Information Content for Quantum States

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A method of representing probabilistic aspects of quantum systems is introduced by means of a density matrix on the space of pure quantum states. In particular, a maximum entropy argument allows us to obtain a natural density function that only reflects the information provided by the density matrix. This result is applied to derive the Shannon entropy of a quantum state. The information theoretic quantum entropy thereby obtained is shown to have the desired concavity property, and to differ from the the conventional von Neumann entropy. This is illustrated explicitly for a two-state system.

In standard quantum mechanics, the information about physical observables is contained in the state of the system, which is represented by a density matrix $\rho$. This is because the expectation of an observable $F_\alpha$ in the state $\rho_\beta$ is given by the trace formula

$$\langle F \rangle = \rho_\beta F_\alpha \rho_\beta,$$  \hspace{1cm} (1)

and it is through such expectations that the statistical properties of measurement outcomes are determined. Indeed, for a state we require $\rho_\beta$ to be nonnegative and to have trace unity. These properties suggest that the density matrix can be viewed as a probability distribution. For example, if $\rho_\beta$ is nondegenerate, with distinct eigenvalues, then it admits a unique decomposition

$$\rho_\beta = \sum_i w_i \Pi_\beta(x_i).$$  \hspace{1cm} (2)

Here, $\Pi_\beta(x_i)$ denotes the normalised projection operators onto the eigenstates $x_i$ of $\rho_\beta$, and the corresponding probability weights $w_i$ satisfy $w_i > 0$ and $\sum_i w_i = 1$. Some care has to be taken with this interpretation of $\rho_\beta$, because in the present context the underpinnings of classical probability are missing, and the associated terminology can only be used, therefore, by analogy. Nevertheless, von Neumann [1], in pursuit of this analogy, was led by a series of ingenious arguments involving the thermodynamics of a hypothetical gas of independent systems represented by a weighted family of orthogonal pure states, to argue that the quantity

$$S_{vN} = -\rho_\beta \ln \rho_\beta$$  \hspace{1cm} (3)

represents the entropy of the state $\rho_\beta$. In the example of the state $\Pi_\beta(x_i)$, for instance, we have $S_{vN} = -\sum_i w_i \ln w_i$, which is the classical information entropy associated with the probability distribution $w_i$.

It is clear, nevertheless, that the von Neumann entropy is inadequate for some situations. Suppose, for example, we make a measurement of an observable with distinct eigenstates $x_i$. Then the results of the measurement can be represented statistically by the state $\Pi_\beta(x_i)$, where the weighting $w_i$ are given by the familiar transition amplitudes taken with respect to the initial state. In this case, the entropy of the distribution is indeed given by $S_{vN}$, since we know that the measurement results in one of the eigenstates $x_i$ being selected, and that the information gained with the knowledge of the outcome precisely counterbalances the entropy of the state $\rho_\beta$. However, this is a special state of affairs, peculiar to the measurement problem, and there is no a priori justification for assuming in general, given $\rho_\beta$, that the system is in one or another of the eigenstates of $\rho_\beta$. In fact, for a given $\rho_\beta$, the implied minimal information distribution on the space of pure states is of a more general character, as we shall demonstrate in what follows.

In this article we introduce a more realistic formula for the entropy of a quantum state. Our expression for the quantum entropy is in line with that of Shannon; as a consequence, many of the standard results for classical information entropy apply. The quantum entropy introduced here differs, in general, from the von Neumann entropy. However, like the von Neumann entropy, the new entropy can be expressed in terms of the eigenvalues of the density matrix, as we shall illustrate explicitly in the case of a system characterised by a two dimensional Hilbert space. Our methodology has the advantage that it more satisfactorily takes into account the significance of information in modern quantum theory [2]. Indeed, whereas von Neumann specifically accommodates into his thermodynamic analysis as extra information the assumption that the ensemble is composed of a weighted system of pure states, each one of which belongs to a given complete family of orthogonal pure states, we make no such assumption here. Instead, in our approach to the quantum entropy problem, we shall be guided by information theoretic principles.

The other ingredient at our disposal, missing in von Neumann’s theory, is the recognition that the space of pure states in quantum theory has the structure of a
phase space; that is to say, it admits a natural symplectic structure. The quantum phase space $\Gamma$ is a complex projective space endowed with a Hermitian correlation between points and hyperplanes. A point $x \in \Gamma$ represents a pure state, i.e., an equivalence class of wave functions belonging to the same ray in Hilbert space. When viewed as a real manifold, $\Gamma$ is known to have a natural Riemannian geometry, given by the Fubini-Study metric, which has a compatible symplectic structure associated with it. A typical quantum observable $F_\beta$ is given by a function $F(x)$ on $\Gamma$ of the form

$$F(x) = \frac{\bar{\psi}_\alpha(x) F_\beta \psi^\alpha(x)}{\bar{\psi}_\gamma(x) \psi^\alpha(x)},$$

where $\psi^\alpha(x)$ denotes any wave function in the equivalence class associated with the pure state $x$. With a slight departure from the traditional terminology we can refer to the function $F(x)$ itself as the observable. Then if $F(x)$ and $G(x)$ are observables, their Poisson bracket with respect to the symplectic structure is also an observable, given by $i$ times the expectation of the commutator of the corresponding operators, taken in the pure state $x$. The resulting algebra of quantum observables gives $\Gamma$ the structure of a Poisson manifold, and as a consequence the Schrödinger trajectories of pure states are given by the integral curves of the symplectic vector field for which the generator $H(x)$ is the quantum Hamiltonian.

We shall take the view here that a general quantum state is represented by a density function $\rho(x)$ on $\Gamma$, satisfying $\rho(x) \geq 0$ and

$$\int_\Gamma \rho(x)dV = 1,$$

where $dV$ is the volume element associated with the Fubini-Study metric. Thus we can think of $\rho(x)$ as an ensemble on the phase space $\Gamma$. For example, let us consider the measurement of an observable $F(x)$ with distinct eigenstate $x_0$, when initially the system is in a given pure state $x_0$. Then for the density function corresponding to an ensemble consisting of a large number of independent identical copies of the system we can write

$$\rho(x) = \delta(x, x_0) \text{ for the initial state, and } \rho(x) = \sum_i w_i \delta(x, x_i) \text{ after the measurement has been performed.}$$

Here $\delta(x, x_i)$ denotes a delta function on $\Gamma$, concentrated at the point $x_i$, and $w_i$ is the transition amplitude between the states $x_0$ and $x_i$. The expectation of an observable $F(x)$ in the general state $\rho(x)$ is then given by

$$\langle F \rangle = \int_\Gamma F(x) \rho(x) dV.$$

We can regard $\langle F \rangle$ as equating $\langle F \rangle$ with the unconditional expectation of the conditional expectation $F(x)$ in the pure state $x$. The dynamical evolution of $\rho(x)$ is governed by the Liouville equation, where the Poisson bracket between $\rho(x)$ and $H(x)$ is determined by the symplectic structure on $\Gamma$. If $\rho(x)$ is initially given by a delta function concentrated on a single pure state, then subsequently it remains of that form, and the point of concentration follows a Schrödinger trajectory.

Now, suppose we introduce the projection operator

$$\Pi^\beta_\alpha(x) = \frac{\bar{\psi}_\beta(x) \psi^\alpha(x)}{\bar{\psi}_\gamma(x) \psi^\alpha(x)}$$

(7)

corresponding to the pure state represented by a generic point $x \in \Gamma$. Then, the general quantum state can be expanded in terms of its moments $\Pi^\beta_\alpha$. In particular, the lowest moment of $\Pi^\beta_\alpha(x)$ in the state $\rho(x)$ gives rise to the density matrix of ordinary quantum mechanics:

$$\rho^\beta_\alpha = \int_\Gamma \rho(x) \Pi^\beta_\alpha(x) dV.$$ 

(8)

It follows from the formulae above that the expectation $\langle F \rangle$ agrees with the standard trace formula $\langle F \rangle$, provided $F(x)$ is a linear observable of the form $\Pi^\beta_\alpha$, that is, $F(x) = F^\alpha_\beta \Pi^\beta_\alpha(x)$. An advantage of the general expression (8) is that it can also be applied in the case of a nonlinear observable of the Kibble-Weinberg type $\Pi^\beta_\alpha$. It should be emphasised nevertheless that when we consider the statistical properties of ordinary linear observables, this formulation of quantum mechanics on $\Gamma$ is equivalent to the conventional Hilbert space approach.

Under suitable technical conditions the information in the state $\rho(x)$ can be represented by the totality of its moments, and a unique expansion of the form

$$\rho(x) = 1 + \mu^\alpha_\beta \Pi^\beta_\alpha(x) + \mu^\alpha_\beta \Pi^\beta_\alpha(x) \Pi^\alpha_\beta(x) + \cdots$$

(9)

exists, where the $\mu$-coefficients are trace-free and totally symmetric. A calculation then shows that the $n$-th coefficient is given, up to a combinatorial factor, by the trace-free part of the $n$-th moment of $\Pi^\beta_\alpha(x)$. It follows that the density matrix of ordinary quantum mechanics in general does not contain all of the information about the state of the system. This remains the case a fortiori if we relax the technical conditions and allow $\rho(x)$ to belong to a broader class of measures. However, if we wish to consider the statistical properties of linear observables, then, owing to formula (8), it suffices to consider the density matrix exclusively. Because our intention here is to investigate the entropy in ordinary quantum mechanics, we shall therefore examine the consequences of assuming that the information encoded in the density matrix is the only information available to us. In this context it is worth recalling the work of Mielnik, who regards the state in ordinary quantum theory as an equivalence class of density functions each of which gives rise to the same density matrix. We note, however, that there is a subtle deficiency in his approach, because it treats all distributions that give rise to the same density matrix on an equal footing. Clearly, some distributions contain more information than others, and according to the general principles of information theory we must look for the
distribution that is least informative, subject to the condition that it is consistent with the prescribed density matrix.

It should be evident from the foregoing discussion that the appropriate expression for the Shannon entropy of a quantum state \( \rho(x) \) is

\[
S_\rho = -\int_{\Gamma} \rho(x) \ln \rho(x) dV. \tag{10}
\]

Because \( \rho(x) \) is a probability density function defined on the smooth manifold \( \Gamma \), it follows that \( S_\rho \) possesses the standard properties of the Shannon entropy. The question we have to address here is thus: given a density matrix \( \rho_\alpha^\beta \), how do we express the corresponding quantum entropy \( S_\rho \), in terms of it? Clearly, for a generic density matrix, there exist many different density functions \( \rho(x) \) that give rise to the same \( \rho_\alpha^\beta \). Therefore, it is not obvious which \( \rho(x) \) we should select. This problem can be resolved by recalling our assumption that the density matrix is the only information available to us. This implies that the relevant density function \( \rho(x) \) is the one with minimum information, or maximum entropy among all \( \rho_\alpha^\beta \)'s subject to the constraint \( \int_{\Gamma} \rho(x) dV = 1 \). If we let \( \lambda_\alpha^\beta \) denote the Lagrange multiplier required for this extremisation problem, then the solution is a distribution of the canonical form

\[
\rho(x) = \exp\left(-\lambda_\alpha^\beta \Pi_\alpha^\beta(x) - \ln Z(\lambda)\right), \tag{11}
\]

where the normalisation is given by the generating function

\[
Z(\lambda) = \int_{\Gamma} \exp\left(-\lambda_\alpha^\beta \Pi_\alpha^\beta(x)\right) dV. \tag{12}
\]

The Lagrange multiplier \( \lambda_\alpha^\beta \) is determined, up to an arbitrary trace term, by the constraint

\[
-\frac{\partial \ln Z(\lambda)}{\partial \lambda_\alpha^\beta} = \rho_\alpha^\beta. \tag{13}
\]

The result \( \lambda_\alpha^\beta \) is perhaps surprising because in the literature of quantum theory the canonical distribution function arises typically in the thermal context.

It follows from the expression for the minimum information distribution function that the quantum Shannon entropy associated with the density matrix \( \rho_\alpha^\beta \) is given by a Legendre transformation

\[
S_\rho = \lambda_\alpha^\beta \rho_\alpha^\beta + \ln Z(\lambda), \tag{14}
\]

where \( \lambda_\alpha^\beta \) is determined by the relation \( \lambda_\alpha^\beta \). Alternatively, we can combine \( \lambda_\alpha^\beta \) and \( \lambda_\alpha^\beta \) and define \( S_\rho \) according to the scheme

\[
S_\rho = \sup_{\lambda} \left( \lambda_\alpha^\beta \rho_\alpha^\beta + \ln Z(\lambda) \right). \tag{15}
\]

In fact, one can show that \( \ln Z(\lambda) \) is convex on the vector space obtained by eliminating the trace of \( \lambda_\alpha^\beta \). The argument, as we indicate below, is reminiscent of the reasoning used to demonstrate the positivity of the heat capacity in statistical mechanics. It follows that \( \ln Z(\lambda) \) is the convex dual of the entropy, and that \( S_\rho \) is concave over the space of density functions. More specifically, we find that

\[
\frac{\partial^2 \ln Z}{\partial \lambda_\alpha^\beta \partial \lambda_i} = \int_{\Gamma} \rho(x) \left( \Pi_\alpha^\beta - \rho_\alpha^\beta \right) \left( \Pi_i^\beta - \rho_i^\beta \right) dV, \tag{16}
\]

which shows that the Hessian of \( \ln Z(\lambda) \) is given by the covariance of the projection operator \( \Pi_\alpha^\beta(x) \), which is positive definite for trace-free displacements in the value of \( \lambda_\alpha^\beta \). Indeed, the Hessian is independent of \( \lambda_\alpha^\beta \), since under the transformation \( \lambda_\alpha^\beta \rightarrow \lambda_\alpha^\beta + \mu \rho_\alpha^\beta \) we have \( Z(\lambda) \rightarrow e^{-\mu} Z(\lambda) \). It thus follows that \( \langle \Pi_\alpha^\beta \rangle \) defines a Riemannian metric, known as the Fisher-Rao metric, on the parameter space of the distribution \( \rho_\alpha^\beta \). Therefore, by convex duality \( \lambda_\alpha^\beta \), we conclude that \( S_\rho \) is concave in the sense that if \( \rho_\alpha^\beta(i) \) are density matrices for \( i = 1, 2, \cdots, n \) and if \( \{w_i\} \) is a set of probability weights, then

\[
S_\rho \left[ \sum_i w_i \rho_\alpha^\beta(i) \right] \geq \sum_i w_i S_\rho \left[ \rho_\alpha^\beta(i) \right], \tag{17}
\]

where \( S_\rho [\rho_\alpha^\beta] \) denotes the entropy \( \langle \Pi_\alpha^\beta \rangle \) associated with a given density matrix \( \rho_\alpha^\beta \).

This is our main result for the quantum entropy. To see that \( S_\rho \) differs from \( S_{vN} \) by a constant \( A \), independent of \( \rho_\alpha^\beta \), such that \( S_\rho = S_{vN} + \ln A \). Then solving for \( \rho_\alpha^\beta \) by use of \( \lambda_\alpha^\beta \) and \( \lambda_\alpha^\beta \) we obtain \( \rho_\alpha^\beta = A \exp(-\lambda_\alpha^\beta)/Z(\lambda) \), which implies that \( \int_{\Gamma} \Pi_\alpha^\beta \exp(-\lambda_\alpha^\beta \Pi_\alpha^\beta(x)) dV = A \exp(-\lambda_\alpha^\beta) \) holds for all \( \lambda_\alpha^\beta \). Expanding each side to first order in \( \lambda_\alpha^\beta \), we reach a contradiction.

We have demonstrated that if the information available at our disposal is given solely by the density matrix \( \rho_\alpha^\beta \), then the corresponding entropy is given by \( \langle \Pi_\alpha^\beta \rangle \). Conversely, any other form of entropy, such as that of von Neumann, implies the knowledge of information other than \( \rho_\alpha^\beta \), even if the entropy itself can be expressed in terms of \( \rho_\alpha^\beta \). Hence, in a strict sense, any other choice of entropy goes beyond the category of linear quantum mechanics, as is consistent with the fact that the von Neumann entropy gives the correct result in the case of a two state system. We choose the basis where the density matrix is diagonal, with elements \( \rho_1 \) and \( \rho_2 = 1 - \rho_1 \). Because \( \lambda_\alpha^\beta \) commutes with \( \rho_\alpha^\beta \), in this basis \( \lambda_\alpha^\beta \) is also diagonal, with eigenvalues \( \lambda_1 \) and
\( \lambda_2 \). The \( \Gamma \)-space integration for the generating function \( Z(\lambda) \) can be lifted to \( \mathbb{C}^2 \) with a spherical constraint on \( \psi^\alpha(x) \). The integration involves a Gaussian (cf. \( [\mathbb{I}] \)), and we obtain \( Z(\lambda) = (2\pi)^3 (e^{-\lambda_2} - e^{-\lambda_1})(\lambda_1 - \lambda_2)^{-1} \), from which it follows that

\[
\rho_1 = \frac{1}{\lambda_1 - \lambda_2} + \frac{1}{1 - e^{\lambda_1 - \lambda_2}}.
\] (18)

Then because the dependence on \( \lambda_2^2 \) is only up to the eigenvalue difference, we can set \( \lambda_2 = \lambda \) and \( \lambda_1 = -\lambda \). With these expressions at hand, we can compare the quantum entropy with the von Neumann entropy. The qualitative behaviours of \( S_\rho(\lambda) \) and \( S_{\rho_{vN}}(\lambda) \) in this example turn out to be similar, though not identical, as illustrated in Fig. 1, where we compare plots for the \( \lambda \)-derivatives of the two entropies. The two curves agree in the pure-state limits \( \lambda \to \pm \infty \).

![FIG. 1. The plots for the entropy derivative](image)

Although we have only shown explicit results for a two-state system, it is worth remarking that the \( \Gamma \)-space integration for the general generating function is invariably a Gaussian, and that the derivation of the entropy thus remains tractable for all finite dimensionalities.

In summary, we have introduced the idea of a probability density function \( \rho(x) \) on the space of rays through the origin of the Hilbert space that only reflects the information provided by the density matrix. Based upon this we were able to obtain the Shannon entropy for a quantum state, which, from an information theoretic point of view, is superior to von Neumann’s proposal for the entropy. The utility of the distribution \( [\mathbb{I}] \) does not exclusively reside, however, in studying the entropy of quantum states. In fact, it can be applied to numerous other probabilistic and information theoretic aspects of quantum mechanics, as well as quantum estimation theory. For example, the Lagrange multiplier \( \lambda_3^2 \) in the foregoing analysis can be viewed as parameterising the quantum state \( \rho_3^2 \) of the system. Then, in the problem of estimating an unknown quantum state \( [\mathbb{I}] \), it is of interest to consider the Fisher information matrix which determines the variance lower bound (cf. \( [\mathbb{I}] \)). In the present context, this is given by the Hessian \( [\mathbb{I}] \) of the generating function \( \ln Z(\lambda) \), which can be computed explicitly for a given \( \rho_3^2 \). The use of the minimal information state \( \rho(x) \) can also be applied to the theory of quantum communication. We hope that the approach introduced here will offer further insights into the understanding of quantum theory.

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