Creating ensembles of dual unitary and maximally entangling quantum evolutions

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Maximally entangled bipartite unitary operators or gates find various applications from quantum information to being building blocks of minimal models of many-body quantum chaos, and have been referred to as 1-unitalies and dual unitaries. Such dual operators that can create the maximum entanglement on the average when acting on product states have to satisfy additional constraints. These are referred to as 2-unitalies and are examples of perfect tensors that can be used to construct absolutely maximally entangled states. Hitherto no systematic methods exist, in all local dimensions, which result in the formation of such special classes of unitary operators. We outline an iterative protocol, a map on the space of unitary operators, that creates ensembles that are arbitrarily close to being dual unitaries, while for qutrits and ququads we find that a slightly modified protocol yields a plethora of 2-unitalies.

Entanglement, the quintessential quantum property that the whole is in a definite state but the parts are not, has been appreciated since almost the inception of quantum mechanics [11, 12], but much more so in the ongoing extensive studies of quantum information, wherein it has acquired the status of a resource [3]. Operators, as quantum gates, observables or time-evolution propagators are also central to quantum mechanics and unentangled states are often entangled due to action of entangling unitary operators in the circuit paradigm of quantum computing [4]. Thus how entangled unitary operators themselves are (measured by entanglement power) [6], and how much entanglement they can produce acting on unentangled states (measured by entangling power) [6] are of primary interest. They have also started forming a means to characterize complexity in many-body systems [7, 9], and earlier applications include quantum transport in light-harvesting complexes [10] and characterization of quantum chaos [11, 12]. They form a state-independent characterization of entanglement growth with time, including approach to thermalization [13, 14]. Other studies of operator nonlocality as a resource include [15, 18], while the studies in [19, 20] characterize of unitary gates and their powers in the case of qubits.

The existence of two-party operators with maximal entanglement properties imply the existence of absolutely maximally entangled states (AME) [21, 22] of four parties, wherein all bipartite cuts are maximally entangled. These are 2-unitalies or “perfect tensors” of rank-4 which are ingredients of holographic quantum states and codes [23]. Further motivation comes from recent observations concerning lattice models wherein a space-time duality allows for some analytical results, even for nonintegrable systems [24, 25]. More explicitly, using a “dual unitary” [25], as nearest neighbor interactions in many-body systems leads to solvable correlation functions. It is not hard to see that these dual unitary operators are in fact equivalent to maximally entangled ones [28, 29], and it also follows that using 2-unitalies, or equivalently maximally entangling operators, as building blocks gives rise to maximally chaotic, but solvable many-body systems.

Maximally entangled bipartite states such as the prototypical Bell states of two qubits, and its generalization to any dimension: \( \sum_{i=1}^{d} |i_A i_B \rangle / \sqrt{d} \) (where \( |i_A, i_B \rangle \) form a complete orthonormal basis in each of the particle spaces) is straightforward to construct and characterize. On the contrary, while it is easy to state conditions under which an operator may have maximal operator entanglement or entangling power, it seems surprisingly difficult to construct their Bell state equivalents, let alone to characterize and parameterize them [22]. One exception is the class of permutation matrices based on orthogonal Latin squares which provide a discrete set of maximally entangling unitary operators for any local dimension other than 2 and 6 [30].

In this Letter we outline a protocol that given non-maximally entangled unitary operators, including unentangled ones, a systematic and largely monotonic increase of the operator entanglement is achieved iteratively, leading to operators that are arbitrarily close to being maximally entangled or dual unitary operators. A subset of these could also be maximally entangling or perfect tensors, but we outline an alternative strategy that while not monotonic, leads to near perfect tensors. In particular for the case of local dimension \( d = 3 \) (qutrits) and to some extent \( d = 4 \) we show that the procedure leads to a large measure of perfect tensors, or equivalently AME states. It maybe noted that for \( d = 2 \), the qubit case, such AME states do not exist [5, 31]. Starting from random unitary matrices selected uniformly from the group \( U(d^2) \), the circular unitary ensemble or CUE of random matrix theory (RMT), these protocols produces an ensemble of dual unitaries for all local dimensions and an ensemble of perfect tensors for
Definitions and preliminaries: Consider the bipartite Hilbert space $\mathcal{H}_{AB}^d = \mathcal{H}_A^d \otimes \mathcal{H}_B^d$ and let $U(d^2)$ be the set of unitary operators in it. If $U \in U(d^2)$, its operator Schmidt decomposition is given by $U = \sum_{j=1}^{d^2} \sqrt{\lambda_j} m_j^A \otimes m_j^B$, where $m_j^A, m_j^B$ form local orthonormal operator bases under the Hilbert-Schmidt inner product \[ \| \cdot \|_{HS} \], that is $\langle m_{jk}^{A,B} | m_{pq}^{A,B} \rangle = \delta_{jk}$. The unitarity of $U$ implies that $\sum_{j=1}^{d^2} \lambda_j / d^2 = 1$, hence defining $p_j = \lambda_j / d^2$, the Tsallis-entropies

$$S_q(U) = \frac{1 - \sum_{j} p_j^q}{q - 1}$$

are measures of operator entanglement. In particular the case of $q = 2$ is the linear entropy $E(U) = 1 - \sum_{j} \lambda_j^2 / d^2$, referred simply as the operator entanglement is extensively used below, although the case of $q = 1/2$ will turn out to be important as well. The entropy $S_q(U) = 0$ iff the operator is of product form, when $\lambda_1 = d^2$ and the rest vanish, while the maximum possible value (for the case of $S_2(U) = E(U)$ it is $E(U)_{\text{max}} = 1 - 1/d^2$), is obtained when all $\lambda_i = 1$. However, to construct such maximally entangled (or simply dual) unitary operators the constraints required of the $2d^2$ operators $m_j^{A,B}$ are difficult to satisfy. Hence while there are known operators such as swap, and the Fourier transform in arbitrary dimensions that are dual operators, systematic constructions, with the exception of qubits, are lacking.

If $\langle nm | U^R | \alpha \beta \rangle = \langle na | U | mb \rangle$ is the realignment or reshaping, it is easy to see that $(X \otimes Y)^R = |X\rangle \langle X^*|$ \( |Y\rangle \langle Y^*| \), where $|X\rangle$ is the row-vectorization of the matrix $X$ and $*^\dagger$ is the complex conjugation. It then follows from the Schmidt decomposition of $U$ that $U^R = \sum_{j=1}^{d^2} \sqrt{\lambda_j} |m_j^A\rangle \langle m_j^B|^\dagger$, the spectral decomposition of $U^R U^R = \sum_{j=1}^{d^2} \lambda_j |m_j^A\rangle \langle m_j^B|^\dagger \otimes |m_j^B\rangle \langle m_j^A|$, and $E(U) = 1 - \text{tr} \left( (U^R U^R)^R / \lambda_1 \right) / d^4$. Hence iff $U^R$ is also unitary are all the eigenvalues $\lambda_j = 1$ and $U$ is dual unitary or maximally entangled. This somewhat abstract definition of operator entanglement has a well-known operational meaning via how much entanglement it can engender acting on product states, which is recalled further below, but we turn to the main task of constructing such unitaries.

The realignment-nearest-unitary map and its iteration: Two stages define the map $M: U(d^2) \mapsto U(d^2)$, first is the linear one $U \mapsto U^R$, and the second is the nonlinear one that maps $U^R \mapsto V$, where $V$ is the nearest unitary operator to $U^R$, which is simply given by the polar decomposition $U^R = VH$, where $H = \sqrt{U^R \dagger U^R}$ is a positive matrix. Given any unitary $U_0$, we find $U_n = M_n(U_0)$. It seems plausible that $U_n$ tends to become dual unitary, in particular that, the Tsallis entropy with $q = 2$, $E(U_n)$ increases with $n$ and ideally towards the maximum possible value of $E(S) = 1 - 1/d^2$. While we found overwhelming numerical evidence for this, we found a few exceptions for $d = 3$ alone when $U_0$ is restricted to the subgroup of orthogonal matrices. This is borne out, as shown in Fig. 1, where we start from typical representatives from the CUE and the increase is not only monotonic but remarkably it is asymptotic to the maximum possible value of $E(U)$, thus getting arbitrarily close to dual ones. For qubits, $d = 2$, the approach appears to be exponential, while for qutrits, $d = 3$, the convergence of $E(U)$ to the maximum value of $8/9$ could be exponentially fast or a much slow power law depending on the initial $U_0$, as shown in Fig. 2. The approach for $d > 4$ seems to be a power law on the average, with $\Delta_n = E(U)_{\text{max}} - E(U_n)$ the deviation from the maximum, vanishing as $\approx n^{-1.3}$.

From extensive numerical evidence, we conjecture that under the $M_R$ map, almost all unitaries sampled according to the CUE monotonically tend arbitrarily close to being dual. Additionally, we are able to prove the following:

**Theorem 1.** For any $d$, the $q = 1/2$ Tsallis entropy
of operator entanglement $S_{1/2}(U_n) = 2(d \operatorname{tr} \sqrt{U_n^{R} U_n^{R*}} - 1)$ and the corresponding extensive Rényi entropy $2 \log \left( \frac{\operatorname{tr} \sqrt{U_n^{R} U_n^{R*}}}{d} \right)$ are non-decreasing under the $M_R$ map: $S_{1/2}(U_{n+1}) \geq S_{1/2}(U_n)$.

Proof. This is a consequence of the following lemma.

**Lemma 1.** For any $d$, the trace-norm $\|U_R^R\|_1 = \operatorname{tr} \sqrt{U_R^R U_R^{R*}}$ is non-decreasing under the $M_R$ map: $\|U_{n+1}^R\|_1 \geq \|U_n^R\|_1$.

Proof. Let

$$D_n^2 = \min_{W \in U(d^2)} \|U_n^R - W\|^2_F = \|U_n^R - U_{n+1}^R\|^2_F$$

as $U_{n+1}$ is the nearest unitary to $U_n^R$ under any unitarily invariant norm. Here $\|X\|_F = \sqrt{\operatorname{tr}(X^* X)}$ is the Frobenius norm. From the observations that (i) the realignment is involutive, that is $(X^R)^R = X$, and (ii) the Frobenius norm is invariant $\|X^R\|_F = \|X\|_F = \sqrt{\sum_{ij} \left| X_{ij} \right|^2}$ under realignment as it is simply a permutation of the matrix elements, it follows that

$$D_{n+1}^2 = \min_{V \in U(d^2)} \|U_n^R - V\|^2_F,$$

hence using the Eq. (1), it follows that $D_{n+1}^2 \leq D_n^2$. From Eq. (2) we get

$$D_n^2 = 2d^2 - 2 \operatorname{Re} \operatorname{tr} \left( U_n^R U_n^R \right) = 2d^2 - 2 \operatorname{tr} \left( \sqrt{U_n^R U_n^R} \right).$$

Hence the trace-norm of $U_n^R$ is a non-decreasing function of $n$.

Numerical evidence also points to the increase of any of the Tsallis entropies, indicating that a majorization of the kind $U_{n+1}^R U_{n+1}^R < U_n^R U_n^R$ generically holds.

**Characterization of dual unitaries and the entangling power.** An important characterization of the dual unitaries created by the other invariant $E(U S) = \frac{1}{d} S_n^R$ for any $d$, where $S$ is the swap operator, or equivalently its entangling power. The connection of the operator entanglements of $U$ and $US$ introduced above to state entanglement in the bipartite space is via the entangling power, which is defined as the average linear entropy produced while operating on product states. Let $\langle \psi_{AB} \rangle = U|\psi_A\rangle|\psi_B\rangle$, and $\rho_A = \operatorname{tr}_B(|\psi_{AB}\rangle\langle \psi_{AB} |)$, then $e_p(U) = \langle (1 - \operatorname{tr}_A(\rho_A^2) \rangle$, where the $\langle \rangle$ brackets indicate averaging with respect to an ensemble of single particle states $|\psi_{AB}\rangle$. In particular if these are chosen from the Haar measure, the $e_p(U) = d^2 E(U) + E(US) - E(S)/\langle d+1 \rangle^2$.

Note that for dual or unitaries, $e_p(U)$ is simply proportional to $E(U S)$, thus the entangling power is the main characterizer of this set. The maximum possible entangling power admitted by the dimensionality of the spaces is $e_p^{\text{max}} = (d - 1)/(d + 1)$, and is achieved by $2$-unitary matrices, which do not exist for $d = 2$ while examples are known to exist in all other dimensions except $d = 6$ in the form of certain special permutations $[30]$. While there are no systematic methods to create ensembles of such unitaries, the procedure outlined below produces an abundance of these, in $d = 3$ and to some extent for $d = 4$.

We construct an ensemble of unitary matrices starting from the CUE and iterating them under the $M_R$ map. Symbolically this ensemble is $M_R^n(\text{CUE})$, which we will refer to simply as “dual-CUE”, although in practice of course we will iterate a finite number of times to find intermediate ensembles. Figure insets show the distribution of $E(U_n)$ for some appropriate choice of $n$ for the dual-CUE and for comparison the distribution of $E(U)$ for the CUE is also shown. The dual-CUE’s entanglement seems to be tending to a Dirac delta function at the maximum value of $E(S) = 1 - 1/d^2$ justifying the adjective, and this happens at smaller number of iterations $n$ for smaller $d$.

In the main part of the figure is shown the distribution of the entangling power for the CUE and the dual-CUE, this also being essentially the distribution of $E(U S)$ for the latter ensemble and there are several notable features. For small dimensions, the entangling power of the dual-CUE is broader and the mean of the entangling power is actually less than that of the CUE. For $d = 2$, there is a divergence of the distribution corresponding to the dual-CUE around the maximum entangling power of $2/9$ (less than $1/3$.
allowed by the dimensions and same as that of the cnot and dcnor gates). In the case of qubits, the Cartan or canonical nonlocal form of two-qubit gates is $\exp(-ic_1\sigma_x\otimes\sigma_x - ic_2\sigma_y\otimes\sigma_y - ic_3\sigma_z\otimes\sigma_z)$ [14]. It is possible to derive a map of the parameter $c_i$ induced by the $M_R$ map [56], and we see that indeed there is a fast convergence of these to $c_1 = c_2 = \pi/4$ and to a value of $c_3$ that depends on the initial unitary. Recent characterizations of 1-unitaries or dual operators for qubits indeed have pointed out such an one-parameter family of Cartan forms [14] [25]. Thus while the full unitary operator may not converge under the map, the nonlocal part of it does.

For the case of qutrits, the dual-CUE distribution is split and there is a peak at the largest possible value of 1/2. In these cases, remarkably, the map $M_R$ has driven random CUE realizations into perfect tensors or 2-unitaries which maximize not just $E(U)$ but also $E(US)$ and hence the entangling power. Approximately about 6% of the CUE end up being of this kind. For the case of $d = 4$, there is still a bimodal distribution, but the peak has shifted away from the maximum possible value of 3/5, while for $d > 4$, the distribution is not bimodal but also the dual-CUE distribution is more entangling than the CUE and the average entangling power is larger now for the dual-CUE.

One may try to maximize $E(US)$ instead of $E(U)$ and this involves replacing realignment with partial transpose as $E(US) = 1 - \text{tr}[(U^T A U^T A)^2]/d^4$. In place of the $M_R$ map, there is now a partial transpose based one denoted $M_T$ that acts within the space $U(d^2)$, the index with respect to which the partial transpose is taken being suppressed. Iteration under this map typically result in operators that maximize $E(US)$, or equivalently $US$ are dual operators. We do not know if there exists a (dream) map that result in 2-unitaries or perfect tensors maximizing the entangling power which is a sum of $E(U)$ and $E(US)$. However, we found that the iteration of the composition $M_{TR}$ wherein $R$ map is followed by the $T$ before finding the nearest unitary, often results in such operators for low dimension and especially for $d = 3$ and $d = 4$.

This is shown in Fig. 4 where we see that while for $d = 2$, the map produces a broad distribution of entangling powers as there are no 2-unitaries in this case, for $d = 3$ we see a large peak at the maximum value of 1/2. Remarkably, more than 95% of the CUE seeded matrices end up being 2-unitaries, this may be contrasted with just the $M_R$ map, see Fig. 3 which led to about 6%. The remaining ones increase the entangling power but asymptote to lower values, as we also see for the case of $d = 4$, where we have a complex set of prominent values. But unlike just the $M_R$ map which did not produce any 2-unitaries, about 20% of those iterated with the $M_{TR}$ map end up being for all practical purposes, 2-unitaries. For $d = 5$, there is only one peak...
seen, but unlike $d = 3, 4$ these do not seem to get arbitrarily close to $2$-unitaries, and instead asymptote to about 98.9% of the maximum allowed value. This leads to the disappointment that this map does not shed any light on the open question of if $2$-unitaries exist in $d = 6$.

As far as the usual RMT properties are concerned, the CUE is indistinguishable from that of the dual-CUE or even the ensemble of $2$-unitaries. We have checked numerically that the next neighbor gap distribution and the form factor are identical for these ensembles. The only way these map driven ensembles are different seem to be their nonlocal properties and their entangling abilities.

**Summary and open problems:** In summary we have introduced maps in the space of bipartite unitary operators whose fixed points are attracting and have generically maximal entangling properties. These produce, starting from the CUE, an ensemble of dual unitaries for any local dimensions and an ensemble of perfect tensors for local dimension 3 and 4, in turn producing a large class of four partite AME states of qutrits and ququads. Many open questions concerning the attractors and basins of attractions of these maps, which are novel dynamical systems in their own right, remain open, including the conjecture of majorization which we found to hold numerically for any dimension except for some orthogonal matrices when $d = 3$.

The statistics of entanglement and nonlocal correlations produced by an ensemble of dual unitaries and perfect tensors acting on product states are of natural interest and will serve to further characterize these sets. Many-body systems built out of such special bi-partite unitaries could further reveal relations between entanglement, complexity and the nature of dynamical evolution. Other open problems include the extension of the current studies to multipartite systems [35], to powers of such special unitaries, and to finding perfect tensors in higher dimensions. The production of large class of four partite AME states of qutrits and ququads helps to improve quantum communication for multi-partite systems.

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