NOTES ON ENTANGLEMENT POLYTOPES FROM A MATHEMATICAL PERSPECTIVE

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Throughout the history of mathematics and physics, these two disciplines have profoundly enriched each other's developments. For instance, symplectic geometry is a geometric framework that was motivated by Hamiltonian mechanics in classical physics; representation theory, the mathematical study of symmetries, is highly relevant for the study of quantum physics and beyond. In this note, we explain an interesting application of symplectic geometry, representation theory, and some closely related combinatorics to the study of quantum entanglement.

Entanglement [4] is a fundamental phenomenon in quantum mechanics, with important applications to quantum information, quantum commucation and quantum computing. Multi-particle entanglement is difficult to understand and quantify. In the paper "Entanglement Polytopes: Multiparticle Entanglement from Single-Particle Information" by Walter, Doran, Grass and Christandl published in the journal "Science" [1], the authors present an interesting story of applying geometry, representation theory and combinatorics to study entanglement classes among pure states as defined by SLOCC(Stochastic local operations and classical communication) operations [9]. More specifically, each SLOCC entanglement class in the space of pure states is associated with a very concrete convex polytope, which is easy to study in practice and relatively robust against experimental noise.

1. Quantum Entanglement

Quantum mechanics, the physics governing nature at very small(atomic and subatomic) scales, is known for being highly counter-intuitive. However, its mathematical formulation is relatively straightforward.

The quantum states for N particles live in the Hilbert space $\mathcal{H} = \mathbb{C}^{d_1} \otimes \cdots \otimes \mathbb{C}^{d_N}$, and they may be pure or mixed. Each state can be represented by a unique density matrix ρ, which is a Hermitian matrix with nonnegative eigenvalues and trace one. The eigenvectors and eigenvalues of a density matrix represent the possible states in a mixed state and their associated probabilities. In particular, the density matrix of a pure state is just a projector to the one-dimensional vector space generated by the state. Note that even if a state is pure globally, it can still be mixed locally. The local density matrices can be obtained from the global ones by taking partial trace [3, 10].

The space of pure states is isomorphic to the projective space $\mathbb{P}(\mathcal{H})$. There are two kinds of pure states: the separable states, which can be written as tensor products of vectors in individual local Hilbert spaces, and the entangled states, which cannot be. Unlike the separable states, the probabilities of measurements on individual particles in an entangled state are correlated. In the case of two particles with $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$, the space of pure states is isomorphic to $\mathbb{P}^3$ and the space of separable states $\mathbb{P}^1 \times \mathbb{P}^1$ embeds in $\mathbb{P}^3$ via the Segre embedding. On the other hand, the famous Bell basis give an example of four maximally entangled states in this case.

Distinct pure states are entangled to "different" extents, and there are multiple ways of measuring such differences. For SLOCC, consider the action of the group $G = SL_{d_1}(\mathbb{C}) \times \cdots SL_{d_N}(\mathbb{C})$, which acts on the Hilbert space by acting on individual particles locally. More explicitly, given a matrix M in an $N-$tuple of matrices in G and a local density matrix ρ, the action of M on ρ is given by $M \cdot \rho \cdot M^\dagger$(normalized such that the trace is one), where $M^\dagger$ is the standard notation for the conjugate transpose of M in quantum mechanics. By definition, the SLOCC entanglement class containing a particular pure state or its corresponding density matrix is its G orbit in $\mathbb{P}(\mathcal{H})$.

2. Symplectic Geometry and Classical Mechanics

To understand how SLOCC entanglement classes can be linked to convex polytopes via local symmetries, let's first take a step back to recall some classical mechanics, whose natural mathematical framework is symplectic geometry. Symplectic manifolds are generalizations of the phase spaces of a close classical system. Given a classical system (M, ω) with the Hamiltonian function $H : M \to \mathbb{R}$, the symplectic form is a pairing between the Hamiltonian vector field, which is derived from the Hamiltonian equations of the system, and the differential $\mathrm{d}H$ [12, 13, 14, 15].

Noether's theorem states that every differentiable symmetry of the action of a physical system has a corresponding conservation law. Consider a symplectic manifold (M, ω) with a Lie group G action that's reasonably nice (more specifically, both symplectic and Hamiltonian). Each element X of the Lie algebra $\mathfrak{g}$ generates a vector field X_M on M. Then the moment map $\mu : M \to \mathfrak{g}^*$ is $G-$equivariant and gives the Hamiltonian function for each vector field X_M generated by a given element X of the Lie algebra $\mathfrak{g}$, by pairing with X. Correspondingly, there is a co-moment map $\gamma : \mathfrak{g} \to C^\infty(M)$ which links the Lie bracket in the Lie algebra $\mathfrak{g}$ and the Poisson bracket in the algebra of smooth functions on the symplectic manifold M. Roughly speaking, this gives a way of systematically computing the result of Noether's theorem on symmetry and conservation laws.

3. Representation Theory and Geometric Quantization

There are mathematical constructions which allow to go back and forth between the classical and quantum settings. Given a classical system, we can quantize it, and given a quantum system, we can take its classical limit. When we start with a symplectic manifold equipped with other structures, we can quantize it via a framework called geometric quantization [5, 6, 7].

To discuss geometric quantization more precisely, we need to briefly introduce the notion of a Khähler manifold. It is a smooth manifold with a compatible trio of structures: a symplectic form ω, a complex structure J, and a Riemannian metric g. Any two of these three structures are enough to determine the third. There are many examples of Khähler manifolds, like complex vector spaces and projective spaces.

To construct Hilbert spaces out of a Khähler manifold M, we introduce L, a complex line bundle on M which is equipped with the following structures: (1) a connection with curvature $i\omega$; this comes from the symplectic structure on M, and is necessary for turning smooth functions on M, the classical observables, into operators on the space of sections of L, the quantum observables; (2) the structure of a holomorphic line bundle; this comes from the complex structure on M, and gives the underlying space for our Hilbert space: the space of holomorphic sections of L; (3) the structure of a Hermitian line bundle; this way we can put an inner product on the space of holomorphic sections of L and actually get a Hilbert space.

Now let's see some interesting examples of geometric quantizations that are relevant for our study of entanglement polytopes.

1. Given a complex Hilbert space $\mathcal{H}$, its classical limit is the corresponding projective space $\mathbb{P}(\mathcal{H})$, which has a canonical Khähler structure. In particular, there is a natural symplectic structure on $\mathbb{P}(\mathcal{H})$ called the Fubini-Study form. The geometric quantization of $\mathbb{P}(\mathcal{H})$ gives us back $\mathcal{H}$. A simple instance of $\mathcal{H}$ is $\mathbb{C}^2$, with the standard inner product. Then its classical limit is $\mathbb{CP}^1$, which is diffeomorphic to S^2 as a real smooth manifold. It has the standard complex structure, a Fubini-Study form as the symplectic form, which is a constant times the area form on S^2, and a Riemannian metric whose geodesics are the great circles on a two sphere.

2. Let G be a complex reductive group, with a Borel subgroup B. Then the flag variety G/B admits some $G-$invariant Khähler structures. By the Borel-Weil Theorem, every finite dimensional irreducible representation of G is isomorphic to the space of holomorphic sections of a unique $G-$equivariant line bundle on the flag variety. When $G = SL_2(\mathbb{C})$, its flag variety is isomorphic to $\mathbb{P}^1$. The $G-$equivariant holomorphic line bundles of $\mathbb{P}^1$ are classified by integers. Given any finite dimensional irreducible representation V of $SL_2(\mathbb{C})$, which is classified by its dimension v, V is isomorphic to the space of holomorphic sections of the line bundle of $\mathbb{P}^1$ that's also labeled by v.

3. Consider the Lie algebra $\mathfrak{g}$, which admits the standard adjoint G action, and the dual of the Lie algebra $\mathfrak{g}^*$, which admit a G action called the coadjoint action that is induced from the adjoint action. Each coadjoint orbit has a canonical symplectic structure, and intersects the positive Weyl chamber in exactly one point p. If this point is an integral highest weight λ, then there exists a map $\mu : T \to S^1$ such that λ equals the derivative of μ. Consider the $G-$equivariant line bundle on the coadjoint orbit containing λ given by $G \times_\mu \mathbb{C}$, where G acts by μ. Then the space of holomorphic sections of this line bundle gives rise to the irreducible $G-$ representation labeled by λ. This is a consequence of Borel-Weil Theorem. If the point p is not integral, then there is simply no such line bundle, since the weight won't integrate to the torus. This corresponds to the fact that there is no finite dimensional irreducible representation of that weight [2].

4. Entanglement Polytopes

After the discussion of general mathematical notions like symplectic geometry, moment maps and geometric quantization, let's get back to our quantum states. Since SLOCC allows local operations and classical communications, we may explore some classical physics and symplectic geometry related to individual particles. Let's consider the classical limit of our Hilbert space $\mathcal{H}$, $\mathbb{P}(\mathcal{H})$, which is isomorphic to the space of pure states in $\mathcal{H}$.

Given the Lie group $G = SL_{d_1}(\mathbb{C})\times\cdots SL_{d_N}(\mathbb{C})$, which acts our Hilbert space $\mathcal{H} = \mathbb{C}^{d_1}\otimes\cdots\otimes\mathbb{C}^{d_N}$, consider its compact subgroup $K = SU_{d_1}(\mathbb{C}) \times \cdots SU_{d_N}(\mathbb{C})$. With the induced action of K on the "classical system" $\mathbb{P}(\mathcal{H})$, it's natural to seek the "conserved quantities" corresponding to the $K-$symmetry under Nother's theorem. So we compute the $K-$equivariant moment map $\Phi : \mathbb{P}(\mathcal{H}) \to \mathfrak{k}^*$, where $\mathfrak{k}^*$ is the dual of the Lie algebra. Note that $\mathfrak{k}^* = \mathfrak{su}_{d_1}(\mathbb{C}) \times \cdots \mathfrak{su}_{d_N}(\mathbb{C})$, where for each $i \in \{1, ..., N\}$, $\mathfrak{su}_{d_i}(\mathbb{C})$ is isomorphic to the group of $d_i \times d_i$ complex Hermitian matrices with trace one. Given a density matrix ρ, let $\rho^{(i)}, i \in \{1, ..., N\}$, denote the corresponding local density matrix for the $i-$th particle, which is obtained from ρ by taking partial trace. It turns out that $\Phi(\rho) = (\rho^{(1)}, ..., \rho^{(N)})$.

Due to the $K-$equivariance of the moment map, $K-$orbits in $\mathbb{P}(\mathcal{H})$ are mapped to the coajoint orbits $\mathfrak{k}^*$. Since the coadjoint action by unitary matrices is equivalent to a change of basis, every element of a coadjoint orbit is labeled by eigenvalues, i.e. $\mathfrak{k}^*/K \cong \mathfrak{t}^*/W$. In particular, every coadjoint orbit intersects the positive Weyl chamber at exactly one point. With our group K, the positive Weyl chamber is the $N-$tuple of diagonal matrices with trace one and weakly decreasing entries, which we denote as $D_\downarrow$.

On the other hand, the SLOCC entanglement classes, i.e. the $G-$orbits, are much bigger than the $K-$orbits in general, so the images of the entanglement classes under the moment map Φ may contain a wider range of eigenvalues. In fact, given an entanglement class $\mathcal{C}$, its entanglement polytope $\Delta_\mathcal{C}$ is defined to be $\Delta_\mathcal{C} = \Phi(\bar{\mathcal{C}}) \cap D_\downarrow$. Moreover, closure relations between entanglement classes are preserved by their corresponding entanglement polytopes.

Note that entanglement polytopes are quite different from the torus equivariant moment polytopes. For instance, when $n = 2$ and $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$, consider the space of separable pure states $\mathbb{P}^1 \times \mathbb{P}^1$. Its entanglement polytope is just a point, but its $T \times T \to SL_2(\mathbb{C}) \times SL_2(\mathbb{C})$-equivariant moment polytope is a square in $\mathbb{R}^2$, with its four vertices being the distinct torus equivariant moment map images of the four $T-$fixed points.

Since the size of the density matrices grow exponentially with the number of particles, it may not always be easy to compute the local density matrices and their spectra. In the entanglement polytopes paper, the authors suggest easier computation methods in Theorem 1 and 2 (Supplementary Text) by making connections to invariant theory [16]. The main mathematical notion used is called "covariants" in the paper, and the definition there contains a small error. Below we present two equivalent and rigorous definitions of covariants.

Recall that the finite-dimensional polynomial irreducible representations of the group $GL_d(\mathbb{C})$ are labeled by highest weights. All the finite-dimensional irreducible representations of $SL_d(\mathbb{C})$ and $SU_d(\mathbb{C})$ are the same, and can be obtained from the polynomial representations of $GL_d(\mathbb{C})$ by restrictions to $SL_d(\mathbb{C})/SU_d(\mathbb{C})$, and are generated by homogeneous polynomials. Then a covariant is an $N-$tuple of homogeneous polynomials which is also an element of a tensor product of irreducible representations $V^{d_1}_{\mu^{(\vec{1})}} \otimes \cdots V^{d_N}_{\mu^{(\vec{N})}}$. Equivalently, by Definition 3.6 and 4.1 of [11], a covariant of degree n is a section of the line bundle $\mathcal{O}(n)$ on $\mathbb{P}(\mathcal{H})$. Note that irreducible representations of G show up in the previous definition because G acts naturally on $\mathbb{P}(\mathcal{H})$ and its coordinate ring.

Finally, examples! First consider two particles. By directly computing the range of possible eigenvalues, I conclude that the entanglement polytope for the maximally entangled Bell basis elements is isomorphic to the square $[0,1]\times[0,1]$. The polytope for all the separable states is just the point $(1,1)$. These two polytopes are all the possible entanglement polytopes in this case, as $G = SL_2(\mathbb{C}) \times SL_2(\mathbb{C}) \cong SO_4(\mathbb{C})$, which only has two orbits on $\mathbb{CP}^3$, one with zero linear inner product, and the other with nonzero inner product. As for three or four particles, see section 5 of the Supplementary text of the paper. The authors used Theorem 2 by collecting some non-vanishing generating covariants as well as their normalized highest weights, and took convex hull. It is likely that the authors used computers to accomplish this invariant theoretic computation.

5. Remarks

By passing a quantum system to its geometric classical limit, the authors of the entanglement polytopes paper [1] discovered a small set of combinatorial objects which shed light on infinitely many really complicated entanglement classes. Hope there will be more applications of geometric quantization to quantum technologies in the future.

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