How ‘hot’ are mixed quantum states?

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Abstract

Given a mixed quantum state $\rho$ of a qudit, we consider any observable $M$ as a kind of ‘thermometer’ in the following sense. Given a source which emits pure states with these or those distributions, we select such distributions that the appropriate average value of the observable $M$ is equal to the average $\text{Tr} M \rho$ of $M$ in the state $\rho$. Among those distributions we find the most typical one, namely, having the highest differential entropy. We call this distribution conditional Gibbs ensemble as it turns out to be a Gibbs distribution characterized by a temperature-like parameter $\beta$. The expressions establishing the liaisons between the density operator $\rho$ and its temperature parameter $\beta$ are provided. Within this approach, the uniform mixed state has the highest ‘temperature’, which tends to zero as the state in question approaches to a pure state.

Keywords: quantum ensembles; differential entropy; Gibbs distribution

Introduction

It is a notorious property of quantum systems that their mixed states can be prepared using non-equivalent ensembles. For instance, having a qubit, if you mix two pure states $(0, 1)$ and $(1, 0)$ with proportion $\frac{1}{2} : \frac{1}{2}$, or three states

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\( \frac{1}{\sqrt{2i}} (9, 10\sqrt{2i}), \frac{1}{\sqrt{194}} (12, 5\sqrt{2i}) \text{ and } \frac{1}{\sqrt{17}} (3i, 2\sqrt{2}) \) in proportion \( \frac{281}{900} : \frac{17}{450} : \frac{17}{36} \),
you get the same mixed quantum state with the density matrix \([1]\):

\[
\rho = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\]

Now consider a continuous probability distribution on the set of all pure states (=one-dimensional projectors \(|\phi\rangle \langle \phi|\)), denote its density by \(\mu(\phi)\). We may view this as a source of particles which are emitted according to the probabilistic distribution \(\mu(\phi)\). To be rigorous, note that the characteristic feature of \(\mu\) is

\[
\int_{\mathbf{S}} \mu(\phi) \, d\phi = 1
\]

where \(\mathbf{S}\) is the set of all pure states and \(d\phi\) is the unitary invariant measure on pure states normalized to integrate to unity. This measure \(d\phi\) is unambiguously defined as \(\mathbf{S}\) is a connected compact manifold with a transitive action of the unitary group \(U(d)\).

Our next step is to fix an observable \(M\), associated with the self-adjoint operator, denote it also by \(M\). For any pure state \(|\phi\rangle \langle \phi|\) the average value of \(M\) is defined equal to \(\langle \phi | M | \phi \rangle\), which is, in turn, a continuous bounded function

\[
\tilde{M}(\phi) = \langle \phi | M | \phi \rangle
\]

on the manifold \(\mathbf{S}\). Averaging the average \((2)\) with respect to the distribution \(\mu(\phi)\), we obtain the average value of the observable \(M\) on the ensemble \(\mu\), which reads

\[
\int_{\mathbf{S}} \tilde{M}(\phi) \mu(\phi) \, d\phi = \left\langle \tilde{M}, \mu \right\rangle
\]

where \(\left\langle \cdot, \cdot \right\rangle\) is the scalar product in the space \(L^2(\mathbf{S}, d\phi)\).

On the other hand we may consider the average value \(\text{Tr} \, M \rho\) of the observable \(M\) in state \(\rho\), and then consider only the ensemble \(\mu\) compatible with \(\rho\), in that sense that, given \(M\) as the only measurement apparatus, we can not distinguish \(\rho\) and any of such \(\mu\). This is expressed as:

\[
\text{Tr} \, M \rho = \left\langle \tilde{M}, \mu \right\rangle
\]
1 The likelihood ratio

The expression (4) specifies for us a class of distributions. This is a broad class, for instance, it contains a delta-like distribution \( \mu(\phi) = \sum \lambda_j \delta(1 - \langle \phi | e_j \rangle) \) where \( \sum \lambda_j \langle e_j | e_j \rangle \) is the spectral decomposition of the density matrix \( \rho \). Our basic suggestion is the following. We fix certain fiducial distribution on the set of pure states—this distribution need not have anything in common with the density matrix \( \rho \). In this paper the uniform distribution over the set of all pure states is chosen as fiducial. Then, we compute a distance between the distribution in question and fiducial one: \( \mu_0(\phi) = 1 \), which averages to completely mixed state

\[
\int |\phi\rangle \langle \phi| \, d\phi = \frac{I}{d} = \begin{pmatrix}
1/d & 0 & \ldots & 0 \\
0 & 1/d & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & 1/d
\end{pmatrix}
\] (5)

There are many ways to define the distance between two distributions; we specify it to be Kullback-Leibler distance [2]:

\[
S(\mu \| \mu_0) = \int \mu(x) \ln \frac{\mu(x)}{\mu_0(x)} \, dx
\] (6)

The reason for this choice is that this distance minimizes the Type I error when discriminating states. Let us dwell on this issue in more detail.

Suppose the sender has two options: either emit states according to the fiducial distribution, or emit them according to the distribution \( \mu \). This is a standard way to send classical messages through quantum channels. The goal of the recipient is to determine what happened on the sender’s side. The recipient makes a null hypothesis—that the fiducial distribution was applied. Another option will be referred to as the concurring hypothesis. The Type I error is to accept the concurring hypothesis in the case when the fiducial ensemble was in fact prepared. The probability of Type I error is, according to Sanov theorem

\[
p(1|0) = e^{-S(\mu \| \mu_0)}
\]

That is why our goal is to minimize this probability, though staying within the restriction [4]. In our setting we have a particular choice [5] for the fiducial distribution, therefore the Kullback-Leibler distance will have the
2 Conditional Gibbs distributions

In this section we are going to solve a variational problem similar to that arising in classical thermodynamics. For a given density matrix $\rho$ and given observable $M$ we search a continuous ensemble, denote its distribution by $\mu(\phi)$, having minimal differential entropy with respect to the uniform ensemble and satisfying the compatibility relation (4):

$$S(\mu) \rightarrow \min, \quad \text{Tr} \, M \rho = \langle \tilde{M}, \mu \rangle$$

—recall that $\langle \cdot, \cdot \rangle$ is the scalar product in the space $L^2(S, d\phi)$. The combination of $\rho$ and $M$ plays here the rôle similar to that of energy in classical thermodynamics. We emphasize that the differential entropy used here is a mixing entropy (it is related to the ensemble $\mu$) rather than von Neumann entropy, which depends only on the density matrix $\rho$. The ensemble which yields the solution of this problem will be called conditional Gibbs ensemble. The appropriate Lagrange function reads:

$$L(\mu) = \int \mu(\phi) \ln \mu(\phi) \, d\phi - \lambda \left( \int \langle \phi| M |\phi \rangle \, \mu(\phi) \, d\phi - \text{Tr}(M \rho) \right)$$

where $\lambda$ is the Lagrange multiple. Making the derivative of $L$ over $\mu$ zero, we get

$$\mu(\phi) = e^{-\beta \langle \phi| M |\phi \rangle} / Z(\beta)$$

where $\beta$ is the optimal value of the Lagrange multiple $\lambda$, which we derive from the constraint (8). The normalizing multiple

$$Z(\beta) = \int e^{-\beta \langle \phi| M |\phi \rangle} \, d\phi$$

is the partition function for (9).

Yet having the explicit formula (9) for the solution of the variational problem (8), we still have to prove its existence for any pair $\rho$ and $M$. To do
that, first note that that the differential entropy (7) is a convex functional with respect to \( \mu \). The restriction \( \text{Tr} \, M \rho = \langle \hat{M}, \mu \rangle \) is, in turn, linear, thus specifying a linear affine manifold in the space \( \mathcal{L}^2(S, d\phi) \). Then the existence of appropriate \( \mu \) directly follows from Gel’fand theorem [4], and the form of \( \mu \) is specified by (9).

3 Analytic expressions

In this section we provide explicit formulas linking the temperature parameter \( \beta \) with the density operator \( \rho \) and the measuring observable \( M \). First let us evaluate the expression for the average value of \( M \), that is, the lhs of (4).

\[
\int_S \tilde{M}(\phi) \mu(\phi) \, d\phi = \sum_{s=1}^d M_s \frac{\partial \ln Z(\beta)}{\partial m_s} = G_M(\beta)
\]

The explicit expressions for the partial derivatives were obtained earlier [5]:

\[
\frac{\partial \ln Z(\beta)}{\partial m_s} = - \frac{\sum_{s=1}^d m_s \left( e^{-\beta m_s} \prod_{j \neq s}^d m_j + \frac{1}{m_s} \prod_{j \neq s}^d m_j \frac{\prod_{j \neq s}^d m_j}{m_s} \right)}{\sum_{k=1}^d \frac{e^{-\beta m_k} \prod_{j \neq k}^d m_j}{m_k}}
\]

where \( m_s \) range over the eigenvalues of \( M \) and \( m_{sj} = m_s - m_j \) (if two or more of them are equal, the appropriate expression is obtained as a limit starting with unequal eigenvalues). Summing them up with the eigenvalues \( m_s \) of \( M \), we get the expression for \( G_M(\beta) \):

\[
G_M(\beta) = - \left( \sum_{s=1}^d m_s \frac{e^{-\beta m_s}}{\prod_{j \neq s}^d m_j} \right) \left/ \left( \sum_{s=1}^d m_s \frac{e^{-\beta m_s}}{\prod_{j \neq s}^d m_j} \right) \right.
\]

(11)

From the expression (10) for \( Z(\beta) \), we infer that \( G \) is a monotonous decreasing function of the argument \( \beta \) whose values range between \( +\infty \) and 0; this takes place for any \( M \neq 0 \). That means, in turn, that the inverse of \( G_M \) exists for any \( M \neq 0 \), denote it by \( F_M \):

\[
F_M = G_M^{-1}
\]

(12)
As a result, we may write down the formula for $\beta$:

$$\beta = F_M (\text{Tr} \ M\rho)$$

(13)

4 Analogs with temperature: equalizing and convexity

Why do we claim that any observable $M$ can be treated as ‘thermometer’? Consider two quantum systems with state spaces $\mathcal{H}$ and $\mathcal{H}'$, respectively. Let their states initially be $\rho$ and $\rho'$. Then, since we consider a non-interacting coupling of the systems, the joint density matrix is $\rho \otimes \rho'$ in the tensor product space $\mathcal{H} \otimes \mathcal{H}'$. Let us measure the sum of values of the observables $M$ and $M'$, that is, introduce the observable $M = M \otimes \mathbb{I} + \mathbb{I} \otimes M'$.

Now let us fix the fiducial distribution (introduced in section 1), in our case this will be the uniform distribution over the set of product pure states. This reflects the fact that we are emitting particles in two independent laboratories. The conditional optimal ensemble with respect to the observable $M$ is the following distribution

$$\mu_M(\psi \otimes \psi') = e^{-\beta_M \langle \psi \otimes \psi'|M|\psi \otimes \psi'\rangle} / Z_M(\beta_M)$$

Like in classical thermodynamics, the partition function of the joint system is the product of subsystems’ partition functions:

$$Z_M(\tau) = \int \int e^{-\tau \langle \psi \otimes \psi'|M|\psi \otimes \psi'\rangle} \, d\phi \, d\phi' = \int \int e^{-\tau \left( \langle \psi|M|\psi\rangle + \langle \psi'|M'|\psi'\rangle \right)} \, d\phi \, d\phi' = Z_M(\tau) \cdot Z_{M'}(\tau)$$

denoting the equalizing property holds

If $\beta_M \leq \beta_{M'}$, then $\beta_M \leq \beta_M \leq \beta_{M'}$

(14)

which means that the conditional ensembles are equilibrium and that $\beta$ plays the rôle of inverse temperature.

As mentioned above, the function $F_M(\beta)$, is a monotone function of $\beta$ when the observable $M$ is fixed. Let us explore $F_M (\text{Tr} \ M\rho)$ as a function of
the density matrix $\rho$, when the ‘thermometer’ $M$ is fixed. From the convexity of $F_M(x)$ we deduce that, when $M$ is fixed, the function $F_M(\text{Tr}\, M\rho)$ is a convex function of $\rho$. That means, in turn, that the least value of the inverse temperature $\beta$ is attained on completely mixed state (5). Conversely, the pure states are the ‘coldest’ yielding the maximum for the temperature parameter $\beta$.

Conclusions

Continuous ensembles of pure states proved their relevance in various aspects of quantum mechanics. From the theoretical perspective, they provide the limit cases on which numerical characteristics of density matrices are attained, for instance, the minimal value of accessible information about the state is attained on ‘Scrooge’ ensemble which is a continuous distribution [6]. Furthermore, I claim that they are relevant from the operationalistic point of view. Even if we are speaking of preparing discrete ensembles, we must also have in mind that their are unavoidably smeared by various noises and, strictly speaking, we have to deal with continuous distributions.

We introduce the notion of fiducial distribution of pure states, which can be seen as given ‘for free’. In our case this is white noise—the uniform distribution on the set $S$ of all pure states of the system [7]. Then we choose an observable $M$. For any given mixed state $\rho$ a continuous ensemble is shown to exist, which (i) has the smallest Kullback-leibler distance from the fiducial one and (ii) reproduces $\rho$ provided we can measure only $M$. The resulting ensemble is described by exponential distribution (9) of pure states:

$$
\left(1/Z_M(\beta)\right) e^{-\beta\langle\psi|M|\psi\rangle}\langle\phi|\langle\phi|d\phi
$$

where the parameter $\beta$ plays a rôle in some respect similar to temperature, in particular, it is shown to possess the equalizing property. The geometric properties of the proposed ensembles were also studied [8].

The proposed ensembles can be applied for producing robust protocols for sending classical messages through noisy quantum channels—this is based on the general idea that in order to attain maximal efficiency of communication, one must feed in mostly robust states which are first of characterized by maximal entropy. Another prospective application of the proposed techniques is quantification of entanglement of mixed states [9].

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Acknowledgments

Profound discussion of the subject provided by prof. A.Kazakov and the participants of St.Petersburg research seminar on Quantum Information and Computation is acknowledged. The work was carried out under the auspices of Russian Basic Research Foundation (grant 04-06-80215a). One of the authors (RRZ) highly appreciates the hospitality of the Organizing Committee of Quantum-2006: III workshop ad memoriam of Carlo Novero (in particular, Marco Genovese) and the Quantum Computation Group of I.S.I. Foundation (Torino, Italy) for valuable suggestions and comments within a research seminar of the EC-funded project TOPQIP.

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