INVARIANT ENTROPY AND COMPLEXITY OF QUANTUM STATES

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The concept of entropy is fundamental for many branches of physics and other sciences dealing with systems which reveal a certain degree of complexity and disorder. As stressed in the monograph 1, "entropy is not a single concept but rather a family of notions". In relation to quantum theory, the mainstream of development is formed by four main overlapping lines. They can be referred to as *thermodynamical* (Boltzmann - Gibbs) entropy, *quantum ensemble* (von Neumann) entropy, *information* (Shannon) entropy and *dynamical* (Kolmogorov - Sinai) entropy. Since the general description of a quantum system, including its interaction with the environment, time development and relaxation to equilibrium, can be given in terms of the density matrix ρ, the von Neumann definition,

$$S = -\mathrm{Trace}\,(\rho\,\ln\rho), \tag{1}$$

seems to be the most fundamental. For a system in an equilibrium with a heat bath, the density matrix (and, accordingly, von Neumann entropy) is eqivalent to that in the canonical or grand canonical thermal ensemble. The evolution of a closed gas-like quantum many-body system *from a random initial state* can be shown to lead to the same values of macroscopic observables as for the thermal equilibrium described by the microcanonical ensemble which has a clear semiclassical limit as the equipopulation on the energy surface in phase space.

The ensemble entropy cannot be represented as an expectation value of a dynamic variable expressed by an operator in Hilbert space. However, being a trace functional of the density matrix, it is *invariant* under unitary basis transformations. For a *pure* wave function, as that of a stationary state $|\alpha\rangle$ in an isolated system, presented as a *superposition* in an arbitrary orthonormal basis $|k\rangle$,

$$|\alpha\rangle = \sum_k C_k^\alpha |k\rangle, \tag{2}$$

the density matrix has matrix elements

$$\rho_{kl}^\alpha = C_k^\alpha C_l^{\alpha *}. \tag{3}$$

This matrix is actually a projector onto the state $|\alpha\rangle$, so it has one eigenvalue equal to 1 (this eigenvector coincides with $|\alpha\rangle$) while all other eigenvalues have a degenerate zero value, and basis-independent von Neumann entropy vanishes. An *incoherent* averaging over independent states $|\alpha\rangle$ with the *weights* w^α (no interference!), creates a *mixed* quantum state with incomplete information. The corresponding density matrix,

$$\rho_{kl} = \sum_\alpha w^\alpha C_k^\alpha C_l^{\alpha *}, \quad \sum_\alpha w^\alpha = 1, \tag{4}$$

obviously has w^α as its eigenvalues, mean occupation numbers of the states $|\alpha\rangle$ in the ensemble described by the density matrix ρ, eq. (4); von Neumann entropy is given by

$$S = -\sum_\alpha w^\alpha \ln w^\alpha. \tag{5}$$

Information entropy, with traditional applications in communication theory, is expressed in terms of *probabilities* P_j rather than amplitudes,

$$I = -\sum_j P_j \ln P_j. \tag{6}$$

Therefore it is *representation dependent* being different for different choices of the set of mutually excluding events. In quantum systems, one can find information entropy of individual states (2) *with respect to a fixed basis*

$$I^\alpha = -\sum_k w_k^\alpha \ln w_k^\alpha. \tag{7}$$

All correlations between the amplitudes of different components of the wave function are suppressed in this definition. Averaging information entropy over some ensemble of quantum states, one gets a measure of average complexity of those states. At this stage, the similarity between information entropy and von Neumann ensemble entropy can emerge if one can establish an appropriate correspondence between the ensembles used in the two approaches and the basis utilized in calculating information entropy 2. Thus, for canonical equilibrium thermal ensembles, the correlations are destroyed by the random interaction with the heat bath so that the density matrix is diagonal in the energy representation for the system. In this case, the eigenvalues of the density matrix give the occupancies of the stationary eigenstates of the isolated system which could be directly used for constructing information (= thermodynamical) entropy.

Information entropy (7), used as a tool for quantifying the degree of complexity of individual quantum states 2, 3, shows delocalization of the wave function in an arbitrary basis. However, as a rule, one can find a basis, or a family of bases, which are singled out by physical arguments specific for each system. The delocalization lengths in such a representation manifest complex character of states and can be quantitatively related to other signatures of quantum chaos. For realistic many-body systems with strong interaction, the *mean field* represents the exceptional basis where the local correlations and fluctuations of adjacent stationary states are separated from their regular evolution along the spectrum (4). As shown in large-scale nuclear shell model calculations 2, the representation dependence of information entropy might be considered in some respects an advantage which provides a useful physical measure of a *mutual relationship* between the eigenbasis of the hamiltonian and the representation basis, for example that of independent particles in a mean field.

Moreover, chaotic dynamics make different states with close excitation energy and the same values of exact constants of motion "look the same", i.e. have similar observable properties. This is nothing but a microscopic picture of *thermal equilibrium* 4. After averaging over a narrow energy window in a high level density region, information entropy in the mean field (shell model) basis becomes a smooth function of excitation energy and carries the same thermodynamic contents as thermal entropy found for the microcanonical distribution from the level density. Being calculated in a *random* basis, the magnitude of information entropy of generic states in a complex system is typically on the level predicted by random matrix theory and does not display any regular evolution along the spectrum.

We explore 5 the possibility of describing the degree of complexity of individual quantum states using the von Neumann definition of entropy (1) and applying an *external noise* which converts a pure state into the mixed one. We assume that the stationary hamiltonian of the system contains random parameter(s) λ which determine the λ-dependent eigenstates $|\alpha;\lambda\rangle$, corresponding amplitudes $C_k^\alpha(\lambda)$, eq.

(2), in an independent basis $|k\rangle$, and the density matrix

$$\rho^{\alpha}_{kl} = \overline{C^{\alpha}_{k}(\lambda)C^{\alpha *}_{l}(\lambda)} \equiv \int d\lambda\,\mathcal{P}(\lambda)C^{\alpha}_{k}(\lambda)C^{\alpha *}_{l}(\lambda), \tag{8}$$

where $\mathcal{P}(\lambda)$ is the normalized distribution function of the noise parameters λ. We do not consider the perturbation to be weak; therefore the resulting mixed state depends explicitly on the noise properties and gives a description of the ensemble "system plus noise". In fact, such a description of a nucleus can be more realistic than the standard one because any hamiltonian in terms of nucleon degrees of freedom only is an effective theory which corresponds to the elimination of the underlying variables (quarks, gluons, mesons, photons and so on). The averaging over mediating fields is essentially equivalent to the consideration the interaction agents as some kind of a random environment.

Multiple *avoided crossings* of the energy terms in a function of parameters reveal strong mixing and drive the system to the chaotic limit. We calculate the density matrix (8), its eigenvalues ν^{α} (mean occupation numbers in the presence of the noise), and von Neumann entropy (1) for a given energy term $|\alpha;\lambda\rangle$. This entropy can be called *correlational* since all correlations of the amplitudes are retained in the definition (8). Using exactly solvable models, we show essential features of representation-independent entropy obtained according to this definition, its similarity to and distinction from information entropy. Even for the simplest systems as a harmonic oscillator in a random uniform field, the resulting steady states are far from trivial. For a Gaussian noise, the radiation from such a system could be characterized by an effective temperature although the distribution function for a number of quanta does not coincide with the Planck distribution so that using the latter for the description of the spectrum, one would get a wrong temperature. We also give an example of a realistic numerical calculation for a many-body system of fermions (a nucleus ^{24}Mg) which shows that our ensemble entropy ("correlational" entropy) is a smooth function of excitation energy and therefore may be used as a measure of the degree of complexity.

References

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