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Quantum Density Matrix and Entropic Uncertainty*

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ABSTRACT

A discussion of the determination of the quantum density matrix from realistic measurements using the maximum entropy principle is presented.

1. Introduction

The application of MAXENT to quantum theory is not a well-developed subject. Indeed, there is only one paper to my knowledge that gives a satisfactory treatment (in the mathematical sense) of this approach.[1] While this treatment lends itself to a discussion of certain questions in Quantum Measurement Theory, a normally esoteric subject of little physical consequence, it was developed with a very practical problem in mind. Namely, how does one choose a quantum density matrix based on realistic and necessarily incomplete measurements. Before answering this, one must answer a simpler question. How does one properly describe the results of a measurement of a variable with a continuous spectrum (such as position or momentum) when the experimental device has finite resolution?

The answer to this question was recently given by Partovi,[2] who based his treatment on a criticism and an idea by Deutsch.[3]

Entropic Uncertainty:

The basic 'trick' of the entropic formulation of uncertainty is to introduce the relevant characteristics of the measuring device into the measure of uncertainty. This inclusion will lead to unexpected physical consequencies. To that end let us introduce the notation of a measuring devive D^A which is used to measure the observable A. Thus a measurement will consist of a partitioning of the spectrum (either continuous or discrete) of A into a collection of subsets α_i. Therefore the state of the system, $|\psi\rangle$, is to be described by a corresponding set of probabilities

$$P_i^A = P_i^A(\psi \mid D^A) . \tag{1.1}$$

The number P_i^A is the probability that the measurement will yield a value in the subset α_i. Since the most common type of subset will be an interval, they will be called 'bins'. The spectrum is a property of A, but the manner in which it is partioned into bins is a property of the measuring device.

The process of binning is represented by the expression for the probability defined above

$$P_i^a = \langle\psi|\, \pi_i^a \,|\psi\rangle \;/\; \langle\psi \mid \psi\rangle \quad . \tag{1.2}$$

The operator π_i^a is the projection onto the subspace relevant to the subset α_i. The completeness relation is transformed into the operator statement

$$1 = \sum_i \pi_i^a \ . \tag{1.3}$$

The entropy associated with the measurement of the observable A using the device D including the uncertainty due to the effects of binning is

$$S(\psi \mid D^A) = -\sum_i P_i^A \ln P_i^A \ , \tag{1.4}$$

where P_i^A is defined in eqn (1.2) .

In the special case that the subset α_i includes only one eigenvalue of the operator A, then the projection operator simplifies to

$$\pi_i^a = |a_i\rangle \ \langle a_i| \ , \tag{1.5}$$

and the measurement entropy reduces to

$$S(\psi \mid D^A) = -\sum_i \mid \langle\psi \mid a_i\rangle \mid^2 \ \ln \ \mid \langle\psi \mid a_i\rangle \mid^2 \tag{1.6}$$

which is the form given in ref.3 . However, in most interesting cases, at least some of the observables of interest will be either continuous or will be a discrete spectra with a limit point.

Duetsch[3] and Partovi[2] showed that a proper definition of the uncertainty in the measurement of the two observables A and B in the state ψ is simply the total entropy

$$U(D^A, D^B; \psi) = S(\psi \mid D^A) + S(\psi \mid D^B), \tag{1.7}$$

This expression has the property that it possesses a lower bound that depends on the measuring devices D^A and D^B but not on the state ψ.

Since the probabilities $P_i^{A or B}$ are normalized, the 'uncertainty' can be rewritten in terms of the joint probability $P_i^A P_j^B$:

$$U(D^A, D^B; \psi) = -\sum_i \sum_j P_i^A P_j^B \ln P_i^A P_j^B \quad . \tag{1.8}$$

This form also provides the physical justification for adding the individual entropic uncertainties and considering that as the proper measure of uncertainty. Note that this has nothing to do with 'simultaneous measurements' but is related to the serial measurement of the observables A and B on an identically prepared beam.

This uncertainty should be interpreted in terms of a higher sample space . It is a generalization of the standard case in that the subsequent samples are not measurements of the same observable. It corresponds to independent measurements of different observables performed on an identically prepared beam. Therefore the product of the two probabilities is expected. The above form also generalizes in a natural way to the case of more than two observables (or in other words to more than two independent samples).

A comparison with the classic Heisenberg's uncertainty principle is facilitated by noting first that by some simple manipulations, we have

$$P_i^A \, P_j^B \; \leq || \; \pi_i^A \; + \; \pi_j^B \; ||^2 \; /4 \; . \tag{1.9}$$

The double brace means the norm of the operator sum. Therefore the uncertainty can easily be shown to satisfy the inequality

$$U(D^A, D^B; \psi) \; \geq \; 2 \; \ln[\, 2 \, / \, sup_{i,j} \; || \; \pi_i^A \; + \pi_j^B \; || \,] \; . \tag{1.10}$$

Since the π_i^a are projection operators, it immediately follows that the left hand side of eqn. (1.9) is between the limits of $1/4$ to 1. It achieves unity only if there is a common eigenfunction of the operators A and B. It is only in this circumstance that the uncertainty as given in eqn. (1.8) can be zero; in all other circumstances it is positive. Any definition of the uncertainty should satisfy this condition if it is to be at all reasonable and even consistent.

REMARK: It is interesting to note that the most popular extension of the uncertainty principle (as judged by the literature), namely

$$[\langle A^2 \rangle - \langle A \rangle^2 \,] \, [\langle B^2 \rangle - \langle B \rangle^2 \,] \, \geq \, | \, \langle [A, B] \rangle \, |^2 \; /4 \; , \tag{1.11}$$

where the expectation values are taken in the state ψ, does not satisfy this condition (for example, let A and B have opposite symmetry. Then the right-hand side vanishes if the state has a definite symmetry).

The Density Matrix:

The object of this section will be to argue that the measurement entropy defined above is more general than the standard form yet will reduce to the familiar form for the ensemble entropy in the correct physical limit. The measurement entropy will, however, allow the proper inference of the density matrix ρ from any set of necessarily incomplete measurements.

We shall always consider that a measurement is performed only once on a particular copy of the system. We imagine an 'oven' that produces a beam of identical copies of the basic system that is overall stationary in its properties, and thereby reproducible. To describe such a system, we introduce the standard density matrix by the replacement

$$|\psi\rangle \; \langle\psi| \; \rightarrow \rho \; , \tag{1.12}$$

and

$$\langle\psi| \; \pi_i^a \; |\psi\rangle \;\; \rightarrow tr(\rho\pi_i^a \;) \; . \tag{1.13}$$

There is a considerable amount of physics behind this innocent looking replacement involving an average over the output of the oven and possible correlations.

The measurement entropy of the ensemble corresponding to the operator A is then taken to be

$$S(\psi \mid D^A \,) \; = \; -\sum_i tr(\rho\pi_i^A \;) \; \ln tr(\rho\pi_i^A \;) \; , \tag{1.14}$$

which is a joint property of the system and the measuring device D.

The question that must now be answered is **what operator should we choose for A so that S corresponds to the entropy of the ensemble?** It should come as no surprise (a similar result was proven by von Neumann- his argument can be carried over to the present case with only a minimum of thought) that the unique choice for A is ρ itself. Since the density matrix describes all that can be known about the system and contains nothing superfluous, it is the operator that has the least uncertainty/entropy about the system. The motivation behind this argument and this choice for the operator we term the **maximum uncertainty principle** .

Now note that $tr\rho = 1$ and $tr\rho^2 \leq 1$. Therefore the density matrix has a purely discrete spectrum. Following the discussion of eqn. (1.5), if the measuring device is sufficiently fine-binned, then the projection is

$$\pi_i^{\rho} = |i\rangle \langle i| , \tag{1.15}$$

where the state $|i\rangle$ is an eigenfunction of the density matrix:

$$\rho |i\rangle = \rho_i |i\rangle . \tag{1.16}$$

The entropy then becomes

$$S = -\sum_i \rho_i \ln \rho_i , \tag{1.17}$$

which can be immediately written in the familiar abstract form

$$S = -tr[\rho \ln \rho] . \tag{1.18}$$

Thus we see that when the measuring device is made sufficiently accurate, the ensemble entropy defined above reduces to the usual form. However, for 'cruder' (and more physical) devices, the finite resolution implicit in the projection operators plays a crucial and new role. Thus we have given a formalism that provides a unified physical description of both the microscopic and macroscopic situations.

The procedure now follows in analogy to the previous sections. The ensemble entropy is maximized subject to the measurement constraints ($a = 1, ..A$)

$$P_i^a = tr(\rho \pi_i^a) . \quad (1.19)$$

The result is

$$\rho = Z^{-1} \exp[-\sum_{a,i} \lambda_i^a \pi_i^a] . \quad (1.20)$$

The multipliers λ_i^a are determined from

$$Z = tr(\exp[-\sum_{a,i} \lambda_i^a \pi_i^a]) , \quad (1.21)$$

and

$$P_i^A = Z^{-1} tr(\pi_i^A \exp[-\sum_{a,i} \lambda_i^a \pi_i^a]) . \quad (1.22)$$

It should be stressed that while the form, eqn. (1.20) , of the density matrix resembles the classical one, it is an operator. The projection operators in the exponent can be quite complicated in form, since they do not in general commute with each other. The density matrix must be evaluated with some care.

Some Examples:

In this paragraph we shall give two examples that illustrate the utility and simplicity of the entropic uncertainty approach. The examples are chosen for reasons of simplicity of presentation and relevance.

The first is the well-discussed problem of the correct form of the uncertainty relation for compact variables. We choose for an example the polar angle and its conjugate angular momentum. Thus the relevant operators are $A = \phi$ and $B = L_z$. The apparatus will be assumed to be able to measure the angle only to the extent that the result can be assigned to N bins, where $N = 2\pi/\delta\phi$

with $\delta\phi$ being the width of the angular bins, while the angular momentum can be measured and resolved down to a single value (which is integer). From eqn. (1.9) it is seen that we need to evaluate the maximum eigenvalue of the operator $\pi_i^A + \pi_j^B$. This eigenvalue equation takes the form

$$(\pi_i^\phi + \pi_m^{L_z})\,|v\rangle = \lambda\,|v\rangle \ , \tag{1.23}$$

where (the bin boundaries are located at ϕ_i)

$$\pi_i^\phi = \Theta(\phi - \phi_i)\Theta(\phi_{i+1} - \phi) \tag{1.24}$$

and the angular momentum projector is the integral operator

$$\pi_m^{L_z} = \frac{1}{2\pi}\int_o^{2\pi} d\phi'\, exp[\, im(\phi - \phi')\,]\ . \tag{1.25}$$

The solution corresponding to the maximum eigenvalue is found to be

$$|v_{max}\rangle = [1 + (\delta\phi/2\pi)^{1/2}\pi_i^\phi\,]\ |m\rangle \ , \tag{1.26}$$

where the state $|m\rangle$ is an eigenfunction of the angular momentum operator with eigenvalue m, with

$$\lambda_{max} = 1 + (\delta\phi/2\pi)^{1/2}. \tag{1.27}$$

The final result for the minimum uncertainty is

$$U(D^A, D^B; \psi) \geq 2\ \ln[\,2\,/\,[1 + (\delta\phi/2\pi)^{1/2}\,]\ . \tag{1.28}$$

Note that $\delta\phi$ is the resulution of the measuring device, <u>not</u> the variance. It is helpful in interpreting this result to note the following: if the angle ϕ is found to be in a particular bin while the angular momentum is measured to have a definite value m, then the joint probability has an upper bound given by

$$P_i^{\phi}\, P_m^{L_z} \,\leq\, \frac{1}{4}\,[1\,+\,(\delta\phi/2\pi)^{1/2}\,]^2\;. \tag{1.29}$$

This is a much more reasonable expression of the physics in the uncertainty relation than is given by the standard Heisenberg-type inequality involving variances.

Finally, I will just quote the corresponding result for continuous variables and for comparison purposes will chose the classic pair x and p. For details, see ref. 1 . The position bins are of width δx and the momentum bins are of width δp. The general case is not worth working out in detail, but in the limit that $(\delta x\, \delta p) \lesssim 1$, the joint probability satisfies

$$P_i^x\, P_j^p \,\leq\, \frac{1}{4}\,(1\,+\,[(\delta x\,\delta p)/2\pi]^{1/2}\,)^2\;. \tag{1.30}$$

It is interesting to note that the wave function that saturates the above bound is localized in the appropriate bins but falls off only as a power-law, hence the variances used in the Heisenberg form are infinite for this wave function that is optimum for the 'bin' case.

REFERENCES

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