates in the table CNOT and $\sqrt{\text{SWAP}}$ are perfect entanglers. The Heisenberg Hamiltonian can produce only two perfect entanglers ($\sqrt{\text{SWAP}}$ or its inverse), while $\sigma_y\sigma_y$ - only CNOT. At the same time, the interaction $\hat{\sigma}_\perp\hat{\sigma}_\perp$ produces a set of perfect entanglers if the system evolves for time $t$ with $\cos t \leq 0$.

To conclude, we have presented complete sets of local polynomial invariants of two-qubit gates (3 real invariants) and two-qubit mixed states (18 invariants) and demonstrated how these results can be used to optimize quantum logic circuits and to study entangling properties of unitary operations.

I am grateful to G. Burkard, D.P. DiVincenzo, M. Grassl, G. Schöhn, and A. Shnirman for fruitful discussions.

---

[1] The subgroup $SU(2)^{\otimes 2}$ of single-bit operations in $SU(4)$ consists of operators $u \otimes v$, where $u$ acts only on the first and $v$ on the second qubit.

[2] D.P. DiVincenzo, Phys. Rev. A 51, 1015 (1995).

[3] S. Lloyd, Phys. Rev. Lett. 75, 346 (1995).

[4] D. Deutsch, A. Barenco, A. Ekert, Proc. R. Soc. Lond. A 449, 669 (1995).

[5] A. Barenco et al., Phys. Rev. A 52, 3457 (1995).

[6] G. Burkard, D. Loss, D.P. DiVincenzo, and J.A. Smolin, Phys. Rev. B 60, 11404 (1999).

[7] E.M. Rains, preprint, quant-ph/9704042 (1997).

[8] M. Grassl, M. Rötteler, and T. Beth, Phys. Rev. A 58, 1833 (1998). They presented 21 invariants, which included $\text{tr }\hat{\rho}$, equal to 1 for physical states.

[9] This function can be non-polynomial. For instance, the values of the invariants $I_{19} = (s_1, s_2, \beta, \bar{\beta}, \hat{\beta}, \bar{\beta}, \hat{\beta}, \ldots)$ and $I_{20} = (\beta, \beta, \beta, \beta, \hat{\beta}, \bar{\beta}, \hat{\beta}, \bar{\beta}, \bar{\beta}, \hat{\beta})$ are completely determined by $I_{1-18}$ but are not polynomial functions of them. As shown by M. Grassl (private communication), $I_{1-20}$ generate the same polynomial ring as invariants from Ref. [8].

[10] A. Shnirman, G. Schöhn, and Z. Hermon, Phys. Rev. Lett. 79, 2371 (1997).

[11] Yu. Makhlin, G. Schöhn, and A. Shnirman, Nature 386, 305 (1999).

[12] D. Loss and D.P. DiVincenzo, Phys. Rev. A 57, 120 (1998).