On the eigenvalue representation of observables and probabilities in a high-dimensional euclidean space and its relation to informational geometry

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In this work we will present the basic concepts of the Eigenvalue Representation of Observables and Probabilities in a High-dimensional Euclidean (EROPHILE) space (Boulougouris Georgios C. .; Theodorou, Doros N. Journal of Chemical Physics , 2009, 130, 044905):. EROPHILE is a general approach that it was initially designed to address discrete systems where the dynamics can be described using a Master Equation and where detail balance is expected to hold. The main aspect of the EROPHILE is that describes perturbations from thermodynamic Equilibrium using the Eigenvectors of the Master Equation (or the time evolution operator in the more general case) and results in a geometrical description of both the dynamics and thermodynamics around Thermodynamic Equilibrium expressing statistical quantities as inner products in a Euclidian space. In systems that obey detail balance it has been shown the Eigenvalue Representation of Observables and Probabilities in a High-dimensional Euclidean (EROPHILE) approach can be used to identify relaxation modes in dynamical response experiments and most importantly express in the same Euclidian space both probabilities and observables as vectors providing us with the possibility of expressing either the deviation from equilibrium based on observables or the variances of observables as a function of the eigenvectors of the time evolution operator. For example, it has been shown that sub glass relaxations modes in atactic polystyrene simulations can be identified as the net result of the redistribution of the population of inherent structures that coincide with one of the eigenvector of the Master Equation that describes the dynamical transitions between inherent states. Alternatively the subglass relaxation mode can be identified as the observable for which the autocorrelation has only one characteristic time (decay via a single exponential that corresponds to a single eigenvalue). Finally, we will present its relation to the Information Geometry approach used to describe equilibrium thermodynamics.

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