

---

# Expansion Coefficients Evaluation of the Free Energy at High Temperatures using Micro-canonical Numerical Simulations.

Elizabeth Moreno-Hilario<sup>\*†1</sup>, Maria Sotelo-Serna<sup>\*‡1</sup>, Francisco Sastre<sup>§1</sup>, and Alejandro Gil-Villegas<sup>¶1</sup>

<sup>1</sup>División de Ciencias e Ingenierías. Universidad de Guanajuato. (DCI-UG) – Lomas del Bosque 103. Lomas del Campestre. 37150, León, Guanajuato., Mexico

## Abstract

In statistical systems, the free energy can be expressed by infinite power expansions of the inverse temperature. In the canonical ensemble, the evaluation of the expansion coefficients requires knowledge of the energy fluctuations, this implies a hard numerical effort. Furthermore, this calculations must be held in the limit where the temperature tends to infinite. However, it is observed that the equation of state in the micro-canonical ensemble  $S(U)$  has a maximum in this limit and it is a smooth function whose derivate can be fitted with a quadratic polynomial around this maximum. Using a method proposed in reference [1] it is possible to evaluate with high accuracy the inverse temperature curves as a function of the internal energy for fluids with square well potential. From here we can obtain reliable values for the expansion coefficients of the free energy expansion. [1] F. Sastre, A. L. Benavides, J. Torres and A. Gil-Villegas, PRE 92, 033303. (2015)

---

\*Speaker

†Corresponding author: [morenohe2013@licifug.ugto.mx](mailto:morenohe2013@licifug.ugto.mx)

‡Corresponding author: [sotelosm2013@licifug.ugto.mx](mailto:sotelosm2013@licifug.ugto.mx)

§Corresponding author: [sastre@fisica.ugto.mx](mailto:sastre@fisica.ugto.mx)

¶Corresponding author: [gil@fisica.ugto.mx](mailto:gil@fisica.ugto.mx)