Observing Geometry of Quantum States in a Three-Level System

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In quantum mechanics, geometry has been demonstrated as a useful tool for inferring nonclassical behaviors and exotic properties of quantum systems. One standard approach to illustrate the geometry of quantum systems is to project the quantum state space onto the Euclidean space via measurements of observables on the system. Despite the great success of this method in studying two-level quantum systems (qubits) with the celebrated Bloch sphere representation, it is still difficult to reveal the geometry of multidimensional quantum systems. Here we report the first experiment measuring the geometry of such projections beyond the qubit. Specifically, we observe the joint numerical ranges of a triple of observables in a three-level photonic system, providing a complete classification of these ranges. We further show that the geometry of different classes reveals ground-state degeneracies of a Hamiltonian as a linear combination of the observables, which is related to quantum phases in the thermodynamic limit. Our results offer a versatile geometric approach for exploring the properties of higher-dimensional quantum systems.

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Arising from Euclid’s first attempt to establish its axiomatic form, geometry has become an essential method for understanding the physical world, especially in the field of quantum physics [1–4]. One exemplary use of geometric method was the creation of statistical mechanics in the 1870s, when Gibbs introduced a geometric means to infer thermodynamic properties (e.g., energy or entropy) of a system by considering a convex body constituted by all possible values of physical quantities [5]. Shifting to systems in which the behaviors are governed by quantum physics, the possible expectation values of physical quantities are instead acquired over the entire space of quantum states, mathematically the set of all semidefinite matrices of trace one \( \mathcal{M}_d = \{ \rho : \rho \geq 0, \text{Tr}(\rho) = 1 \} \) in a \( d \)-dimensional Hilbert space. The convex body formed by joint expectation values of different observables on all quantum states can be used as a geometric representation of quantum state space. One of the most successful examples is the Bloch sphere of qubit state space [6], which has become the fundamental model in quantum information [7]. Many works are devoted to studying the geometry of higher-dimensional systems, such as generalizing the Bloch vector [6,8–10] and visualizing a single qutrit state [11]. However, there is no satisfactory geometric ways to visualize the whole higher-dimensional state space, which possesses properties dissimilar to those of qubits that are starting to play indispensable roles in quantum information processing [12–14].

In this Letter, we investigate the geometry of quantum states by projecting the state space \( \mathcal{M}_d \) onto the \( n \)-dimensional Euclidean space \( \mathbb{R}^n \) via measurements of \( n \) observables on the system [15–18]. This geometric construction allows the exploration of the complicated structure and physical properties of high-dimensional quantum systems through their lower-dimensional projections. Behind this construction is the concept of the numerical range in mathematical terminology. Back in 1916, Toeplitz [15] introduced the numerical range of a \( d \times d \) complex matrix \( F \), which is defined as \( \mathcal{W}(F) = \{ z = \langle \psi | F | \psi \rangle : | \psi \rangle \in \mathbb{C}^d, (| \psi \rangle \langle \psi |) = 1 \} \). Here \( F = F_1 + iF_2 \) involves two Hermitian matrices \( F_1 \) and \( F_2 \). The conjecture by Toeplitz that \( \mathcal{W}(F) \) is convex was later proved by Hausdorff in 1919 [15,16]. A natural extension, termed the
inward-pointing unit vector in $R^n$. The state space projection via these matrices, which allows the statistical mixture of pure states $|\psi\rangle$, is simply the convex hull of the JNR

$$L(\mathcal{F}) = \{\text{Tr}(\rho F_1), \ldots, \text{Tr}(\rho F_n) : \rho \in \mathcal{M}_d\}. \quad (2)$$

In the following, we are mainly concerned with the set $L(\mathcal{F})$ and do not distinguish it from $W(\mathcal{F})$ (see Supplemental Material, Sec. I A [19]).

In recent years, the topic of the numerical range has been reviewed in the study of quantum phase transitions [25–28], the derivation of uncertainty relations [29] and entanglement criterion [30], and error correcting codes in quantum computing [31,32]. Yet many characteristics of JNRs are still unknown for dimensions as low as 3. Recently, Szymański, Weis, and Zyczkowski made a crucial step toward resolving this problem by proving the complete classification of the JNR in the case $d = n = 3$ [33]. However, experimentally recovering the geometry of a JNR, together with its classification, demands sampling adequate data, which is a nontrivial problem requiring the ability to implement arbitrary unitary operations on a qudit system [34,35]. Here we perform the first experiment allowing the complete observation of state space projections beyond qubit systems.

As mentioned above, a simple example in a qubit system is the JNR of three Pauli operators known as the Bloch sphere [6], whereas the JNR of other Hermitian matrices is equivalent to a transformation of the Bloch sphere, as shown in Fig. 1(a). Extended to higher-dimensional systems, the geometry of the JNR is associated with a class of system Hamiltonians $H(h) = \sum h_i F_i$ parameterized by $h = (h_1, \ldots, h_n)$ in the basis $\mathcal{F}$. It is intuitive that surface points (extreme points) of the JNR are generated by ground states of $H(h)$ (see Supplemental Material, Sec. I B [19]). Geometrically, each parameter vector $h$ represents an inward-pointing unit vector in $R^n$ and corresponds to a supporting hyperplane tangent to the surface of the JNR, as depicted in Fig. 1(b). The tangent point is acquired by the ground state $|\psi(h)\rangle$ of $H(h)$, while the corresponding ground-state energy $E_g(h)$ can be obtained by projecting the point $\{F_1|\psi(h)\rangle, \ldots, F_n|\psi(h)\rangle\}$ onto the $h$ direction. When continuously varying the parameter vector $h$, the envelope of all supporting hyperplanes constitutes the surface of the JNR, which can be generated by all ground states $|\psi_j(h)\rangle$.

Therefore, this indicates ground-state degeneracy in the sense that different ground states are associated with one system Hamiltonian, $H(h)$ [28].

In the case $d = n = 3$, the image of the JNR forms a three-dimensional oval that can be classified in terms of its one- or two-dimensional faces, that is, segments or filled ellipses. These faces are invariant under linear transformation and translation. According to the number of segments (s) and filled ellipses (e) on the surface, all the JNRs can be divided into ten possible categories [33]. Among these, the eight unitarily irreducible categories that we measured are as follows (the other two categories correspond to reducible operator sets, which can be derived by lower-dimensional JNRs; see Supplemental Material, Sec. II D [19]):

$$s = 0; e = 0, 1, 2, 3, 4 \quad \text{and} \quad s = 1; e = 0, 1, 2.$$

To measure the JNR, one can prepare identical copies of quantum states and obtain a triple of expectation values of $\mathcal{F}$ by separately measuring each of the three observables on the same states. Experimentally, qutrit states can be encoded in the photons’ different degrees of freedom.
Here we prepare a single photon in the superposition of three modes that is equivalent to a spin-one particle. The single photon, generated in a heralded manner by the parametric downconversion process, projects input states onto the three eigenstates of the observable $F_i$, so that the expectation values of $F_i$ can be estimated through the measured probability distribution $\{p_j\}$. The wave plates in the measurement stage can be configured in different settings, thus enabling measurements of different observables with respect to the same set of states.

For each class of the JNR, we provide an example of the 3-tuple of observables $F$ (see Supplemental Material, Sec. II B [19]) being measured in our experiment. Given that the set of the JNR is convex for $n = 3$ [40] and any interior point can be obtained by the mixture of surface states, measuring pure surface states is enough for the observation of the JNR. We randomly sample 300 ground states $|\psi_g(\theta, \phi)\rangle$ of system Hamiltonians

$$H(\theta, \phi) = \sin \theta \cos \phi F_1 + \sin \theta \sin \phi F_2 + \cos \theta F_3$$

for each class (see Supplemental Material, Sec. II A [19]). Here $(\theta, \phi)$ defines the unit vector $\vec{u} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$. Then we measure the expectation values of the three observables with respect to these ground states.

Figure 3 illustrates the experimental results for the exemplary JNRs of eight classes. The experimental results are in line with the theoretical predictions, as they are very close to the surface of the theoretical predictions. The average similarity $S$ between experimentally measured probability distributions $\{p_j\}$ and the theoretical values $\{p_j^\text{th}\}$ is above 0.994, with $S = \left( \sqrt{p_0 p_{0}^\text{th}} + \sqrt{p_1 p_{1}^\text{th}} + \sqrt{p_2 p_{2}^\text{th}} \right)^2$. The
convex hulls of the experimental data also show the same geometrical features (the number of $s$ and $e$). Deviations between the observed data and the theoretical values are mainly attributed to systematic errors in the settings of experimental parameters (see Supplemental Material, Sec. II E [19]). Apart from the first class, the remaining seven classes of the JNR are different from either a sphere or an ellipsoid, showing distinct properties of qutrit state space from those of qubits.

Following the complete observation of the geometric bodies, we show how the geometry of JNRs in Fig. 3 determines the ground-state energies and degeneracies of the system Hamiltonians. In Fig. 4, by combining all the experimental results $\langle F_1, F_2, F_3 \rangle$ of $\mathcal{F}$ with their
corresponding unit vector $(\theta, \phi)$, we obtain the expectation value $E$ of the system Hamiltonian $H(\theta, \phi)$ and give the diagrams of $E$ (red dots) versus $\theta$ and $\phi$. The resulting energies are in line with the theoretical prediction of ground-state energies (the lower colored surfaces) within experimental errors. In particular, there is a clear correspondence between the segments and ellipses in Fig. 3 and the degeneracy points in Fig. 4. For example, the first class [Fig. 4(a)] corresponds to a gaped Hamiltonian and there is no flat portion on the surface of its JNR. As for the case $s = 1, e = 2$, there are three degeneracy points in the band structure diagram. Two are cone-shaped, which are non-analytic in all directions and correspond to the two ellipses on the JNR. The other is $\Lambda$-shaped, which is non-analytic only in one direction and corresponds to the segment. These various band structure diagrams, which can be geometrically revealed by the surfaces of the JNRs, also show the distinct features of three-level quantum systems compared to two-level systems.

For quantum matters at the zero temperature, the ground states associated with a class of Hamiltonians are regarded as “quantum phases” of the matter. The degeneracy of ground states, usually indicating a gap closing, is an important indicator of different quantum phases [41] such as symmetry-breaking, topological-ordered, and gapless phases. As demonstrated in our experiment, the flat surfaces (ellipses and segments in the case $d = n = 3$) on an image of the JNR indicate ground-state degeneracies of the Hamiltonian $H(\vec{h})$ and thus represent different phases of the system. Therefore, the surface of the JNR can be viewed as an intuitive geometric representation of quantum phases on which different regions represent different phases.

We experimentally identify the geometry of a three-level quantum system by observing the complete classification of the JNRs of three observables. The results highlight the distinct difference between high-dimensional quantum systems and qubits. Furthermore, we elucidate the relation between the geometric characters of the JNR and the ground-state degeneracies of the system Hamiltonians. Our work opens an avenue to experimentally explore fascinating phenomena of quantum systems via their state space projections. This geometric method is also applicable to many-body systems when the set of observables happens to be the local Hamiltonians of the system, which may be easier to implement than the global ones [42]. Besides this, the concept of the JNR has shown a wide range of potential applications. As convex sets, JNRs have been adopted in the $N$-representability problem [26,43] and the quantum marginal problem [44] for visualizing the set of reduced density matrices. In the field of quantum information, JNRs find applications in the derivation of entanglement witnesses [30,45] and uncertainty relations [29,46] and provide theoretical foundations for the self-characterization of quantum devices [47,48]. We expect this versatile concept to promote further investigations in understanding the geometry of quantum systems, inferring intriguing phases and properties of quantum matters, as well as developing novel technologies in quantum information science.

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