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The information entropy of quantum-mechanical states

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Abstract. – It is well known that a Shannon-based definition of information entropy leads in the classical case to the Boltzmann entropy. It is tempting to regard the von Neumann entropy as the corresponding quantum-mechanical definition. But the latter is problematic from the quantum information point of view. Consequently, we introduce a new definition of entropy that reflects the inherent uncertainty of quantum-mechanical states. We derive for it an explicit expression, and discuss some of its general properties. We distinguish between the minimum uncertainty entropy of pure states, and the excess statistical entropy of mixtures.

The statistical state of a system (ρ) is specified in classical mechanics using a probability function, while in the quantum-mechanical case it is specified by a probability matrix. The information entropy $S[\rho]$ is a measure for the amount of extra information which is required in order to predict the outcome of a measurement. If no extra information is needed, we say that the system is in a definite statistical state with $S = 0$. A classical system can be in principle prepared in a definite state. But this is not true for a quantum-mechanical system. Even if the system is prepared in a pure state, still there is an inherent *uncertainty* regarding the outcome of a general measurement. Therefore, the minimum information entropy of a quantum-mechanical state is larger than zero.

It is clear that the common von Neumann definition of quantum-mechanical entropy does not reflect the inherent uncertainty which is associated with quantum-mechanical states [1, 2]. For a pure state it gives $S = 0$. Let us assume that we prepare two spins in a (pure) singlet state. In such a case the von Neumann entropy of a single spin is $S = \ln(2)$, while the system as a whole has $S = 0$. If it were meaningful to give these results an information theoretic interpretation, it would be implied that the amount of information which is needed to determine the outcome of a measurement of a subsystem is larger than the amount of information which is required in order to determine the outcome of a measurement of the whole system. This does not make sense.

Thus we are faced with the need to give a proper definition for the (information) entropy of a quantum-mechanical state. As in the case of the von Neumann entropy, it can be regarded as a measure for the lack of purity of a general (mixed) state. But unlike the von Neumann entropy it does not give $S = 0$ for pure states, and does not coincide with the thermodynamic entropy in case of a thermal state.

In this letter we introduce a Shannon-based definition of quantum-mechanical information entropy; derive explicit expressions for the calculation of this entropy; and discuss some of its

properties. For further motivations and review of the traditional definition of entropy in the context of quantum computation and quantum information, see [3].

The statistical state of a classical system, that can be found in one of N possible states r , is characterized by the corresponding probabilities p_r , with the normalization $\sum p_r = 1$. The amount of information which is required in order to know what is going to be the outcome of a measurement is given by the Shannon formula: $S = -\sum_r p_r \ln(p_r)$. Note that $S = 0$ if the system is in a definite state, while $S = \ln(N)$ in the worst case of a uniform distribution. This definition coincides with the Boltzmann definition of entropy if r are regarded as phase space cells.

In the quantum-mechanical case the statistical state of a system is described by a probability matrix ρ . A measurement requires the specification of a basis of (pure) states $|a\rangle$. Without any loss of generality, it is convenient to define a given basis by specifying a Hermitian operator \mathcal{A} . We note that in a semiclassical context the basis \mathcal{A} can be regarded as a *partitioning* of phase space into cells. The probability to have a as the outcome of a measurement is $\langle a|\rho|a\rangle$. Therefore the information entropy for such a measurement is

$$S[\rho|\mathcal{A}] = -\sum_a \langle a|\rho|a\rangle \ln(\langle a|\rho|a\rangle). \quad (1)$$

Our notation emphasizes that this is in fact a conditional entropy: one has to specify in advance what is the measurement setup. In particular, there is a basis \mathcal{H} in which ρ is diagonal, $\rho = \text{diag}\{p_r\}$. In this basis $S[\rho|\mathcal{A}]$ attains its *minimum* value,

$$S_{\text{H}}[\rho] = S[\rho|\mathcal{H}] = -\sum_r p_r \ln(p_r) = -\text{trace}(\rho \ln \rho), \quad (2)$$

which is known as the von Neumann entropy. We would like to emphasize that from the *strict* information theory point of view, the quantity $S_{\text{H}}[\rho]$ can be interpreted as information entropy (*à la* Shannon) only if we assume *a priori* knowledge of the preferred basis that makes ρ diagonal. In equilibrium statistical mechanics the interest is in stationary states. This means that ρ is diagonal in the basis that is determined by the Hamiltonian \mathcal{H} . Therefore, if we measure the energy of the system, the information entropy is indeed $S_{\text{H}}[\rho]$. In particular, for a canonical state $\rho \propto \exp[-\beta\mathcal{H}]$, it reduces to the thermodynamic definition of entropy.

For a pure quantum-mechanical state $\rho = |\Psi\rangle\langle\Psi|$, the von Neumann definition gives $S_{\text{H}}[\rho] = 0$. This seems to imply that a pure quantum-mechanical state is lacking a statistical nature. This is of course not correct. For a general measurement we have *uncertainty*. An absolute definition of an information entropy of a quantum-mechanical state should not assume any special basis. This implies a *unique* definition of the *absolute* entropy. Using standard information theory argumentation we conclude that⁽¹⁾

$$S[\rho] = \overline{S[\rho|\mathcal{A}]} = S_0(N) + F(p_1, p_2, \dots) \equiv S_0(N) + S_{\text{F}}[\rho], \quad (3)$$

where the overline indicates averaging over all possible basis sets with uniform measure (no preferred basis). We would like to emphasize that the averaging procedure is *unique*: A choice of a basis is like a choice of “direction” in a $(2N - 1)$ -dimensional space (in the case of spin 1/2 this direction can be interpreted as the geometrical orientation of our xyz axes in the physical space). The second equality in eq. (3) gives an explicit expression for the absolute entropy,

⁽¹⁾If we regard the measurement apparatus as a part of the system, then information theory tells us that the total entropy is $S_{\text{total}} = S[\mathcal{A}] + \sum_{\mathcal{A}} P(\mathcal{A})S[\rho|\mathcal{A}]$. The probability $P(\mathcal{A})$ describes our lack of knowledge regarding the state of the apparatus, and $S[\mathcal{A}]$ is its corresponding entropy. Quantum mechanics assumes that there is no preferred basis.

which we are going to derive below. The result is written as a sum of two terms: The first term is the *minimum uncertainty entropy* of a quantum-mechanical state, achieved by a pure state, while the second term gives the deviation from purity. We shall call the second term excess statistical entropy, and will use for it the notation $S_F[\rho]$. Conceptually, it is meaningful to ask to what extent $S_F[\rho]$ is correlated with $S_H[\rho]$. We shall discuss this issue later on.

Assume that $\rho = \text{diag}\{p_r\}$ is diagonal in some basis \mathcal{H} . We can regard all the possible \mathcal{A} basis sets, as unitary “rotations” of \mathcal{H} . This means that any $a \in \mathcal{A}$ in the rotated basis is obtained from a state $r \in \mathcal{H}$ in the preferred basis by an operation U . Consequently,

$$S = \overline{\sum_a f\left(\sum_r p_r |\langle r|a\rangle|^2\right)}^{\mathcal{A}} = \overline{\sum_s f\left(\sum_r p_r |\langle r|U|s\rangle|^2\right)}^{\mathcal{U}} \quad (4)$$

$$= \overline{Nf\left(\sum_r p_r |\langle r|\Psi\rangle|^2\right)}^{\Psi} = \overline{Nf\left(\sum_r p_r (x_r^2 + y_r^2)\right)}^{\text{sphere}} = N \int_0^\infty f(s) P(s) ds, \quad (5)$$

where we use the notation $f(s) = -s \ln(s)$. Each averaged $|\langle r|U|s\rangle|^2$ in eq. (4) is equal to $|\langle r|\Psi\rangle|^2$ averaged over all possible Ψ , which leads to eq. (5). It is important to re-emphasize that the quantum-mechanical “democracy” uniquely defines the measure for this Ψ average. This becomes more transparent if we define x_r and y_r as the real and imaginary parts of $\Psi_r = \langle r|\Psi\rangle$. The normalization condition is $\sum_r (x_r^2 + y_r^2) = 1$. Hence in the final expression the average is over all possible directions in a $(2N - 1)$ -dimensional space. In the final expression we introduce the notation

$$s = \sum_r p_r |\Psi_r|^2 = \sum_r p_r (x_r^2 + y_r^2) \quad (6)$$

and its probability distribution is denoted $P(s)$. In what follows we discuss the calculation of $P(s)$ and its integral with $f(s)$.

In case of a maximally mixed state $P(s)$ is delta-distributed around $s = 1/N$, and hence $f(s) = \ln(N)/N$. The corresponding information entropy is therefore $S[\rho] = \ln(N)$, as expected. If the state is not maximally mixed, then $P(s)$ becomes non-trivial. In case of a pure state $s = |\Psi_1|^2$ and its distribution is well known [4]:

$$P(s) = (N - 1)(1 - s)^{N-2}. \quad (7)$$

Thus we get an expression for the “*minimum uncertainty entropy*” which is N -dependent:

$$S_0(N) = \sum_{k=2}^N \frac{1}{k} \approx \ln(N) - (1 - \gamma) + \frac{1}{2N}. \quad (8)$$

Using the asymptotic approximation in the last equality we see that the difference between the S of a maximally mixed state, and that of a pure state, approaches a universal value $(1 - \gamma)$, where γ is Euler’s constant. Using different phrasing, we see that the excess statistical entropy is universally bounded:

$$S_F[\rho] < 1 - \gamma. \quad (9)$$

To get an actual expression for the excess statistical entropy, due to lack of purity, requires some more effort. The first stage is to calculate $P(s)$ leading to (see appendix)

$$P(s) = (N - 1) \sum_{(p_r > s)} \left[\prod_{r'(\neq r)} \frac{1}{p_r - p_{r'}} \right] (p_r - s)^{N-2}. \quad (10)$$

The second stage is to calculate the integral of eq. (5) using

$$\int_0^p (p-s)^{N-2} s \ln(s) ds = \frac{p^N}{N(N-1)} \left[\ln(p) - \sum_{k=2}^n \frac{1}{k} \right]$$

and then to use the identity (see appendix)

$$\sum_r p_r^N \prod_{r'(\neq r)} \frac{1}{p_r - p_{r'}} = \sum_r p_r = 1. \quad (11)$$

Hence one obtains

$$F(p_1, p_2, \dots) = - \sum_r \left[\prod_{r'(\neq r)} \frac{p_r}{p_r - p_{r'}} \right] p_r \ln(p_r). \quad (12)$$

This expression is independent of N . Namely, extra zero eigenvalues do not have any effect on the result. Some particular cases are of interest. For a mixture of two states we get

$$F(p_1, p_2) = - \frac{1}{p_1 - p_2} (p_1^2 \ln(p_1) - p_2^2 \ln(p_2)). \quad (13)$$

For a uniform mixture of n states we get

$$S_F[\rho] = \ln(n) - \sum_{k=2}^n \frac{1}{k}, \quad (14)$$

$$S[\rho] = \ln(n) + \sum_{n < k \leq N} \frac{1}{k}. \quad (15)$$

Either $S_H[\rho]$ or $S_F[\rho]$ can serve as a measure for lack of purity. In fig. 1 we present results of calculation of $S_F[\rho]$ vs. $S_H[\rho]$ for a set of representative states, both uniform and non-uniform mixtures. We see that there is a very strong correlation between these two (different) measures of purity.

Our definition of entropy has some interesting mathematical properties. One simple property is concavity: Given $0 < \lambda < 1$ and two sets of probabilities, we have

$$F(\lambda p_r + (1-\lambda)q_r) \geq \lambda F(p_r) + (1-\lambda)F(q_r). \quad (16)$$

This follows from the concavity of $f(s)$ in eq. (5). Concavity and symmetry with respect to the variables p_i imply that $S[\rho]$ attains its maximum for maximally mixed states and its minimum for pure states. This property is helpful for justifying argumentations that are based on ‘‘worst case’’ calculations. Below we list some less trivial properties which are of physical interest.

Consider a system in a state ρ , and its subsystem which is in some state σ . Technically, the reduced probability matrix σ is obtained from ρ by tracing over the irrelevant indices. From general information theoretic considerations we expect

$$S[\sigma] < S[\rho]. \quad (17)$$

This means that determination of a state of a subsystem requires less information. As explained in the introduction, this inequality is violated by the von Neumann entropy. But

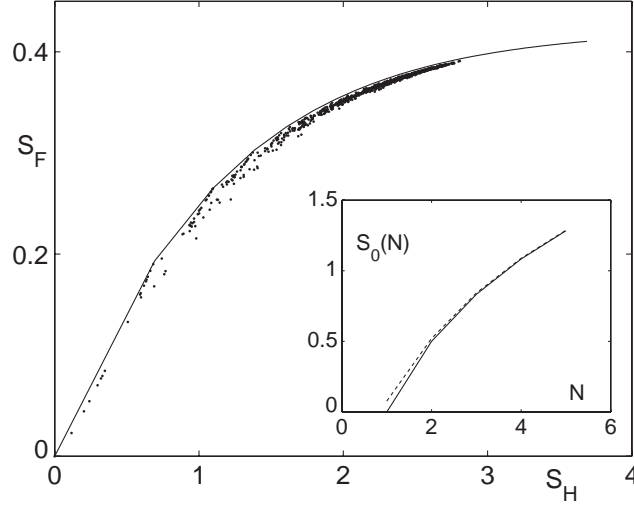


Fig. 1 – The excess information entropy of a mixed quantum-mechanical state S_F vs. the von Neumann entropy S_H . The solid line is for uniform mixtures, while the dots are for randomly chosen (non-uniform) mixtures. Inset: The information entropy of a pure quantum-mechanical state as a function of the Hilbert space dimension N . See eq. (8). The dashed line is the asymptotic approximation.

with our definition $S[\rho] \geq S_0(MN) \geq S_0(2N) > \ln(N) > S[\sigma]$, where N and MN are the dimensions of σ and ρ , respectively.

Another common physical situation is having a state $\rho = \sigma_A \otimes \sigma_B$, where σ_A and σ_B are states of subsystems that were prepared independently(!). Obviously, we have the property

$$S[\rho|\mathcal{A} \otimes \mathcal{B}] = S[\sigma_A|\mathcal{A}] + S[\sigma_B|\mathcal{B}]. \quad (18)$$

But for the absolute information entropy we expect

$$S[\rho] \geq S[\sigma_A] + S[\sigma_B]. \quad (19)$$

This comes about because there are bases which are not “external tensor product” of \mathcal{A} -basis and \mathcal{B} -basis. Thus, this inequality reflects the greater uncertainty that we have in the state determination of the combined system. Note that if our world were classical, we would get an equality, which is the case with the Boltzmann entropy, and in fact also with the von Neumann entropy. In order to better establish eq. (19) we can consider a worst case scenario. Let N and M be the dimensions of σ_A and σ_B , respectively. Assume that these states are uniform mixtures of n and m states, respectively, then ρ is a uniform mixture of nm states in dimension NM . Using eq. (15) and the inequality

$$\begin{aligned} \sum_{k=nm+1}^{NM} \frac{1}{k} &= \sum_{k=nm+1}^{mN} \frac{1}{k} + \sum_{k=mN+1}^{NM} \frac{1}{k} = \\ &= \sum_{k_1=n+1}^N \sum_{l_1=0}^{m-1} \frac{1}{k_1 m - l_1} + \sum_{k_2=m+1}^M \sum_{l_2=0}^{N-1} \frac{1}{k_2 N - l_2} > \sum_{k=n+1}^N \frac{1}{k} + \sum_{k=m+1}^M \frac{1}{k}, \end{aligned}$$

we confirm that eq. (19) is indeed satisfied. A particular case of the inequality of eq. (19) is that the minimum uncertainty entropy satisfies

$$S_0(NM) > S_0(N) + S_0(M). \quad (20)$$

But what about the excess statistical entropy? Our conjecture is that

$$S_F[\rho] \leq S_F[\sigma_A] + S_F[\sigma_B]. \tag{21}$$

We can again establish this inequality for uniform mixtures of n and m states in dimensions N and M , respectively: Using eq. (14) we observe that

$$S_F[\rho] - S_F[\sigma_A] - S_F[\sigma_B] = S_0(n) + S_0(m) - S_0(nm),$$

which is negative by eq. (20). It is important to realize that eq. (20) overcompensates the inequality eq. (21) leading to eq. (19). It is well known that for the von Neumann entropy we have the general inequality

$$S_H[\rho] \leq S_H[\sigma_A] + S_H[\sigma_B], \tag{22}$$

which holds for any subdivision of a system into two (correlated) subsystems. We already observed (fig. 1) that $S_F[\rho]$ is strongly correlated with $S_H[\rho]$. Moreover, this correlation is *sublinear*. It follows that we expect the easier inequality eq. (21) to hold in general, also in case of correlated subsystems.

The effect of quantum measurements on the entropy is of special interest. Let P_i be a complete orthogonal set of projectors ($\sum_i P_i = 1$). The state after a projective measurement is $\sigma = \sum_i P_i \rho P_i$. Consequently, the state of the system becomes more mixed. This is indeed reflected by an increase in the von Neumann entropy of the systems. Also our entropy is a measure for lack of purity. Therefore, it is reasonable to expect $S[\sigma] \geq S[\rho]$. We were not able to prove this assertion.

Summary. – The von Neumann entropy $S[\rho|\mathcal{H}]$ is useful in the thermodynamic context, where the interest is *a priori* limited to stationary (equilibrium) states. If we want to study the growth of entropy during an ergodization process, we may consider $S[\rho|\mathcal{A}]$, where \mathcal{A} is a basis (or a “partition” of phase space) that does not commute with \mathcal{H} . See, for example, ref. [5], where entropy is defined with respect to the position representation. In the latter case the entropy of a pure state is in general non-zero. In the present study we have derived an explicit expression for the minimum uncertainty entropy $S_0(N)$ of pure states. This can be associated with the *average* over the minimum entropic uncertainty [6]. We also have derived an expression for the excess statistical entropy $S_F[\rho]$ of mixtures. The latter can be used as a measure for lack of purity of quantum-mechanical states, and it is strongly correlated with the von Neumann entropy $S_H[\rho]$. It is bounded from above by $(1 - \gamma)$, where γ is Euler’s constant. The total information entropy $S[\rho]$, unlike the von Neumann entropy, has properties that do make sense from the quantum information point of view.

APPENDIX

Switching to the variables $s_r = x_r^2 + y_r^2$ the definition of $P(s)$ takes the form

$$\begin{aligned} P(s) &= \left\langle \delta \left(s - \sum_r p_r (x_r^2 + y_r^2) \right) \right\rangle_{\text{sphere}} = (N-1)! \int_0^\infty ds_1 \dots ds_N \delta \left(1 - \sum_r s_r \right) \delta \left(s - \sum_r p_r s_r \right) \\ &= (N-1)! \int_0^\infty ds_1 \dots ds_N \int \frac{d\omega d\nu}{(2\pi)^2} e^{(1-\sum_r s_r)(i\nu+0) + i(s-\sum_r p_r s_r)\omega}, \end{aligned}$$

where the infinitesimal 0 has been introduced to insure convergence once the order of integration is changed. Thus, after the integration over $ds_1 \dots ds_N$, one has

$$P(s) = (N-1)! \int \frac{d\omega d\nu}{(2\pi)^2} e^{i\nu+i\omega s} \prod_r \frac{1}{i\omega p_r + i\nu + 0} = \int \frac{d\omega}{2\pi} \frac{(N-1)!}{(i\omega)^{N-1}} \sum_r e^{i\omega(s-p_r)} \prod_{r'(\neq r)} \frac{1}{p_{r'} - p_r}.$$

One can show (see below) that there is no singularity in the integral at $\omega = 0$, so one can deform the contour of integration in such a way that it will go slightly above the point $\omega = 0$. Then one can make the integral term by term leading to the final result eq. (10). Namely, if $p_r < s$ the contour is closed in the upper half plane leading to zero, while if $p_r > s$ the contour is closed in the lower half plane leading to a non-zero contribution from the $\omega = 0$ pole.

The above manipulation was based on the observation that the integrand *as a whole* is non-singular: The $1/\omega^{N-1}$ singularity of the individual terms cancel upon summation over r . This cancellation can be established by expanding the exponent in powers of ω , and using the identity

$$\sum_r (s - p_r)^n \prod_{r'(\neq r)} \frac{1}{p_r - p_{r'}} = 0 \quad \text{for } n \leq (N - 2).$$

Both this identity and also eq. (11) can be proved by the following procedure:

$$\sum_r g(p_r) \prod_{k(\neq r)} \frac{1}{p_r - p_k} = \oint \frac{dz}{2\pi i} g(z) \prod_k \frac{1}{z - p_k} = \oint \frac{dz}{2\pi i} z^{N-2} g(1/z) \prod_k \frac{1}{1 - p_k z},$$

where in the last step one changes $z \mapsto 1/z$.

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