

Quantum Discord and Total Quantum Correlations in a N -partite Quantum State

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Understanding quantum correlations is a fundamental problem facing science.

Last two decades, this problem is approached via entanglement separability scenarios, with its successes and failures.

Successes : Quantum information processing (Teleportation, Superdense coding, Algorithms, Cryptography),
Physical processes (Quantum phase transitions, BE condensation, Quantum-to-classical transitions, Open quantum systems)

Failures : No viable measure for entanglement in mixed states.

Entanglement does not account for the total quantum correlations or 'quantumness' of a quantum state. Separable quantum states can have correlations responsible for some quantum tasks which cannot be achieved by classical means. Well known instance :
DQC1. Knill Laflamme : Phys. Rev. Lett. **81**, 5672 (1998).
A.Datta, A.Shaji and C.M.Caves : Phys. Rev. Lett. **100**, 050502 (2008).

Another approach : Quantum verses classical paradigm. First proposed by

H. Ollivier and W. H. Zurek : Phys. Rev. Lett. **88**, 017901 (2001)
and L. Henderson and V. Vedral : J. Phy. A **34**, 6899 (2001).

Basically, for a bipartite state, Total quantum correlation (Mutual information) - Classical correlation = Quantum correlation (Quantum discord).

An alternative formulation for quantum discord :
Minimal loss of correlation caused by a non-selective von-Neumann projective measurement on one part of the system.

$$D(\rho) = \min_{\Pi^a} \{I(\rho) - I(\Pi^a(\rho))\}$$

where

$$\Pi^a(\rho) = \sum_i (\Pi_i^a \otimes I^b) \rho (\Pi_i^a \otimes I^b) \quad (1)$$

Here the minimum is over von Neumann measurements $\Pi^a = \{\Pi_i^a\}$ on a part say a of a bipartite system ab in a state ρ with reduced density operators ρ^a and ρ^b and $\Pi^a(\rho)$ is the resulting state after the measurement. $I(\rho) = S(\rho^a) + S(\rho^b) - S(\rho)$ is the quantum mutual information, $S(\rho) = -\text{tr}(\rho \ln \rho)$ is the von Neumann entropy and I^b is the identity operator on part b .

This formulation of QD based on mutual information is difficult to generalize to multipartite case. We can overcome this hurdle by introducing a geometric measure of quantum discord as a distance of the given state to the closest classical quantum (or the zero discord) state.

Dakic, Vedral, and Brukner [Phys. Rev. Lett. 105,190502 (2010)],
Lin Chen, Eric Chitambar, Kavan Modi, and Giovanni Vacanti,
arXiv: 1005.4348.

QUANTUM DISCORD IN A N -PARTITE STATE

Consider a multipartite system $\mathcal{H} = \mathcal{H}^1 \otimes \mathcal{H}^2 \otimes \dots \otimes \mathcal{H}^N$ with $\dim(\mathcal{H}^m) = d_m$, $m = 1, 2, \dots, N$. Let $L(\mathcal{H}^m)$ be the Hilbert-Schmidt space of linear operators on \mathcal{H}^m with the Hilbert-Schmidt inner product

$$\langle X^{(m)} | Y^{(m)} \rangle := \text{tr} X^{(m)\dagger} Y^{(m)}.$$

We can define The Hilbert-Schmidt space $L(\mathcal{H}^1 \otimes \mathcal{H}^2 \otimes \dots \otimes \mathcal{H}^N)$ similarly. Let $\{X_i^{(m)} : i = 1, 2, \dots, d_m^2, m = 1, 2, \dots, N\}$ be set of Hermitian operators which constitute orthonormal bases for $L(\mathcal{H}^m)$, then

$$\text{tr} X_i^{(m)} X_j^{(m)} = \delta_{ij},$$

and $\{X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \dots \otimes X_{i_N}^{(N)}\}$ constitutes an orthonormal basis for $L(\mathcal{H}^1 \otimes \mathcal{H}^2 \otimes \dots \otimes \mathcal{H}^N)$.

QUANTUM DISCORD IN A N -PARTITE STATE

(... continued)

In particular, any N -partite state $\rho_{12\dots N} \in L(\mathcal{H}^1 \otimes \mathcal{H}^2 \otimes \dots \otimes \mathcal{H}^N)$ can be expanded as

$$\rho_{12\dots N} = \sum_{i_1 i_2 \dots i_N} c_{i_1 i_2 \dots i_N} X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \dots \otimes X_{i_N}^{(N)} ; i_m = 1, \dots, d_m^2 ; m = 1, \dots$$

with $\mathcal{C} = [c_{i_1 i_2 \dots i_N}] = [\text{tr}(\rho_{12\dots N} X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \dots \otimes X_{i_N}^{(N)})]$ is a N -way array (tensor of order N) with size $d_1^2 d_2^2 \dots d_N^2$.

We can define the geometric measure of quantum discord for a N -partite quantum state corresponding to the von Neumann measurement on the k th part as

$$D_k(\rho_{12\dots N}) = \min_{\chi_k} \|\rho_{12\dots N} - \chi_k\|^2,$$

where the minimum is over the set of zero discord states χ_k [i.e. $D_k(\chi_k) = 0$]. A state $\chi_k \in L(\mathcal{H}^1 \otimes \mathcal{H}^2 \otimes \dots \otimes \mathcal{H}^N)$ is of zero discord if and only if it is a classical-quantum state

$$\chi_k = \sum_{l=1}^{d_k} p_l |l\rangle\langle l| \otimes \rho_{[k]|l},$$

where $[k]$ stands for $12\dots k - 1k + 1\dots N$, $\{p_l\}$ is a probability distribution over the terms in the sum, $\{|l\rangle\}$ is an arbitrary orthonormal basis in \mathcal{H}^k , and $\{\rho_{[k]|l}\}$ is a set of arbitrary states (density operators) acting on

(... continued)

$\mathcal{H}^1 \otimes \mathcal{H}^2 \otimes \dots \otimes \mathcal{H}^{k-1} \otimes \mathcal{H}^{k+1} \otimes \dots \otimes \mathcal{H}^N$). It follows that the quantum discord corresponding to measurement on different subsystems is different, that is, $D_k(\rho) \neq D_l(\rho)$; $k \neq l$.

We need to define a product of a tensor with a matrix, the n -mode product. The n -mode (matrix) product of a tensor \mathcal{Y} (of order N and with dimension $J_1 \times J_2 \times \cdots \times J_N$) with a matrix A with dimension $I \times J_n$ is denoted by $\mathcal{Y} \times_n A$. The result is a tensor of size $J_1 \times J_2 \times \cdots \times J_{n-1} \times I \times J_{n+1} \times \cdots \times J_N$ and is defined elementwise by

$$(\mathcal{Y} \times_n A)_{j_1 j_2 \cdots j_{n-1} i j_{n+1} \cdots j_N} = \sum_{j_n=1}^{J_n} y_{j_1 j_2 \cdots j_N} a_{i j_n}.$$

Recently, for a bipartite system ab ($N = 2$) with states in $\mathcal{H}^a \otimes \mathcal{H}^b$, $\dim(\mathcal{H}^a) = d_a$, $\dim(\mathcal{H}^b) = d_b$, S. Luo and S. Fu (Phys. Rev. A **82**, 034302 (2010)) introduced the following form of geometric measure of quantum discord

$$D_a(\rho) = \text{tr}(CC^t) - \max_A \text{tr}(ACC^tA^t),$$

where $C = [c_{ij}]$ is an $d_a^2 \times d_b^2$ matrix and the maximum is taken over all $d_a \times d_a^2$ -dimensional isometric matrices $A = [a_{li}]$ such that $a_{li} = \text{tr}(|l\rangle\langle l|X_i) = \langle l|X_i|l\rangle$, $l = 1, 2, \dots, d_a$; $i = 1, 2, \dots, d_a^2$ and $\{|l\rangle\}$ is any orthonormal basis in \mathcal{H}^a . we generalize this result to N -partite quantum states.

Theorem 1. Let $\rho_{12\dots N}$ be a N -partite state defined before, then

$$D_k(\rho_{12\dots N}) = \|\mathcal{C}\|^2 - \max_{A^{(k)}} \|\mathcal{C} \times_k A^{(k)}\|^2,$$

where $\mathcal{C} = [c_{i_1 i_2 \dots i_N}]$ is defined by the state $\rho_{12\dots N}$, the maximum is taken over all $d_k \times d_k^2$ -dimensional isometric matrices $A^{(k)} = [a_{li_k}]$, $A^{(k)}(A^{(k)})^t = I_k$, such that

$a_{li_k} = \text{tr}(|l\rangle\langle l| X_{i_k}^{(k)})$, $l = 1, 2, \dots, d_k$; $i_k = 1, 2, \dots, d_k^2$ and $\{|l\rangle\}$ is any orthonormal basis for \mathcal{H}^k .

Sketch of the proof : By expanding $\rho_{12\dots N}$ and χ_k in the basis $\{X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \dots \otimes X_{i_N}^{(N)}\}$ and making a valid choice for the coefficients of expansion of $\rho_{[k]l}$ states we can show that

$$\|\rho_{12\dots N} - \chi_k\|^2 = \|\mathcal{C}\|^2 - \|\mathcal{C} \times_k A^{(k)}\|^2.$$

Since the tensor \mathcal{C} is determined by the state $\rho_{12\dots N}$, we have,

$$D_k(\rho_{12\dots N}) = \min_{\chi_k} \|\rho_{12\dots N} - \chi_k\|^2 = \|\mathcal{C}\|^2 - \max_{A^{(k)}} \|\mathcal{C} \times_k A^{(k)}\|^2,$$

where the maximum is taken over $A^{(k)}$ specified in the theorem, thus completing the proof.

For a bipartite system, \mathcal{C} is a $d_1^2 \times d_2^2$ matrix while $A^{(1)}$ and $A^{(2)}$ are $d_1 \times d_1^2$ and $d_2 \times d_2^2$ matrices respectively. Using the definition of the n-mode product and the norm of a tensor it follows that

$$D_1(\rho) = \text{tr}(CC^t) - \max_{A^{(1)}} \text{tr}(A^{(1)}CC^tA^{(1)t}),$$

and

$$D_2(\rho) = \text{tr}(CC^t) - \max_{A^{(2)}} \text{tr}(A^{(2)}C^tCA^{(2)t}).$$

Following its definition in terms of von-Neumann measurements, it seems more natural and simple to define the geometric measure of quantum discord as

$$\overline{D}_k(\rho_{12\dots N}) = \min_{\Pi^k} \|\rho_{12\dots N} - \Pi^k(\rho_{12\dots N})\|^2,$$

where the minimum is over von Neumann measurements

$\Pi^k = \{\Pi_i^k\}$ on system \mathcal{H}^k , and $\Pi^k(\rho_{12\dots N}) =$

$\sum_i (I_1 \otimes I_2 \otimes \dots \otimes \Pi_i^k \otimes \dots \otimes I_N) \rho_{12\dots N} (I_1 \otimes I_2 \otimes \dots \otimes \Pi_i^k \otimes \dots \otimes I_N)$.

It is easy to prove that $D_k(\rho_{12\dots N}) = \overline{D}_k(\rho_{12\dots N})$.

EXACT FORMULA FOR A N -QUBIT STATE

We get an exact expression for the QD in a N -qubit case. We have to find the maximum in the equation

$$D_k(\rho_{12\dots N}) = \|\mathcal{C}\|^2 - \max_{A^{(k)}} \|\mathcal{C} \times_k A^{(k)}\|^2,$$

The maximum is to be obtained over 2×4 isometric matrices $A^{(k)}$ whose row vectors can be shown to have the form

$$\vec{a}_1 = \frac{1}{\sqrt{2}}(1, \hat{e}_1),$$

$$\vec{a}_2 = \frac{1}{\sqrt{2}}(1, -\hat{e}_1).$$

and the vector $\hat{e}_1 \in \mathbb{R}^3$ must be the coherence vector of a orthonormal basis state in a single qubit Hilbert space. However, every unit vector in \mathbb{R}^3 satisfies this requirement so that this constraint on optimization becomes redundant. This enormous simplification facilitates the explicit construction of the required maximum.

The isometric 2×4 matrix $\tilde{A}^{(k)}$ which maximizes $\|\mathcal{C} \times_k A^{(k)}\|^2$ can be explicitly constructed as

$$\tilde{A}^{(k)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \hat{e}_{max} \\ 1 & -\hat{e}_{max} \end{pmatrix},$$

where \hat{e}_{max} is the eigenvector of $G^{(k)}$ which is a 3×3 real symmetric matrix, defined as

$$G^{(k)} = \vec{s}^{(k)}(\vec{s}^{(k)})^t + \sum_{k_1 \in \mathcal{N}-k} (T^{\{k_1, k\}})^t T^{\{k_1, k\}} + \sum_{2 \leq M \leq N-1} \mathbb{T}^{(M+1)},$$

for its highest eigenvalue η_{max} .

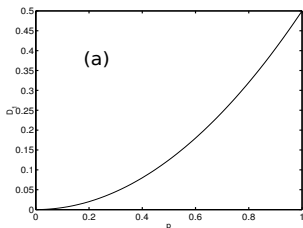
We can then compute

$$D_k(\rho_{12\dots N}) = \|\mathcal{C}\|^2 - \|\mathcal{C} \times_k \tilde{A}^{(k)}\|^2.$$

The first example comprises the 3-qubit mixed states

$$\rho = p|GHZ\rangle\langle GHZ| + \frac{(1-p)}{8}I_8, \quad 0 \leq p \leq 1$$

where $|GHZ\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ and I_8 is the identity matrix. Figure 1(a) shows the variation of $D_1(\rho)$ with p . We see that $D_1(\rho)$ increases continuously from $p = 0$ state (random mixture) to $p = 1$ state (pure GHZ state), as expected.



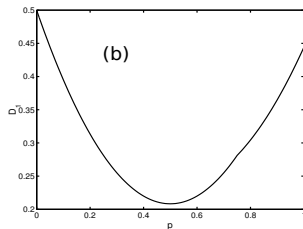
Second example is the set of 3-qubit states

$$\rho = p|W\rangle\langle W| + (1 - p)|GHZ\rangle\langle GHZ|, \quad 0 \leq p \leq 1$$

where $|W\rangle = \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle)$. Figure 1(b) shows the variation of $D_1(\rho)$ with p . It is straightforward to check that this state cannot be written as a classical quantum state for any value of p , including $p = \frac{1}{2}$. This explains the nonzero discord at $p = \frac{1}{2}$. Further, we observe that discord for the pure GHZ state exceeds that for the pure W state, in conformity with similar behavior of entanglement in these states.

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The rate of increase of the discord diminishes discontinuously at $p = \frac{3}{4}$ as the $|W\rangle$ state increasingly dominates the classical mixture with increasing p . This interesting observation needs further analysis.



As the last example we consider the set of 3-qubit states

$$\rho = p|GHZ_{-}\rangle\langle GHZ_{-}| + (1 - p)|GHZ\rangle\langle GHZ|, \quad 0 \leq p \leq 1;$$

where $|GHZ_{-}\rangle = \frac{1}{\sqrt{2}}(|000\rangle - |111\rangle)$. Figure 1(c) shows the variation of $D_1(\rho)$ with p . The discord is symmetric about $p = \frac{1}{2}$ at which it vanishes. For $p = \frac{1}{2}$ the state can be written as

$$\frac{1}{2}|000\rangle\langle 000| + \frac{1}{2}|111\rangle\langle 111|$$

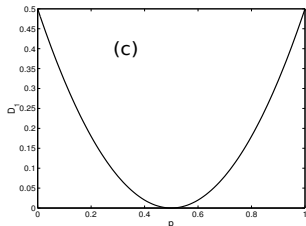
which is a classical quantum state, so that discord vanishes at $p = \frac{1}{2}$.

Example

(... continued)

Again, discord is maximum and equal for pure $|GHZ\rangle$ state and pure $|GHZ_-\rangle$ state, similar to the behavior of entanglement in these two states.

We note that, in all these examples, $D_1(\rho) = D_2(\rho) = D_3(\rho)$ as all the states are symmetric with respect to the swapping of qubits.



TOTAL QUANTUM CORRELATIONS IN A BIPARTITE STATE

Consider a bipartite state ρ and denote by $\tilde{\Pi}^{(1)}$ the von Neumann measurement minimizing $\|\rho - \Pi^{(1)}(\rho)\|^2$. It is straightforward to check that the state after the measurement $\tilde{\Pi}^{(1)}(\rho)$ is a zero discord state, that is $D_1(\tilde{\Pi}^{(1)}(\rho)) = 0$. However, the state $\tilde{\Pi}^{(1)}(\rho)$ may have $D_2(\tilde{\Pi}^{(1)}(\rho)) \neq 0$. Thus the state $\tilde{\Pi}^{(1)}(\rho)$ can have some non-zero quantum correlations. Thus neither $D_1(\rho)$ nor $D_2(\rho)$ gives us a measure of the total quantum correlations in the state ρ . But this analysis suggests that quantity

$$Q(\rho) = D_1(\rho) + D_2(\tilde{\Pi}^{(1)}(\rho))$$

gives the required measure of the total quantum correlations in the state ρ .

In order to find the optimal von Neumann measurement $\tilde{\Pi}^{(1)}$ on ρ which minimizes $\|\rho - \tilde{\Pi}^{(1)}(\rho)\|^2$ we have to find the corresponding orthonormal basis $\{|\tilde{q}\rangle\}$ in \mathcal{H}^1 such that $\{\tilde{\Pi}_q^{(1)}\} = \{|\tilde{q}\rangle\langle\tilde{q}|\}$. The expansion of these 1-D projectors $|\tilde{q}\rangle\langle\tilde{q}|$ in the basis $X_i = \{I_1, \lambda_i\}$

$$|\tilde{q}\rangle\langle\tilde{q}| = \sum_i^{d_1^2} \tilde{a}_{qi} X_i \quad ; \quad q = 1, \dots, d_1$$

with

$$\tilde{a}_{qi} = \langle\tilde{q}|X_i|\tilde{q}\rangle, \quad q = 1, 2, \dots, d_1; \quad i = 1, \dots, d_1^2$$

must then give the matrix $\tilde{A}^{(1)}$ which maximizes $\text{tr}(A C C^t A^t)$ which in turn gives $D_1(\rho)$.

To get the state $\tilde{\Pi}^{(1)}(\rho)$ we proceed as follows. As noticed above, any post measurement state $\Pi^{(1)}(\rho)$ is a zero discord state satisfying $D_1(\Pi^{(1)}(\rho)) = 0$. Hence $\Pi^{(1)}(\rho)$ must have the form of classical quantum state as in for $N = 2$ namely,

$$\Pi^{(1)}(\rho) = \sum_{q=1}^{d_1} p_q |q\rangle\langle q| \otimes \rho_q.$$

We expand the state $p_q \rho_q$ in terms of the basis $\{X_j^{(2)}\}$ to get

$$p_q \rho_q = \sum_j b_{qj} X_j^{(2)},$$

where $b_{qj} = \text{tr}(p_q \rho_q X_j^{(2)})$.

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We know from theorem 1 that, for the above equation to hold, we must have

$$b_{qj} = \sum_i \tilde{a}_{qi} c_{ij}.$$

Now, we substitute these equations in the expression for the general post measurement state to get the state $\tilde{\Pi}^{(1)}(\rho)$ which easily reduces to

$$\tilde{\Pi}^{(1)}(\rho) = \sum_{lj} (\tilde{A}^{(1)t} \tilde{A}^{(1)} C)_{lj} X_l^{(1)} \otimes X_j^{(2)},$$

where $\tilde{A}^{(1)}$ is the matrix which maximizes $\text{tr}(A^{(1)} C C^t A^{(1)t})$. This expression can be exactly evaluated in two qubit case.

TOTAL QUANTUM CORRELATIONS IN A N -PARTITE STATE

Consider a N -partite state $\rho_{12\dots N}$ and denote by $\tilde{\Pi}^{(k)}$ the von Neumann measurement giving QD D_K . It is straightforward to check that the state after the measurement $\tilde{\Pi}^{(k)}(\rho_{12\dots N})$ is a zero k -discord state, that is $D_k(\tilde{\Pi}^{(k)}(\rho_{12\dots N})) = 0$. However, the state $\tilde{\Pi}^{(k)}(\rho_{12\dots N})$ may have $D_l(\tilde{\Pi}^{(k)}(\rho_{12\dots N})) \neq 0$, $l \neq k$. Thus the state $\tilde{\Pi}^{(k)}(\rho_{12\dots N})$ can have some non-zero quantum correlations. Thus $D_k(\rho_{12\dots N})$ cannot give us a measure of the total quantum correlations in the state $\rho_{12\dots N}$. This analysis suggests a geometric measure of total quantum correlations present in a N -partite state $\rho_{12\dots N}$.

TOTAL QUANTUM CORRELATIONS IN A N -PARTITE STATE

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We can now use the above considerations to investigate the total quantum correlations present in a state $\rho_{12\dots N}$. Let us assume that the non-selective von Neumann projective measurements $\tilde{\Pi}^{(1)}, \tilde{\Pi}^{(2)}, \dots, \tilde{\Pi}^{(N)}$ are performed successively on N parts $12\dots N$, k th successive measurement being performed on the k th part, leading to $D_k(\mu_{12\dots N}) = 0$, where $\mu_{12\dots N}$ is the state produced after $(k - 1)$ th successive measurement. Clearly, the corresponding post-measurement states are given by

$$\tilde{\Pi}^{(1)}(\rho_{12\dots N}), \tilde{\Pi}^{(2)}(\tilde{\Pi}^{(1)}(\rho_{12\dots N})), \dots, \tilde{\Pi}^{(N)}(\dots(\tilde{\Pi}^{(1)}(\rho_{12\dots N})\dots)).$$

Here the measurement $\tilde{\Pi}^{(k)}$ minimizes the loss of correlations in the state produced after the first $k - 1$ successive measurements on $k - 1$ parts.

Thus the geometric measures of quantum discord of these successive measurement states are given by

$$\begin{aligned}
 &D_1(\rho_{12\dots N}), \\
 &D_2(\tilde{\Pi}^{(1)}(\rho_{12\dots N})), \\
 &D_3(\tilde{\Pi}^{(2)}(\tilde{\Pi}^{(1)}(\rho_{12\dots N}))), \\
 &\vdots \\
 &D_N(\tilde{\Pi}^{(N-1)}(\dots(\tilde{\Pi}^{(1)}(\rho_{12\dots N})))\dots).
 \end{aligned}$$

Therefore, the geometric measure of total quantum correlations present in a N-partite quantum state $\rho_{12\dots N}$ is given by

$$\begin{aligned}
 Q(\rho_{12\dots N}) = &D_1(\rho_{12\dots N}) + D_2(\tilde{\Pi}^{(1)}(\rho_{12\dots N})) + D_3(\tilde{\Pi}^{(2)}(\tilde{\Pi}^{(1)}(\rho_{12\dots N}))) + \dots \\
 &\dots + D_N(\tilde{\Pi}^{(N-1)}(\dots(\tilde{\Pi}^{(1)}(\rho_{12\dots N})))\dots), \quad (2)
 \end{aligned}$$

which is a multipartite generalization of the bipartite measure.

We can show that

$$Q(\rho_{12\dots N}) = \|\mathcal{C}\|^2 - \|\mathcal{C} \times_1 \tilde{A}^{(1)} \times_2 \tilde{A}^{(2)} \times_3 \dots \times_{N-1} \tilde{A}^{(N-1)} \times_N \tilde{A}^{(N)}\|^2.$$

where $\tilde{A}^{(k)}$ is the matrix optimizing the k th measurement. This formula applies to an arbitrary N -partite quantum state. However, $Q(\rho_{12\dots N})$ can be actually computed only for a N -qubit state, because the matrices $\tilde{A}^{(k)}$ as well as the states $\tilde{\Pi}^{(k)}(\rho_{12\dots N})$, $k = 1, \dots, N$ can be explicitly constructed in this case. Further, for N -qubit states, this formula can be experimentally implemented, as all the elements of all the matrices can be determined by measuring Pauli operators on individual qubits. We can show that $Q(\rho_{12\dots N})$ is invariant under the permutation of parts, that is, it does not matter in which order the measurements are made.