NUMERICAL CALCULATION OF THE DENSITY OF STATES FOR A CLASSICAL NON-IDEAL SYSTEM

Larkin A.S.,* Filinov V.S., Levashov P.R.

JIHT RAS, Moscow, Russia

**alexanderlarkin@rambler.ru*

The density of states $g(E)$ of a classical system is the number of microscopic states lying in the range of potential energies from E to $E + \mathrm{d}E$, related to the length of this interval [1]. Knowing this value allows one to calculate thermodynamic functions and quantities, such as the statistical sum, free and internal energy, entropy, heat capacity, etc. directly from the product of $g(E)$ and the Boltzmann exponent $\exp(-E/kT)$. At the same time, the density of states itself depends only on the number of particles, the occupied volume and the type of interparticle interaction, so that it is universal for all temperature values T. In this work, we consider the problem of calculating the density of states using the Wong-Landau algorithm [2] in the case of discrete and continuous potential energy spectra. This method belongs to the family of "histogram" Monte Carlo methods and consists of sequence of steps between the cells of the histogram of the density of states $g(E)$ with simultaneous refinement. The authors propose a modification of this algorithm, which differs in a much more efficient way of parallelizing the program for multiprocessor systems with shared memory and an improved criterion for the "flatness" of the energy histogram. As an example, calculations of the density of states and derivatives of thermodynamic functions are performed for such systems as 2D Ising model, N non-interacting classical oscillators and N particles with a Lennard-Jones potential.

---

1. F. Wang, D. P. Landau *Phys. Rev. Lett.*, 86, 2021.
2. F. Moreno, S. Davis, J. Peralta Computer Physics Communications, 274,2022.