

# Geometric Quantum State Estimation

Fabio Anza\* and James P. Crutchfield†

*Complexity Sciences Center and Physics Department,  
University of California at Davis, One Shields Avenue, Davis, CA 95616*

(Dated: August 20, 2020)

Density matrices capture all of a quantum system’s statistics accessible through projective and positive operator-valued measurements. They do not completely determine its state, however, as they neglect the physical realization of ensembles. Fortunately, the concept of geometric quantum state does properly describe physical ensembles. Here, given knowledge of a density matrix, possibly arising from a tomography protocol, we show how to estimate the geometric quantum state using a maximum entropy principle based on a geometrically-appropriate entropy.

PACS numbers: 05.45.-a 89.75.Kd 89.70.+c 05.45.Tp

Keywords: Quantum mechanics, geometric quantum mechanics, maximum entropy estimation, density matrix

## I. INTRODUCTION

Quantum mechanics defines a system’s state  $|\psi\rangle$  as an element of a Hilbert space  $\mathcal{H}$ . These are the *pure states*. To account for uncertainties in a system’s actual state  $|\psi\rangle$  one extends the definition to *density operators*  $\rho$  that act on  $\mathcal{H}$ . These operators are linear, positive semidefinite  $\rho \geq 0$ , self-adjoint  $\rho = \rho^\dagger$ , and normalized  $\text{Tr} \rho = 1$ .  $\rho$  then is a pure state when it is also a projector:  $\rho^2 = \rho$ .

The spectral theorem guarantees that one can always decompose a density operator as  $\rho = \sum_i \lambda_i |\lambda_i\rangle \langle \lambda_i|$ , where  $\lambda_i \in [0, 1]$  are its eigenvalues and  $|\lambda_i\rangle$  its eigenvectors. *Ensemble theory* gives the decomposition’s statistical meaning [1, 2]:  $\lambda_i$  is the probability that the system is in the pure state  $|\lambda_i\rangle$ . Thus, if we concede that an operational procedure aimed at preparing a system in a pure state  $|\psi\rangle$  will not always be perfectly executed, we must admit uncertainties of this kind. Moreover, if we admit limited knowledge of the interactions a system has with its environment, uncertainties of this kind will be dynamically generated.

Most generally, density operators  $\rho = \sum_k p_k |\psi_k\rangle \langle \psi_k|$  are convex combinations of pure states. Given a preparation scheme, they say that a system is in pure state  $|\psi_k\rangle$  with probability  $p_k$ . In this sense, they are probability measures whose sample space is  $\mathcal{H}$ . This is formalized using *geometric quantum mechanics* (GQM)—an equivalent formulation that exploits tools from differential geometry to describe the states and dynamics of quantum systems [3–18]. In GQM the states of a quantum system with Hilbert space  $\mathcal{H}$  of dimension  $D$  are points in the projective manifold  $\mathcal{P}(\mathcal{H}) = \mathbb{C}P^{D-1}$ .

Adopting GQM’s perspective, one realizes that pure states are Dirac-delta measures on the pure-state manifold  $\mathcal{P}(\mathcal{H})$ , while *mixed states* are discrete convex com-

binations of Dirac-delta measures. This suggests considering continuous mixed states as generic probability measures on  $\mathcal{P}(\mathcal{H})$ . This notion of state, which we here dub *geometric quantum state*, straightforwardly generalizes the density matrix formalism, to which it reduces in appropriate cases. The primary benefit is an informationally-richer concept of quantum state than the density matrix.

Geometric quantum states have been sporadically considered in the literature [9, 19–21], though mostly in special cases. Companion works, Refs. [22, 23], give a formal definition, invariant under changes of coordinates, in terms of the infinite limit of finite convex combinations, together with an extended geometric formalism that addresses the notion of partial trace in a more flexible way. While efforts have been invested to develop the tools of GQM, to the best of our knowledge the notion of continuous mixed state has remained (almost) exclusively a mathematical tool. With this in mind, the following lays a bridge between density matrices and geometric quantum states. The goal is to introduce a protocol for estimating a geometric quantum state, starting from experimental data.

Our development proceeds as follows. We briefly introduce geometric quantum mechanics, highlighting its relation to the more familiar density-matrix formalism. Then, we show how to set up a maximum entropy estimate for geometric quantum states, starting from knowledge of the density matrix. Eventually, we draw out several consequences and discuss future challenges.

## II. GEOMETRIC QUANTUM MECHANICS

The following briefly covers geometric quantum mechanics and its tools. More complete discussions are found in the relevant literature [3–18] and in two companion works [22, 23].

*Manifold of quantum states.* Given a system with a  $D$ -dimensional Hilbert space  $\mathcal{H}$ , in GQM its pure states

\* fanza@ucdavis.edu

† chaos@ucdavis.edu

are points in the complex projective manifold  $\mathcal{P}(\mathcal{H}) = \mathbb{C}P^{D-1}$ . To give coordinates we fix an arbitrary basis  $\{|e_\alpha\rangle\}_{\alpha=0}^{D-1}$  of  $\mathcal{H}$ . In this way, a pure state  $|\psi\rangle$  is parametrized by  $D$  complex and homogeneous coordinates  $Z = \{Z^\alpha\}$ , up to normalization and an overall phase:

$$|\psi\rangle = \sum_{\alpha=0}^{D-1} Z^\alpha |e_\alpha\rangle ,$$

where  $Z \in \mathbb{C}^D$ ,  $Z \sim \lambda Z$ , and  $\lambda \in \mathbb{C}/\{0\}$ . In the case of a single qubit, for example, we have  $Z_{\text{qubit}} = (\sqrt{p_0}e^{i\nu_0}, \sqrt{p_1}e^{i\nu_1})$ .

*Measurements.* Quantum measurements on  $\mathcal{H}$  are modeled using *positive operator-valued measurements* (POVMs) as follows.  $\{E_j\}_{j=1}^n$  are collections of Hermitian, nonnegative operators  $E_j \geq 0$ , called *effects*. They are decompositions of the identity  $\sum_{j=1}^n E_j = \mathbb{I}$ . In GQM they are described by finite collections of  $n$  real and non-negative functions  $E_j(Z) \geq 0$  on  $\mathcal{P}(\mathcal{H})$ :

$$E_j(Z) = \sum_{\alpha,\beta} (E_j)_{\alpha,\beta} Z^\alpha \bar{Z}^\beta ,$$

where  $E_{\alpha,\beta} = E_{\beta,\alpha}^*$  and whose sum is always equal to the constant function 1:  $\sum_{j=1}^n E_j(Z) = 1$ . For POVMs, observables  $\mathcal{O}$  are also real quadratic functions:

$$\mathcal{O}(Z) = \sum_{\alpha,\beta=1}^D \mathcal{O}_{\alpha,\beta} Z^\alpha \bar{Z}^\beta ,$$

where  $\mathcal{O}_{\alpha,\beta} = \mathcal{O}_{\alpha,\beta}^*$ .

*Geometric quantum states.* Complex projective spaces, such as  $\mathcal{P}(\mathcal{H})$ , have a preferred metric  $g_{FS}$  and a related volume element  $dV_{FS}$ , called the *Fubini-Study volume element*. The details surrounding these go beyond our present purposes. Fortunately, it is sufficient to give  $dV_{FS}$ 's explicit form in the coordinate system we use for concrete calculations. The latter is the ‘‘probability + phase’’ coordinate system:  $Z^\alpha = \sqrt{p_\alpha}e^{i\nu_\alpha}$ :

$$\begin{aligned} dV_{FS} &= \sqrt{\det g_{FS}} \prod_{\alpha=0}^{D-1} dZ^\alpha d\bar{Z}^\alpha \\ &= \prod_{\alpha=1}^{D-1} \frac{dp_\alpha d\nu_\alpha}{2} . \end{aligned}$$

In GQM, quantum states convey information about the ways real values are associated to observables and POVMs. Thus, it is quite natural to describe the latter as real-valued functionals  $P[\mathcal{O}]$  that, via a probability measure on  $\mathcal{P}(\mathcal{H})$ , associate a number to an element  $\mathcal{O}$  of the algebra  $\mathcal{A}$  of observables:

$$P_q[\mathcal{O}] = \int_{\mathcal{P}(\mathcal{H})} q(Z) \mathcal{O}(Z) dV_{FS} ,$$

where  $\mathcal{O} \in \mathcal{A}$  and  $q(Z) \geq 0$  is the normalized distribution associated with the functional  $P$ :

$$P_q[\mathbb{I}] = \int_{\mathcal{P}(\mathcal{H})} q(Z) dV_{FS} = 1 .$$

In this setting, since pure states  $|\psi_0\rangle$  are points in  $\mathcal{P}(\mathcal{H})$ , they are associated to functionals with Dirac-delta distributions  $p_0(Z) = \tilde{\delta}[Z - Z_0]$ :

$$P_0[\mathcal{O}] = \int_{\mathcal{P}(\mathcal{H})} \tilde{\delta}(Z - Z_0) \mathcal{O}(Z) dV_{FS} ,$$

where  $\tilde{\delta}(Z - Z_0)$  is shorthand for a coordinate-covariant Dirac-delta in arbitrary coordinates. In homogeneous coordinates this reads:

$$\tilde{\delta}(Z - Z_0) := \frac{1}{\sqrt{\det g_{FS}}} \prod_{\alpha=0}^{D-1} \delta(X - X_0) \delta(Y - Y_0) ,$$

where  $Z = X + iY$ . In  $(p_\alpha, \nu_\alpha)$  coordinates this becomes:

$$\tilde{\delta}(Z - Z_0) = \prod_{\alpha=1}^{D-1} 2\delta(p_\alpha - p_\alpha^0) \delta(\nu_\alpha - \nu_\alpha^0) ,$$

where the coordinate-invariant nature of the functionals  $P_p[\mathcal{O}]$  is manifest. Mixed states  $\rho = \sum_j \lambda_j |\lambda_j\rangle \langle \lambda_j|$  are thus convex combinations of these Dirac-delta functionals:  $p_{\text{mix}}(Z) = \sum_j \lambda_j \tilde{\delta}(Z - Z_j)$ , where  $Z_j \leftrightarrow |\lambda_j\rangle$ . The distribution  $q(Z)$  is called a *geometric quantum state*.

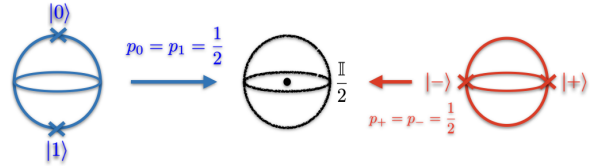


Figure 1. If the barycenter of two density matrices is the same, as for  $\rho_A$  and  $\rho_B$ , the standard formalism of quantum mechanics regards them as identical, while they are not. The difference is seen using the geometric formalism.  $P_A$  and  $P_B$  are two Dirac-delta distributions peaked on different antipodal points of the Bloch sphere.

*Density matrix formalism.* Geometric quantum states are logically prior to density matrices, essentially for two reasons. First, the latter can be computed from the former, as follows:

$$\rho_{\alpha\beta}^q = P_q[Z^\alpha \bar{Z}^\beta] \quad (1)$$

$$= \int_{\mathcal{P}(\mathcal{H})} dV_{FS} q(Z) Z^\alpha \bar{Z}^\beta . \quad (2)$$

Second, the correspondence is many-to-one: many different geometric quantum states can have the same density matrix. Indeed, while the geometric quantum state  $q(Z)$  addresses the system's state, the density matrix addresses

the statistics of POVM outcomes, provided that the state is  $q(Z)$ . Going from  $q(Z)$  to  $\rho_{\alpha\beta}^q$  actually erases most information about the detailed statistics of the quantum state and preserves only its POVM statistics.

Figure 1 illustrates this. Prepare an ensemble with equally-likely copies of states  $|0\rangle$  and  $|1\rangle$  or of states  $|+\rangle$  and  $|-\rangle$ . While the density matrix is the same for both, the geometric quantum state  $q(Z)$  of the system is not. Due to this, the density matrix contains no information about the physical realization of the ensemble of a quantum system. For a more thorough discussion on this point see Ref. [22].

This observation is particularly relevant in information processing, as found in quantum computing. There, one is not only interested in measurement outcomes, but must understand, predict, and control how a quantum system changes its behavior due to external signals. By focusing only on the density matrix we lack an appropriate characterization of the ensemble producing the pure states and, therefore, miss a wealth of information that can help in manipulating quantum states.

With this set up and the key issues of state representation laid out, we are now ready to imagine a state preparation protocol and a tomographically-complete [24] set of POVMs that allows to recover the density matrix from measurements. As we argued, this information is insufficient to recover the geometric quantum state. To fill the gap we invoke the maximum entropy paradigm, which provides a principled and well-understood procedure with which to infer a probability distribution from partial knowledge.

### III. MAXIMUM GEOMETRIC QUANTUM ENTROPY

*Maximum entropy estimation* [25–27] is applied ubiquitously in science and engineering. Its predictive power has enjoyed marked empirical successes, especially when addressed to systems consisting of large numbers of degrees of freedom or when confronted with much missing microscopic information. Here, we adapt this well-known technique to geometric quantum mechanics.

The relevant entropy is the equivalent of Shannon’s differential entropy [27] on a manifold. We call it *geometric quantum entropy*. Given a continuous and smooth probability distribution  $q(Z)$  it is defined:

$$H_G = - \int_{\mathcal{P}(\mathcal{H})} dV_{FS} q(Z) \log q(Z) . \quad (3)$$

This was first considered, to the best of our knowledge, by Ref. [28]. Its role in quantum thermodynamics and statistical mechanics was recently explored by the authors in Ref. [23]. Here, we do not dwell on the conceptual implications of using  $H_G$  in place of the von Neumann

quantum entropy  $S$ . We simply note that  $H_G$  is a generalized version of the latter, to which it reduces when  $q(Z)$  is a convex sum over Dirac-delta distributions.

The goal in maximum entropy estimation is to find  $H_G$ ’s maximum given the constraints  $\mathcal{C}_N = 0$  (normalization) and  $\mathcal{C}_{\alpha\beta} = 0$  (a fixed density matrix  $P_q[Z^\alpha \bar{Z}^\beta] = \rho_{\alpha\beta}$ ):

$$\mathcal{C}_N := \int_{\mathcal{P}(\mathcal{H})} dV_{FS} q(Z) - 1 , \quad (4a)$$

$$\mathcal{C}_{\alpha,\beta} := \int_{\mathcal{P}(\mathcal{H})} dV_{FS} q(Z) Z^\alpha \bar{Z}^\beta - \rho_{\alpha\beta} , \quad (4b)$$

for all  $\alpha$  and  $\beta$ .

Applying Lagrange multipliers for the maximization, we define:

$$\Lambda[\vec{\lambda}, \gamma, q(Z)] = H_G[q(Z)] - \sum_{\alpha,\beta} \lambda_{\alpha\beta} \mathcal{C}_{\alpha\beta} - \gamma \mathcal{C}_N . \quad (5)$$

Variation with respect to the Lagrange’s multipliers  $\gamma$  and  $\{\lambda_{\alpha\beta}\}$  impose the constraints  $\mathcal{C}_{\alpha\beta} = 0$  for all  $\alpha, \beta$  and  $\mathcal{C}_N = 0$ . Note that since  $\rho = \rho^\dagger$  not all  $\lambda$ s are linearly independent as  $\lambda_{\alpha\beta} = \lambda_{\beta\alpha}^*$ . The functional derivative with respect to the probability distribution  $q(Z)$  gives:

$$\log q(Z) = -(1 + \gamma) - \sum_{\alpha,\beta} Z^\alpha \bar{Z}^\beta \lambda_{\alpha\beta} .$$

This eventually turns into the following maximum entropy estimate:

$$q_{\text{ME}}(Z) = \frac{e^{-\sum_{\alpha,\beta=1}^D \lambda_{\alpha\beta} Z^\alpha \bar{Z}^\beta}}{\mathcal{Z}(\lambda_{\alpha\beta})} \quad (6a)$$

$$\mathcal{Z}(\lambda_{\alpha\beta}) := \int_{\mathcal{P}(\mathcal{H})} dV_{FS} e^{-\sum_{\alpha,\beta=1}^D \lambda_{\alpha\beta} Z^\alpha \bar{Z}^\beta} . \quad (6b)$$

In this, we used  $\mathcal{Z} = e^{\gamma+1}$ . This fixes the probability distribution’s functional form to be exponential.

To guarantee that  $q_{\text{ME}}$  satisfies Eq. (4)’s constraints, the Lagrange multipliers  $\lambda_j$  must satisfy the following nonlinear equations:

$$-\frac{\partial \log \mathcal{Z}(\lambda_{\alpha\beta})}{\partial \lambda_{\alpha\beta}} = \rho_{\alpha\beta} , \quad (7)$$

for all  $\alpha, \beta = 1, \dots, D$ . Equivalently, defining  $F(\lambda_{\alpha\beta}) = -\log \mathcal{Z}(\lambda_{\alpha\beta})$  and using the Legendre transform of  $H_G$ :

$$\Gamma(\lambda_{\alpha\beta}) = \sum_{\alpha,\beta=1}^D \lambda_{\alpha\beta} \rho_{\alpha\beta} - F(\lambda_{\alpha\beta}) ,$$

one can straightforwardly show that Eq. (7) is equivalent to:

$$\frac{\partial \Gamma}{\partial \lambda_{\alpha\beta}} = 0 . \quad (8)$$

for all  $\alpha, \beta = 1, \dots, D$ .

Moreover, one can also show that the functional  $\Gamma(\lambda_{\alpha\beta})$  is everywhere convex, thus proving that if a stationary point—Eq. (8)—exists, it must be an absolute minimum. This statement then transfers to the entropy maximum since, by solution Eq. (6), we have  $\Gamma(\lambda_{\alpha\beta}) = -H_G[q(\vec{\lambda})]$ .

Convexity of the functional  $\Gamma(\lambda_{\alpha\beta})$  is established simply by showing that its Hessian  $\Gamma_{\alpha\beta;\tilde{\alpha}\tilde{\beta}}^{(2)}$  matrix is positive semidefinite. This is done by noticing that:

$$\begin{aligned} \Gamma_{\alpha\beta;\mu\nu}^{(2)} &= \frac{\partial^2 \Gamma}{\partial \lambda_{\alpha\beta} \partial \lambda_{\mu\nu}} \\ &= \mathbb{E} \left[ Z^\alpha \bar{Z}^\beta Z^\mu \bar{Z}^\nu \right] - \mathbb{E} \left[ Z^\alpha \bar{Z}^\beta \right] \mathbb{E} \left[ Z^\mu \bar{Z}^\nu \right] \\ &= \mathbb{E} \left[ Z^\alpha \bar{Z}^\beta Z^\mu \bar{Z}^\nu \right] - \rho_{\alpha\beta} \rho_{\mu\nu} . \end{aligned} \quad (9)$$

As with any covariance matrix, this is positive semidefinite. Thanks to this reformulation and despite the fact that a closed solution to Eq. (7) is not known, good iterative procedures that provide sufficiently-accurate solutions can be employed [29]. For example, gradient-descent optimization can be directly leveraged to find the minimum of  $\Gamma(\lambda_{\alpha\beta})$ . (For more in-depth discussion see Refs. [30–32].)

Taking advantage of its particularly simple form, we can extract an analytical form for  $\mathcal{Z}(\lambda_{\alpha\beta})$ . Appendix A provides the details; here, we simply quote the result. First, since  $\lambda_{\alpha\beta}$  is a Hermitian and positive-definite matrix we know we can always diagonalize it by means of a unitary matrix  $U$ :  $U\lambda U^\dagger = \lambda_D$ , where  $\vec{\lambda}_D = (\lambda_0, \dots, \lambda_{D-1})$ . By reversing this relation, the unitary matrix diagonalizing  $\lambda_{\alpha\beta}$  provides a set of  $D$  functions such that  $\lambda_j = f_j(\lambda_{\alpha\beta})$ . With these definitions in mind:

$$\mathcal{Z}(\lambda_{\alpha\beta}) = \sum_{k=0}^{D-1} \frac{e^{-f_k(\lambda_{\alpha\beta})}}{\prod_{j \neq k} [f_k(\lambda_{\alpha\beta}) - f_j(\lambda_{\alpha\beta})]} .$$

By simple algebraic manipulations, the maximum-entropy estimation  $q_{\text{ME}}(Z)$  can be written as a multivariate Gaussian. Using vector notation  $Z^\alpha = \vec{Z}$  and  $\bar{Z}^\beta = \vec{Z}^*$  and calling  $\vec{\mu} = \langle Z^\alpha \rangle$  and  $\vec{\mu}^* = \langle \bar{Z}^\beta \rangle$ , we find:

$$q_{\text{ME}}(Z) = \frac{1}{Q} e^{-\frac{1}{2}(\vec{Z}^* - \vec{\mu}^*)\Sigma^{-1}(\vec{Z} - \vec{\mu})} \quad (10)$$

$$Q = \int_{\mathcal{P}(\mathcal{H})} dV_{FS} e^{-\frac{1}{2}(\vec{Z}^* - \vec{\mu}^*)\Sigma^{-1}(\vec{Z} - \vec{\mu})} , \quad (11)$$

where  $\Sigma$  is the covariance matrix  $\Sigma_{\alpha\beta} = \mathbb{E} \left[ Z^\alpha \bar{Z}^\beta \right] - \mathbb{E} \left[ Z^\alpha \right] \mathbb{E} \left[ \bar{Z}^\beta \right]$ ,  $\vec{\mu}$  is the average vector  $\mu^\alpha = \mathbb{E} \left[ Z^\alpha \right]$ , and they are linear combinations of the  $\lambda_{\alpha\beta}$ . Fixing  $\Sigma$  and  $\vec{\mu}$  is equivalent to fixing all the  $\lambda_{\alpha\beta}$  and we can use this parametrization to fix the Lagrange multipliers in a func-

tionally simpler way:

$$\begin{aligned} \mu^\alpha &= \mathbb{E} \left[ Z^\alpha \right] , \\ \Sigma_{\alpha\beta} &= \mathbb{E} \left[ Z^\alpha \bar{Z}^\beta \right] - \mathbb{E} \left[ Z^\alpha \right] \mathbb{E} \left[ \bar{Z}^\beta \right] \\ &= \rho_{\alpha\beta} - \mu_\alpha \mu_\beta . \end{aligned}$$

Given knowledge of only the density matrix, we have no input about  $\vec{\mu}$ , which results in  $\vec{\mu} = 0$  and  $\Sigma = \rho$ .

#### IV. CONCLUSIONS

The geometric quantum state  $q(Z)$  is a probability distribution on a system's pure-state manifold  $\mathcal{P}(\mathcal{H})$ . It determines a system's state at a deeper and more refined level than its density matrix  $\rho$ . The latter only contains information about POVM statistics, which are essentially pairwise correlations. And so, to every geometric quantum state  $q(Z)$  there corresponds a unique density matrix  $\rho_q$  that describes  $q(Z)$ 's POVM statistics; see Eq. (2). However, the correspondence is many-to-one: Given a density matrix  $\rho$ , there are various  $q(Z)$  compatible with  $\rho$ 's POVM statistics. One consequence stems from results presented in the two companion works, Refs. [22, 23], where it is argued in fuller detail that the geometric quantum state is a richer characterization of a quantum system's physical state—one that goes beyond its POVMs' statistics. Here, we answered a complementary, operational question, What is the best guess of  $q(Z)$ , assuming knowledge of the density matrix  $\rho$ ?

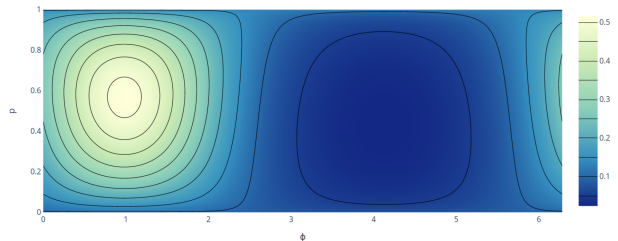


Figure 2. Maximum-entropy geometric quantum state in *probability + phase* coordinates  $(p, \phi)$  determined by functional Eq. (11). Here, we started with density matrix  $\rho$  given by  $\rho_{00} = 1 - \rho_{11} = 0.45$  and  $\rho_{01} = \rho_{10}^* = 0.2 - 0.3i$ .

This was answered using the constrained maximum entropy paradigm, an ubiquitous estimation technique in science and engineering. We showed that the entropy functional appropriate to quantum settings is the geometric quantum entropy of Eq. (3), a transposition into the quantum-state manifold of the classical notion of entropy of a phase space distribution. Due to Eq. (2)'s relation between the density matrix  $\rho$  and the geometric quantum state  $q(Z)$ , the resulting distribution  $q(Z)$  has Eq. (9)'s form of a multivariate Gaussian in which the covariance matrix  $\Sigma$  is directly related to the density matrix  $\rho$ . Given the Gaussian form, fixing its parameters

amounts to an appropriate characterization of its average vector  $\vec{\mu}$  and covariance matrix  $\Sigma$ . Using this functional parametrization we derived the maximum entropy estimate for a geometric quantum state  $q(Z)$  with density matrix  $\rho$ :

$$q_{\text{ME}}(Z) = Q^{-1} e^{-\frac{1}{2} \vec{Z}^* \rho^{-1} \vec{Z}}, \text{ with}$$

$$Q = \int_{\mathcal{P}(\mathcal{H})} dV_{FS} e^{-\frac{1}{2} \vec{Z}^* \rho^{-1} \vec{Z}},$$

when  $\det \rho \neq 0$ .

## ACKNOWLEDGMENTS

F.A. thanks Marina Radulaski, Davide Pastorello, and Davide Girolami for discussions on the geometric for-

malism of quantum mechanics. F.A. and J.P.C. thank Dhruva Karkada for his help with the example, David Gier, Samuel Loomis, Ariadna Venegas-Li for helpful discussions and the Telluride Science Research Center for its hospitality during visits. This material is based upon work supported by, or in part by, a Templeton World Charity Foundation Power of Information Fellowship, FQXi Grant FQXi-RFP-IPW-1902, and U.S. Army Research Laboratory and the U. S. Army Research Office under contracts W911NF-13-1-0390 and W911NF-18-1-0028.

## DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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- [1] R. K. Pathria and Paul D. Beale. *Statistical Mechanics*. Elsevier B.V., 2011. 1
  - [2] W. Greiner, L. Neise, and H. Stöcker. *Thermodynamics and Statistical Mechanics*. Springer New York, New York, NY, 1995. 1
  - [3] F. Strocchi. Complex Coordinates and Quantum Mechanics. *Rev. Mod. Physics*, 38(1):36–40, 1966. 1
  - [4] T. W. B. Kibble. Geometrization of quantum mechanics. *Comm. Math. Physics*, 65(2):189–201, 1979.
  - [5] A. Heslot. Quantum mechanics as a classical theory. *Phys. Rev. D*, 31(6):1341–1348, 1985.
  - [6] G. W. Gibbons. Typical states and density matrices. *J. Geom. Physics*, 8(1-4):147–162, 1992.
  - [7] A. Ashtekar and T. A. Schilling. Geometry of quantum mechanics. In *AIP Conference Proceedings*, volume 342, pages 471–478. AIP, 1995.
  - [8] A. Ashtekar and T. A. Schilling. Geometrical formulation of quantum mechanics. In *On Einstein's Path*, pages 23–65. Springer New York, New York, NY, 1999.
  - [9] D. C. Brody and L. P. Hughston. Geometric quantum mechanics. *J. Geom. Physics*, 38(1):19–53, 2001. 1
  - [10] I. Bengtsson and K. Życzkowski. *Geometry of Quantum States*. Cambridge University Press, Cambridge, 2017.
  - [11] J. F. Cariñena, J. Clemente-Gallardo, and G. Marmo. Geometrization of quantum mechanics. *Theoret. Math. Physics*, 152(1):894–903, 2007.
  - [12] D. Chruściński. Geometric aspects of quantum mechanics and quantum entanglement. *J. Physics Conf. Series*, 30:9–16, 2006.
  - [13] G Marmo and G F Volkert. Geometrical description of quantum mechanics—transformations and dynamics. *Physica Scripta*, 82(3):038117, 2010.
  - [14] J. Avron and O. Kenneth. An elementary introduction to the geometry of quantum states with pictures. *Rev. Math. Physics*, 32(02):2030001, 2020.
  - [15] D. Pastorello. A geometric Hamiltonian description of composite quantum systems and quantum entanglement. *Intl. J. Geom. Meth. Mod. Physics*, 12(07):1550069, 2015.
  - [16] D. Pastorello. Geometric Hamiltonian formulation of quantum mechanics in complex projective spaces. *Intl. J. Geom. Meth. Mod. Physics*, 12(08):1560015, 2015.
  - [17] D. Pastorello. Geometric Hamiltonian quantum mechanics and applications. *International Journal of Geometric Methods in Modern Physics*, 13(Supp. 1):1630017, 2016.
  - [18] J. Clemente-Gallardo and G. Marmo. The Ehrenfest picture and the geometry of quantum mechanics. *Il Nuovo Cimento C*, 3:35–52, 2013. 1
  - [19] D. C. Brody, D. W. Hook, and L. P. Hughston. On quantum microcanonical equilibrium. *J. Physics Conf. Series*, 67:012025, 2007. 1
  - [20] D. C. Brody and L. P. Hughston. The quantum canonical ensemble. *J. Math. Physics*, 39(12):6502–6508, 1998.
  - [21] D. C. Brody and L. P. Hughston. Thermodynamics of quantum heat bath. *J. Physics A Math. Theo.*, 49(42):425302, 2016. 1
  - [22] F. Anza and J. P. Crutchfield. Beyond density matrices: Geometric quantum states. *arXiv:2008.08682*, 2020. 1, 3, 4
  - [23] F. Anza and J. P. Crutchfield. Geometric quantum thermodynamics. *arXiv:2008.08683*, 2020. 1, 3, 4
  - [24] T. Heinosaari and M. Ziman. *The mathematical language of quantum theory*. Cambridge University Press, 2012. 3
  - [25] E. T. Jaynes. Information Theory and Statistical Mechanics. *Phys. Rev.*, 106(4):620–630, 1957. 3
  - [26] E. T. Jaynes. Information Theory and Statistical Mechanics. II. *Phys. Rev.*, 108(2):171–190, 1957.
  - [27] T. M. Cover and J. A. Thomas. *Elements of Information theory*. Wiley-Interscience, New York, 2006. 3
  - [28] D. C. Brody and L. P. Hughston. Information content for quantum states. *J. Math. Physics*, 41(5):2586–2592, 2000. 3
  - [29] F. Anza. New equilibrium ensembles for isolated quantum systems. *Entropy*, 20(10):744, 2018. 4
  - [30] L. R. Mead and N. Papanicolaou. Maximum entropy in the problem of moments. *J. Math. Physics*, 25(8):2404–2417, 1984. 4

- [31] A. Tagliani. Inverse Z transform and moment problem. *Probability Engine. Info. Sci.*, 14(3):393–404, 2000.
- [32] K. Schmudgen. *The moment problem*. Springer International Publishing, 2017. 4

# Geometric Quantum State Estimation

## Supplemental Material

Fabio Anza and James P. Crutchfield

### Appendix A: Calculating the Partition Function

Recall:

$$\mathcal{Z}(\lambda_{\alpha\beta}) = \int_{\mathcal{P}(\mathcal{H})} e^{-\sum_{\alpha,\beta} \lambda_{\alpha\beta} Z^\alpha \bar{Z}^\beta} dV_{FS} .$$

Since  $\lambda_{\alpha\beta}$  are the Lagrange multipliers of  $\mathcal{C}_{\alpha\beta}$  we chose them to be Hermitian as they are not all independent. Thus, we can always diagonalize them with a unitary matrix:

$$\sum_{\alpha\beta} U_{\gamma\alpha} \lambda_{\alpha\beta} U_{\beta\epsilon}^\dagger = l_\gamma \delta_{\gamma\epsilon} .$$

This allows us to define auxiliary integration variables  $X_\gamma = \sum_{\alpha} U_{\gamma\alpha} Z^\alpha$ . Thanks to these, we express the quadratic form in the exponent of the integrand using that  $(U^\dagger U)_{\alpha\beta} = \delta_{\alpha\beta}$ :

$$\begin{aligned} Z \lambda \bar{Z} &= \sum_{\alpha\beta} Z^\alpha \lambda_{\alpha\beta} \bar{Z}^\beta \\ &= \sum_{\alpha\beta} \sum_{\tilde{\alpha}\tilde{\beta}} Z^\alpha \delta_{\alpha\tilde{\alpha}} \lambda_{\tilde{\alpha}\tilde{\beta}} \delta_{\tilde{\beta}\beta} \bar{Z}^{\tilde{\beta}} \\ &= \sum_{\alpha\beta} \sum_{\tilde{\alpha}\tilde{\beta}} \sum_{ab} (Z^\alpha U_{\alpha a}^\dagger) (U_{a\tilde{\alpha}} \lambda_{\tilde{\alpha}\tilde{\beta}} U_{\tilde{\beta} b}^\dagger) (U_{b\beta} \bar{Z}^\beta) \\ &= \sum_a |X_a|^2 l_a . \end{aligned}$$

Moreover, recalling that the Fubini-Study volume element is invariant under unitary transformations, we can simply adapt our coordinate systems to  $X_a$ . And so, we have  $X_a = q_a e^{i\nu_a}$ . This gives  $dV_{FS} = \prod_{k=1}^{D-1} \frac{dq_a d\nu_a}{2}$ . We get to the following simpler functional:

$$\begin{aligned} \mathcal{Z}(\lambda_{\alpha\beta}) &= \int_{\mathcal{P}(\mathcal{H})} e^{-\sum_{a=0}^{D-1} l_a q_a} \prod_{k=1}^{D-1} \frac{dq_a d\nu_a}{2} \\ &= \frac{(2\pi)^{D-1}}{2^{D-1}} \int_{\Delta_{D-1}} e^{-\sum_a l_a q_a} \prod_a dq_a . \end{aligned}$$

Now, we are left with an integral of an exponential function over the  $D - 1$ -simplex. We can use Laplace transform trick to solve this kind of integral:

$$\begin{aligned} I_{D-1}(r) &:= \int_{\Delta_{D-1}} \prod_{k=0}^{D-1} e^{-l_k q_k} \delta\left(\sum_{k=0}^{D-1} q_k - r\right) dq_1 \dots dq_{D-1} \\ \Rightarrow \tilde{I}_{D-1}(z) &:= \int_0^\infty e^{-zr} I_{D-1}(r) dr , \\ \tilde{I}_n(z) &= \prod_{k=0}^n \frac{(-1)^k}{(l_k + z)} \\ &= (-1)^{\frac{n(n+1)}{2}} \prod_{k=0}^n \frac{1}{z - z_k} , \end{aligned}$$

with  $z_k = -l_k \in \mathbb{R}$ .

The function  $\tilde{I}_n(z)$  has  $n+1$  real and distinct poles:  $z = z_k = -l_k$ . Hence, we exploit the partial fraction decomposition of  $\tilde{I}_n(z)$ , which is:

$$(-1)^{\frac{n(n+1)}{2}} \prod_{k=0}^n \frac{1}{z - z_k} = (-1)^{\frac{n(n+1)}{2}} \sum_{k=0}^n \frac{R_k}{z - z_k} ,$$

where:

$$\begin{aligned} R_k &= [(z - z_k)\tilde{I}_n(z)]_{z=z_k} \\ &= \prod_{j=0, j \neq k}^n \frac{(-1)^{\frac{n(n+1)}{2}}}{z_k - z_j} . \end{aligned}$$

Exploiting linearity of the inverse Laplace transform plus the basic result:

$$\mathcal{L}^{-1} \left[ \frac{1}{s + a} \right] (t) = e^{-at} \Theta(t) ,$$

where:

$$\Theta(t) = \begin{cases} 1 & t \geq 0 \\ 0 & t < 0 \end{cases} .$$

We have for:

$$\begin{aligned} I_n(r) &= \mathcal{L}^{-1}[\tilde{I}_n(z)](r) \\ &= \Theta(r) \sum_{k=0}^n R_k e^{z_k r} . \end{aligned}$$

And so:

$$\begin{aligned} Z &= I_{D-1}(1) \\ &= \sum_{k=0}^{D-1} \frac{e^{-l_k}}{\prod_{j=0, j \neq k}^{D-1} (l_k - l_j)} . \end{aligned}$$

Now, consider that  $l_a$  are linear functions of the true matrix elements:

$$\begin{aligned} l_a &= f_a(\lambda_{\alpha\beta}) \\ &= \sum_{\alpha\beta} U_{a\alpha} \lambda_{\alpha\beta} U_{\beta a}^\dagger . \end{aligned}$$

We arrive at:

$$\mathcal{Z}(\lambda_{\alpha\beta}) = \frac{e^{-f_k(\lambda_{\alpha\beta})}}{\prod_{j=0, j \neq k}^{D-1} (l_k(\lambda_{\alpha\beta}) - l_j(\lambda_{\alpha\beta}))} .$$