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LETTER TO THE EDITOR

Entropy in nonlinear quantum mechanics

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Abstract. Peres and Weinberg have debated the definition of entropy in nonlinear quantum mechanics. This issue can be resolved, it is contended, if one adopts an entropy measure consistent with the approach of Guiasu (following work of Wiener and Siegel) in which a probability distribution over the space of wavefunctions is estimated. This is tantamount to rejecting the von Neumann measure (S_N), $-\text{Tr } \rho \ln \rho$, of the entropy of a density matrix (ρ), which is at the basis of Peres' argument. As authority for such a rejection of S_N , a detailed critique of this measure, given by Band and Park in the mid-1970s, can be cited.

Peres [1, 2] has argued in the form of a comment that nonlinear variants of Schrödinger's equation violate the second law of thermodynamics. In a reply, Weinberg [3, 4] has (provisionally) agreed with this position 'if (emphasis added) entropy is defined as it is in ordinary quantum mechanics.' However, Weinberg then proceeded to assert that this ordinary (von Neumann) definition of the entropy (S_N) of a density matrix (ρ), $-\text{Tr } \rho \ln \rho$, upon which Peres' argument is based, is inappropriate in nonlinear theories. Weinberg then found it 'tempting' to take the entropy as an integral over [the] 'phase space' associated with the wavefunctions, but was then faced with the dilemma that such a revised definition does not reduce to S_N as nonlinearities vanish.

This issue has a resolution—I would like to contend here—but only if one views S_N (somewhat unconventionally, it must be admitted) as not only inappropriate in nonlinear quantum mechanical theories, but also in the linear (standard) theory. Band and Park argued this latter point in a number of broad foundational papers [5-8] in the mid-1970s which, however, have had no discernible impact on the subsequent prevalent use of S_N . They were critical of the information-theoretic basis of S_N , as it relies upon the expansion of ρ into (the limited set of) its eigenstates, and not on a decomposition into the continuum of all possible states.

In the spirit of the Band and Park critique, Slater [9, 10] studied a (barycentric/canonical) measure (S_b), which is the minimum relative entropy, with respect to a uniform prior distribution over the continuum of possible pure states (not simply the eigenstates) of the system, of all probability distributions over this continuum which in fact yield ρ . The duality theory of convex programming [11] was employed to determine an algebraic relationship between S_N and S_b for spin- $\frac{1}{2}$ systems.

In somewhat earlier related work, Guiasu [12] (cf [13]) (following work of Wiener and Siegel [14]) had studied an even finer decomposition of ρ , not simply into the continuum of pure states (rays in a Hilbert space), but into the continuum of wavefunctions (vectors in a Hilbert space). Using the related principles of entropy maximization and interdependence minimization, Guiasu estimated the probability density (P) for

the wavefunctions on the basis of ρ . He obtained for P a complex multivariate normal (Gaussian) distribution with zero mean vector and covariance function simply the density matrix (ρ) itself.

Now, a p -variate complex normal distribution can be written as a $2p$ -variate real normal distribution with a covariance matrix Σ_0 of the form [15]

$$\Sigma_0 = \frac{1}{2} \begin{pmatrix} \Sigma_1 & -\Sigma_2 \\ \Sigma_2 & \Sigma_1 \end{pmatrix} \quad (1)$$

where Σ_1 is a real positive-definitive symmetric $p \times p$ matrix and Σ_2 is a real skew-symmetric $p \times p$ matrix, and Σ (the p -dimensional positive-definite Hermitian covariance matrix—which we interpret as ρ) is

$$\Sigma = \Sigma_1 + i \Sigma_2. \quad (2)$$

The entropy of a normal distribution in $2p$ real variables is [16]

$$S_G = p + p \ln 2\pi + \frac{1}{2} \ln(\det \Sigma_0). \quad (3)$$

This can be taken as the ordinary quantum mechanical entropy to which Weinberg's integral over 'phase space' will reduce as nonlinearities vanish, and 'all information about any statistical mixture of states is contained in the density matrix ρ (for instance, the mean value of any observable A is $\text{Tr}(A\rho)$ ' [3]. (Although it might be considered implicit in his work, Guiasu [12] did not discuss the entropy measure (3), and, thus, did not propose it as an alternative to S_N .) Since S_G is an integral over the 'phase space' of wavefunctions, 'one could apply the usual arguments of classical statistical mechanics to show that [S_G] does not decrease' [3].

If π denotes the uniform distribution over the wavefunctions, p^* the Guiasu (multivariate complex normal) distribution over the wavefunctions, and p the relative minimum entropy distribution over the wavefunctions that would yield ρ and also (upon aggregation of the wavefunctions into their rays) the barycentric/canonical representation [9, 10] of ρ , then [17]

$$I(p : \pi) = I(p^* : \pi) + I(p : p^*) \quad (4)$$

where

$$I(p : \pi) = \int_V p(v) \ln[p(v)/\pi(v)] dv \quad (5)$$

is termed the Kullback-Liebler information, cross-entropy, directed divergence, and integration is over the probability space (V) of wavefunctions (v).

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