Determining quantum correlations in bipartite systems - from qubit to qutrit and beyond

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Abstract. We advocate the step change in properties of discrete $d$-level quantum systems, between $d = 2$ and $d \geq 3$. Qubit systems, or multipartite systems containing qubit subsystem, are exceptional in their relative simplicity. One faces a step in complexity in valuating measures of quantum correlations for qutrits and then other higher dimensional qudits. There is a growing number of arguments leading to such conclusion: recently found no-go theorem for generalization of the Peres-Horodecki’s PPT criterion [1], change in geometry of state spaces of qubit and higher degree qudits (the so called ’generalized Bloch ball’ is not a ball anymore), restricted possibilities for diagonalization of correlation matrices for bipartite systems, more difficult way for handling the set of relevant families of orthogonal projectors.

1. Introduction
Quantum correlations in finite dimensional quantum systems are new resources which can fuel quantum information and computing. Their quantification is crucial, but difficult task. Its complexity depends on the chosen correlation, definition of its measure and dimension $d$ of the bipartite $d$-level system. Generic statement valid for all known quantum correlations is: pure states can be uncorrelated or entangled. Historically first and mostly studied correlation is quantum entanglement of qubits, extended also to qutrits [2] and then for qudits [3], but only for limited types of states. Results known for qubit systems can be generalized to some extend to a qubit-qudit case. In that case a lower dimensional system sets the level of the complexity of the problem. An interesting aspect of finding the value of correlation measure is a possibility of relating it to the mean values of a selected observables of a system. One example of such relation is given for qubits, where entanglement measure can be expressed in terms of the mean value of spin [4].

The correlation we want to focus here on is the quantum discord. The general definition of its measure, while it distinguishes the quantum and classical character of correlations in compound systems, is hardly operational, even for qubit systems. That is why we restrict our considerations to the so called measurement-induced one sided quantum geometric discord (MIQGD). It is a version of the geometric measure of quantum correlations related to the distance used in definition. To have measure contractive under completely positive trace preserving maps we chose trace norm (Schatten 1-norm). Such distance used in definition produces proper quantum correlation measure in contrast to the Hilbert-Schmidt distance. We shall discuss the MIQGD for various $d$-level systems, $d = 2, 3, \ldots$. However, properties of bipartite systems with $d \geq 3$ change with restpect to $d = 2$. For two-qutrit states there is no finite set of criteria of separability [1], what means that there is no extension of the Peres-Horodecki’s
necessary and sufficient PPT-criterion valid for qubit-qubit and qubit-qutrit systems\[5, 6\] to higher level systems.

2. Single qudit system quantum state space

In the commonly used notation for su(d) Lie algebras we can describe the one-partite states by the set of generators (we use here uniform notation, where usually for su(2), \( \lambda = \sigma_j \))

\[
\text{tr} \lambda_j = 0, \quad \text{tr} (\lambda_j \lambda_k) = 2 \delta_{jk}, \quad \text{and} \quad \lambda_j \lambda_k = \frac{2}{d} \delta_{jk} \mathbb{I}_d + \sum f_{jkl} (d_{jkl} + i f_{jkl}) \lambda_l
\]

(1)

where \( j, k = 1, \ldots, d^2 - 1 \); the totally symmetric and antisymmetric, respectively, structure constants \( d_{jkl} \) and \( f_{jkl} \) are given by \( d_{jkl} = \frac{1}{d} \text{tr} (\lambda_j (\lambda_k + \lambda_l)) \) and \( f_{jkl} = \frac{1}{d^2} \text{tr} (\lambda_j (\lambda_k | \lambda_l)) \).

- \( su(2) \):
  \[
d_{ijk} = 0, \quad f_{ijk} = \varepsilon_{ijk}
\]

- \( su(3) \):
  \[
d_{ijk} = \begin{cases} 
\frac{1}{2} & \text{for } (ijk) = (146), (157), (256), (344), (355), \\
-\frac{1}{2} & \text{for } (ijk) = (247), (366), (377), \\
\frac{1}{\sqrt{3}} & \text{for } (ijk) = (118), (228), (338), \\
-\frac{1}{\sqrt{3}} & \text{for } (ijk) = (888), \\
-\frac{2}{\sqrt{3}} & \text{for } (ijk) = (448), (558), (668), (778)
\end{cases}
\]

and

\[
f_{ijk} = \begin{cases} 
1 & \text{for } (ijk) = (123), \\
\frac{1}{2} & \text{for } (ijk) = (147), (246), (257), (345), (516), (637), \\
\frac{\sqrt{3}}{2} & \text{for } (ijk) = (458), (678).
\end{cases}
\]

Using these structure constants one can introduce the *-product and \( \wedge \)-products of \( \mathbb{R}^{d^2-1} \) vectors. For \( n, m \in \mathbb{R}^{d^2-1} \) we define

\[
(n \ast m)_j = \frac{\sqrt{d(d-1)}}{2} \frac{1}{d-2} \sum_{kl} d_{jkl} n_k m_l \quad \text{and} \quad (n \wedge m)_j = \frac{\sqrt{d(d-1)}}{2} \frac{1}{d-2} \sum_{kl} f_{jkl} n_k m_l
\]

(2)

Let \( \lambda = (\lambda_1, \ldots, \lambda_{d^2-1}) \) and

\[
\langle n, \lambda \rangle = \sum_n n_j \lambda_j
\]

(3)

The set of states \( \rho \) of \( d \)-level system i.e. the set of hermitian of a unit trace matrices which are positive definite is customarily parameterized in the following way

\[
\rho = \frac{1}{d} \left( \mathbb{I}_d + \sqrt{\frac{d(d-1)}{2}} \langle n, \lambda \rangle \right), \quad n \in \mathbb{R}^{d^2-1},
\]

(4)

where the components of the vector \( n \) are

\[
n_j = \frac{d}{\sqrt{2d(d-1)}} \text{tr} (\rho \lambda_j), \quad j = 1, \ldots, d^2 - 1.
\]

For arbitrary \( d \)-level system, pure states get simple characterization

\[
\langle n, n \rangle = 1 \quad \text{and} \quad n \ast n = n.
\]

(5)
i.e. for solutions of above conditions relevant ρ is a projector. Only in the case of qubits the ∗-product is trivial and above condition select the boundary of the Bloch ball with maximally mixed state laying in its center. Dimension of the quantum state space Q_d is d^2 − 1 and only for the d = 2 one gets direct description of the set of states as the ball embeded in R^3. For higher d this set has much richer structure and is highly difficult to characterize explicitly, what is related also to the fact, that characterization of the positive-definiteness of ρ in terms of vector n for arbitrary d-level system gets complicated and, in fact, is not known for generic case. Nevertheless, for the d > 2 the frequently adopted name in literature for this set is ”generalized Bloch ball” (GBB), what shouldn’t be taken literary. A generic property of the GBB is that as a convex set it has boundary placed in between two spheres, the outsphere of radius R_d and the insphere of the radius r_d, where in the Hilbert-Schmidt distance

\[ R_d = \sqrt{(d−1)/2d}, \quad r_d = \frac{1}{\sqrt{2d(d−1)}}, \]

what means that

\[ R_d = (d−1)r_d. \]

As stated in [7] the Q_d has a constant height, in the sense that

\[ \frac{Ar_d}{V} = d^2 − 1, \]

where A denotes an area of the boundary of the Q_d and V is its volume. More precisely, it was shown in [8] that such property holds for the convex set of separable two qubits states and the set of positive partial transpose states of an arbitrary bipartite system. Let us comment on the generalized Bloch ball Q_d for d = 2,3.

**Bloch ball**

The Q_2 is the simplest quantum state space and its geometry is the best known. Here R_d = r_d and boundary of Q_2, ∂Q_2 is identical with the boundary of outer/inner sphere. Pure states are characterized by < n, n >= 1. The condition n ∗ n = n in this case is not present.

**Single qutrit state space**

Explicit description of the qutrit quantum state space Q_3 and its visualization has been intriguing for some time. As for all Q_d this is a question of describing a convex set with boundary placed between inner and outer spheres, here R_3 = 2r_3. In the Ref. [7] one can find what objects cannot serve as a model of Q_3 and then what information one gets using two-dimensional projections and cross-sections. The question of the ‘visualization’ of the Q_3 was firstly discussed in Ref. [9] and recently published [10]. Tree dimensional ’visualizations’ can be obtained by means of the other parametrizations of the Q_3. As shown in Ref. [11], instead of the vector n one can produce a graphical representation of a qutrit using a three dimensional vector a and a metric tensor η with distribution of eight independent parameters into 3+5 respectively. Qutrit states are described by a and η such that, η ⋅ a ≤ 1.

Using the description of states by means of the vector n, we know, that pure states should satisfy conditions (5), what means that such states are scattered on the outer sphere and discrete rotation is needed to map them geometrically. This is result of the n ∗ n = n condition and non-triviality of the d_{ijk} constants for the su(3) algebra (for qubits arbitrary rotations are allowed).

**Single qudit state space**

Despite some generic properties, there is very little known about generalized Bloch ball for d ≥ 4. As described in the Ref. ([7]) it is easier to enumerate what characteristics that convex set does not have. Let us quote here selected properties o the GBB for qudits from the list given in the Ref. ([7]):
• $Q_d$ has the 'no hair' property i.e. it is a $d^2 - 1$ dimensional convex set topologically equivalent to a ball and it does not have parts of lower dimension.

• $B_{rd} \subset Q_d \subset B_{Rd}$, where $B_r$ denotes a ball with the radius $r$.

• $\partial Q_d$ is $d^2 - 2$ dimensional and contains all states with rank smaller than maximal.

• The set of pure states is $2d - 2$ dimensional and connected. It has zero measure with respect to $\partial Q_d$.

• $Q_d$ has constant height, cf. Eq.(7).

3. Bipartite qudit system state space

Two qubits
The simplest bipartite quantum system in which we can discuss quantum correlations is a system of two qubits. The total space of states is equal to $Q_4$ which detailed geometrical structure is not known. To get some insight into the geometry of $Q_4$, one can consider some lower dimensional sections of this set. In [12] two-dimensional sections of the corresponding space of generalized Bloch vectors were considered. On the other hand, the problem of discrimination between separable and entangled states is in this case completely solved. The separability condition based on the notion of partial transposition [5, 6] is simple and effective. Applied to the above-mentioned sections of the set of states, this condition gives some information about geometrical shapes of the sets of separable and entangled states [12].

Two qutrits and beyond
In the case of two qutrits, the geometry of the space $Q_9$ is yet more complicated. Some aspects of this geometry were studied in the class of so-called Bell-diagonal states which form a simplex living in the nine-dimensional real linear space [13]. This analysis was then extended to the case of general qudits [14]. What mainly differs qutrits from qubits is that in the system of two qutrits separability condition based on partial transposition is not sufficient. It only shows that the states which are not positive after this operation (NPPT states) are entangled. It turns out that all entangled states can be divided into two classes: free entangled states that can be distilled using local operations and classical communication (LOCC); bound entangled states for which no LOCC strategy can be used to extract pure state entanglement [15]. Last but not least recourse, from the pragmatic point of view, might be the Monte Carlo sampling of the quantum state space [16]. It allows obtaining high-quality random samples of quantum states from higher dimensional $Q_d$, respecting the relevant target distributions and allowing to evaluate global extremum of a given correlation measure function. This approach is still to be applied to the geometric quantum discord measures.

New difficulties for higher dimensional systems
Let us point out some difficulties emerging in systems with higher $d$:

(i) Considerably more complex structure of the set of separable bipartite states, quantum-classical states etc.

(ii) Change in structure of universal enveloping algebra for $su(d)$. Vanishing $d_{ijk}$ symmetric structure constants for $su(2)$ became nontrivial for $d \geq 3$ and modify the geometry of state space via $\star$-product.

(iii) Relatively 'shrunken' orthogonal subgroup $R(G)$ originating as the adjoint representation from the unitary transformations $G = \text{SU}(d)$, $\dim \text{SU}(d) = d^2 - 1$ compared to $\dim O(d^2 - 1)$ (Table 1). Only for qubits we have the same dimension of these groups and $SU(2)$ is just universal double cover of $SO(3)$.

(iv) No possibility to diagonalize all correlation matrices i.e. emerging new sectors in comparison to the qubit intuition.

(v) Steep curve of growing complexity; hopeless perspective to perform effectively minimization and produce analytical formulas for correlation measures for arbitrary state.
Table 1. Dimensions of orthogonal subgroups.

| $G$   | $\dim G$ | $\dim R(G)$ | $\dim O(d^2 - 1)$ |
|-------|----------|-------------|-------------------|
| SU(2) | 3        | 3           | 3                 |
| SU(3) | 8        | 8           | 28                |
| SU(4) | 15       | 15          | 105               |
|       | $\ldots$| $\ldots$   | $\frac{1}{2}(d^2 - 1)(d^2 - 2)$ |

(vi) For qubits various correlation measures are equivalent, but split for $d > 3$.

4. Quantifying quantum correlations in bipartite systems - from qubits to qutrits and beyond

Consider now two qudits $\mathcal{A}$ and $\mathcal{B}$. It is convenient to parametrize the set of states of composite system as follows

$$
\rho = \frac{1}{d^2} \left( \mathbb{I}_d \otimes \mathbb{I}_d + \sqrt{\frac{d(d-1)}{2}} \langle x, \lambda \rangle \otimes \mathbb{I}_d + \mathbb{I}_d \otimes \sqrt{\frac{d(d-1)}{2}} \langle y, \lambda \rangle + \sum_{k=1}^{d-1} \langle \mathcal{K}e_k, \lambda \rangle \otimes \langle e_k, \lambda_k \rangle \right)
$$

(8)

where $x, y \in \mathbb{R}^{d^2-1}$ and $\{e_k\}_{k=1}^{d^2-1}$ are the vectors of canonical orthonormal basis of $\mathbb{R}^{d^2-1}$. Notice that

$$
x_j = \frac{d}{\sqrt{2d(d-1)}} \text{tr}(\rho \lambda_j \otimes \mathbb{I}_d), \quad y_j = \frac{d}{\sqrt{2d(d-1)}} \text{tr}(\rho \mathbb{I}_d \otimes \lambda_j)
$$

and the correlation matrix $\mathcal{K}$ has elements

$$
\mathcal{K}_{jk} = \frac{d^2}{4} \text{tr}(\rho \lambda_j \otimes \lambda_k).
$$

The parametrization (8) is chosen is such a way, that the marginals $\text{tr}_\mathcal{B} \rho$ and $\text{tr}_\mathcal{A} \rho$ are given by the vectors $x$ and $y$ as in (4).

Measurement-induced geometric discord

Let us assume that bipartite system $\mathcal{A}\mathcal{B}$ is prepared in a state $\rho$. Any local measurement on the subsystem $\mathcal{A}$ will disturb almost all states $\rho$. This observation yields the definition of a measure of quantum discord. The one-sided measurement induced geometric discord is defined as the minimal disturbance induced by any projective measurement $P_\mathcal{A}$ on subsystem $\mathcal{A}$ [17, 18, 19]. A distance in the set of states is given by the trace norm. Namely,

$$
D_1(\rho) = \min_{P_\mathcal{A}} ||\rho - P_\mathcal{A}(\rho)||_1, \quad ||\sigma||_1 = \text{tr} |\sigma|.
$$

(9)

Local projective measurement $P_\mathcal{A}$ is given by the one-dimensional projectors $P_1, P_2, \ldots, P_d$ on $\mathbb{C}^d$, such that

$$
P_1 + P_2 + \cdots + P_d = \mathbb{I}_d, \quad P_j P_k = \delta_{jk} P_k,
$$

$$
P_\mathcal{A} = P \otimes \mathbb{1}.
$$

where

$$
P(\sigma) = P_1 \sigma P_1 + P_2 \sigma P_2 + \cdots + P_d \sigma P_d.
$$
By $P_k^0$ we shall denote canonical projections on standard orthonormal basis in $C^d$ and respective projections on orthogonal complement spaces by $M_0 = \mathbb{1} - P_0$, $M = \mathbb{1} - P$. The disturbance of the state after the measurement $P_A$ can be written as

$$ S(M) \equiv \rho - P_A(\rho) = \frac{1}{d^2} \left[ \sqrt{\frac{d(d-1)}{2}} \langle Mx, \lambda \rangle \otimes \mathbb{1}_d + \sum_k \langle MKe_k, \lambda \rangle \otimes \langle e_k, \lambda \rangle \right] $$

(10)

$$ D_1(\rho) = \frac{d}{2(d-1)} \min_M \sqrt{Q(M)} \quad Q(M) \equiv S(M)S(M)^*, $$

(11)

where minimum is taken over all $M$ corresponding to measurements on subsystem $A$.

**Simplifications**

Even such defined measure of quantum discord, more operational then general one, is still difficult to calculate and some simplifying assumptions are necessary. Let us consider class of locally maximally mixed states $\rho$

$$ \text{tr}_{\bar{A}} \rho = \mathbb{1}_d, \quad \text{tr}_A \rho = \frac{\mathbb{1}_d}{d}. $$

(12)

In the chosen parametrization this corresponds to $x = y = 0$ what results in simplified states of the form

$$ \rho = \frac{1}{d^2} \left( \mathbb{1}_d \otimes \mathbb{1}_d + \sum_{j=1}^{d^2-1} \langle MKe_j, \lambda \rangle \otimes \langle e_j, \lambda \rangle \right) $$

(13)

Note that the set of correlation matrices defining above states is convex and is contained in the ball

$$ B_2 = \left\{ A \in M_{d^2-1}(\mathbb{R}) : \|A\|_2 \leq \frac{d}{2} \sqrt{d^2-1} \right\} $$

(14)

Maximally entangled pure states of this class are defined by correlation matrices lying on the boundary of the ball $B_2$. However, not every matrix lying on the border corresponds to some state. Detailed characterization of the set of correlation matrices is not known.

For the states under consideration the disturbance after measurement has the form

$$ S(M) = \frac{1}{d^2} \sum_{j=1}^{d^2-1} \langle MKe_j, \lambda \rangle \otimes \langle e_j, \lambda \rangle, $$

(15)

and

$$ Q(M) = \frac{1}{d^4} \left[ \frac{4}{d^2} \sum_j \langle MKe_j, MKe_j \rangle \mathbb{1}_d \otimes \mathbb{1}_d + \frac{2}{d^2} \sum_j \langle MKe_j \otimes MKe_j, \lambda \rangle \otimes \mathbb{1}_d ight. 

$$

$$ + \frac{2}{d^2} \sum_{jk} \langle MKe_j \otimes MKe_k, \lambda \rangle \otimes \langle e_j \otimes e_k, \lambda \rangle + \frac{1}{d^2} \sum_{jk} \langle MKe_j \otimes MKe_k, \lambda \rangle \otimes \langle e_j \otimes e_k, \lambda \rangle 

$$

$$ - \frac{1}{d^2} \sum_{jk} \langle MKe_j \otimes MKe_k, \lambda \rangle \otimes \langle e_j \otimes e_k, \lambda \rangle \right] $$

(16)

The spectrum of $Q(M)$ for arbitrary correlation matrix is rather difficult to obtain, but interestingly enough, one can find a universal lower bound for $D_1$ and for analogous quantum discord measure based
on the Hilbert–Schmidt distance $D_2$ [20]. Let $\mathcal{K}$ defines the corresponding locally maximally mixed state $\rho$, then

\[
D_2(\rho) \geq \frac{4}{d^3(d-1)} \Xi(\mathcal{K}) \quad \text{and} \quad D_1(\rho) \geq \frac{1}{d(d-1)} \sqrt{\Xi(\mathcal{K})}, \quad \text{where} \quad \Xi(\mathcal{K}) = \sum_{j=d}^{d^2-1} \eta_j^j.
\]

By the $\{\eta_j^j\}$ we denote the collection of eigenvalues of $\mathcal{K} \mathcal{K}^T$ taken in non-increasing order. Let us observe that states related to correlation matrices with rank $\mathcal{K} \geq d$ have non-zero quantum discord.

However, to get more specific information one has to admit further restrictions on the form of the correlation matrices. For $\mathcal{K} = t V_0$, and $V_0 \in O(d^2 - 1)$ one can prove that [20]

\[
Q(\mathcal{M}) = \frac{t^2}{d^4} \left[ \frac{4(d-1)}{d} \mathbb{1}_d \otimes \mathbb{1}_d + \frac{2}{d} \mathbb{1}_d \otimes \sum_k X_k \lambda_k + \sum_{j,k} Y_{jk} \lambda_j \otimes \lambda_k \right]
\]

where

\[
X_k = \text{tr} (\mathcal{M} V_0 \Delta_k V_0^T), \quad Y_{jk} = \text{tr} (V_0^T \mathcal{M} \Delta_j \mathcal{M} V_0 \Delta_k + V_0^T \mathcal{M} F_j \mathcal{M} V_0 F_k)
\]

and $(\Delta_k)_i = d_{ijkl}, (F_k)_i = f_{ijkl}$. Let us observe that terms involving $Y_{jk}$ are related to $\ast$ and $\wedge$ products in $\mathbb{R}^{(d^2 - 1)}$.

Above form of the $Q(\mathcal{M})$ can be starting point to obtain analytical expression for trace-norm quantum discord. The additional conditions on the correlation matrices one has to impose come from the case study of the system of two qutrits [19, 20]. Final answer valid for two-qudit systems can be formulated as follows: there two families of correlation matrices defining states for which analytical formula for MIQGD can be obtained. They are given by correlation matrices of the form

\[
\mathcal{K}^a = t V, \quad V \in R(SU(d))
\]

and

\[
\mathcal{K}^{aa} = t \mathcal{T}, \quad \mathcal{T} = V_1 I_0 V_2^T, \quad V_1, V_2 \in R(SU(d)),
\]

where

\[
(I_0)_{kk} = \frac{1}{2} \text{tr}(\lambda_k^T \lambda_k), \quad k = 1, \ldots, d^2 - 1
\]

For the first family we obtain

\[
Q^a(\mathcal{M}) = \frac{t^2}{d^4} \left[ \left( \frac{2}{d} \right)^2 d(d-1) \mathbb{1}_d \otimes \mathbb{1}_d - 2 \sum_{k=2}^d U \lambda_{k^2-1} U^\ast \otimes \tau_V(U) \tau_F(\lambda_{k^2-1}) \tau_V(U^\ast) \right]
\]

and for the second one

\[
Q^{aa}(\mathcal{M}) = \frac{t^2}{d^4} \left[ \left( \frac{2}{d} \right)^2 d(d-1) \mathbb{1}_d \otimes \mathbb{1}_d + 2 \left( (d-2) \sum_k \lambda_k \otimes \tau_F(\lambda_k) \right. \right.
\]

\[
+ \left. \sum_{k=2}^d U \lambda_{k^2-1} U^\ast \otimes \tau_F(U^\ast) \tau_F(\lambda_{k^2-1}) \tau_F(\lambda_{k^2-1}) \tau_F(U) \right]
\]

where $\tau_V$ and $\tau_F$ are Jordan automorphisms and antiautomorphism of the $M_d(\mathbb{C})$ (for details cf. Ref. [20]).

For above classes of states one gets explicit formulas:

(i) for $\rho \in \mathcal{E}^a$

\[
D_1(\rho) = \lvert t \rvert, \quad -\frac{d}{2(d-1)} \leq t \leq \frac{d}{2(d+1)}
\]
(ii) for $\rho \in \mathcal{E}^{aa}$

$$D_1(\rho) = \frac{2}{d} |t|, \quad -\frac{d}{2(d^2-1)} \leq t \leq \frac{d}{2}$$

(24)

It is interesting to compare above families to the two known distinguished classes of states: Werner states and isotropic states. Condition defining Werner states is

$$\rho = U \otimes U \rho U^* \otimes U^*, \quad U \in SU(d)$$

(25)

In turns out that these states fall into the class $\mathcal{E}^a$ and property (4) means that

$$Q^a(\mathcal{M}) = U \otimes U Q^a(\mathcal{M}_0) U^* \otimes U^T.$$

Condition defining the so called isotropic states is

$$\rho = U \otimes U \rho U^* \otimes U^T, \quad U \in SU(d)$$

(26)

These states fall into the class $\mathcal{E}^{aa}$ and for them

$$Q^{aa}(\mathcal{M}) = U \otimes U Q^{aa}(\mathcal{M}_0) U^* \otimes U^T.$$

Hence, in both cases a minimization procedure is not needed.

**Conclusions**

In our work we have presented some aspects of the complex problem of finding values of quantum correlation measures. As an illustration we have discussed the measurement-induced one sided quantum geometric discord based on the trace distance. While, on the one hand we enlist and comment types of difficulties arising for the higher $d$-level systems and stress the step change between $d = 2$ and $d \geq 3$ systems, on the other hand we show that there are important instances, where one can effectively avoid troublesome minimization procedure and obtain strict results for the MIQGD.

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