The unconstrained ensemble and its use in the study of quantum and classical nonadditive systems

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In statistical mechanics, the unconstrained ensemble can be defined only for nonadditive systems. In this ensemble the control variables are temperature, pressure and chemical potential, namely all intensive variables, while the extensive variables, i.e., energy, volume and number of particles, are all free to fluctuate. These conditions are called completely open. Macroscopic systems with short-range interactions are additive, so that temperature, pressure and chemical potential cannot be varied independently (as evidenced by the Gibbs-Duhem relation), preventing the definition of the unconstrained ensemble. On the other hand, nonadditive systems, like small systems, or systems with long-range interactions, are inherently nonadditive, and this causes the presence of an additional thermodynamic degree of freedom, allowing, e.g., to vary independently the chemical potential at fixed pressure and temperature (apart from some particular cases that will be specified). The above considerations hold independently from the nature of the nonadditive system under scrutiny, classical or quantum. In this presentation we will give specific examples of the study of both classical and quantum systems in the framework of the unconstrained ensemble. We wil also describe the issues that arise in the definition of completely open conditions in concrete cases. The bibliography lists some earlier works in which: the peculiar thermodynamic properties of nonadditive systems are described; how it is possible to perform Monte Carlo simulation in the unconstrained ensemble; the application to a concrete model presenting phase transitions.

References

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