

# Configurational temperature in constrained systems: The case of spin dynamics

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© 2018 IOP Publishing Ltd. A general mathematical expression to estimate the temperature in computer simulations of constrained systems is obtained. Using a recently derived theorem which relates the ensemble average of thermodynamics conjugate variables we obtain a family of temperature estimators for constrained systems based solely on the configurational state. We present explicit formulas for the case of a classical spin system governed by Heisenberg type Hamiltonians. The expressions can be considered an extension of the equipartition theorem for spin variables, and are useful in practical situations to monitor the temperature in spin dynamics simulation, as well as to gain a deeper understanding of the meaning of temperature.