

Correlation as a measure of Information Entropy

Information theory studies the quantification, storage, and communication of information. It was originally proposed by Claude E. Shannon in 1948 to find fundamental limits on signal processing and communication operations such as data compression, in a landmark paper entitled “A Mathematical Theory of Communication”.

A key measure in information theory is “entropy”. Entropy quantifies the amount of uncertainty involved in the value of a random variable or the outcome of a random process. Simply, Entropy is the amount of information contained in a system. This is a term that reveals about the amount of disorderliness in the system.

In a plain hypothetical system with no disorder or in perfect order has no information, only when the disorder sets into the system it starts having information which is proportional to the disorder in the system. Any random variable has an expectation/mean probability which is an inverse measure of its information or Entropy. Higher the probability lower is the information.

In the independent –electron model the effect of electronic repulsion, globally referred to as correlation is disregarded. The correlation effect can, however, have major influence on measurable quantities in atomic systems. The ‘Hartree and Ingman 1933’ type wave function has been used to derive an analytical model to calculate single-particle wave functions in coordinate-space and its momentum-analog using the Fourier Transform of the wave functions to quantify the correlation of two-electron systems. Subsequently, its response to the correlation effect of bare or uncorrelated single-particle charge densities of two-electron systems both in position - and momentum –space has been observed and examined its momentum-space analog that could serve as candidates for the correlation measure of two-electron systems. On the one hand the charge densities obtained by our method can be used to compute numbers for position-space information entropy (s_ρ) and momentum-space information entropy (s_γ). It has been suggested that such numbers for s_ρ and s_γ can be used as an electron –correlation tool. On the other hand, our single particle wave functions will be useful to study the effect of correlation on position-space Fisher information (I_ρ) and momentum-space Fisher information (I_γ).

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