NUMERICAL CALCULATION OF DENSITY OF STATES OF CLASSICAL NON-IDEAL MANY-PARTICLE SYSTEM WITH MODIFIED WANG–LANDAU ALGORITHM

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The density of states $G(E)$ for a classical system is defined as the number of microscopic state with energy on the interval $[E, E+\mathrm{d}E]$ related to $\mathrm{d}E$. According to the Gibbs distribution, the probability that a system at a temperature T has energy E is proportional to $G(E)\exp(-E/T)$. An important feature of this approach is that thermodynamic quantities such as partition function, free energy, entrophy, internal energy, heat capacity etc. can be calculated via simple numerical integration in the entire temperature range from one universal function $G(U)$.

The density of states can be calculated numerically using the Wang–Landau algorithm related to so-called histogram Monte–Carlo methods [1]. In this work we present the modification of this algorithm, which is applicable to classical systems with continuous spectrum, consisting of identical particles with interaction via pair potential. To improve the convergence and guarantee the ergodicity of the random walks, we introduced in the algorithm special steps replacing the microscopic state with the other one having the same energy. The software implementation of the algorithm allows parallel computing on multiprocessor systems with shared memory.

We applied the developed implementation of the Wang–Landau algorithm to a soft-sphere system consisting of particles with a repulsive pair interaction described by the inverse twelfth-power potential $\varphi(r) = \varepsilon(\sigma/r)^{12}$. The density of states $G(E)$ has been calculated for the densities ρ from $0.1\sigma^{-3}$ to $0.5\sigma^{-3}$. It has been used to calculate the partition function $Z(T)$, free energy $F(T)$, internal energy $\bar{E}(T)$, heat capacity $C_V(T)$ and entropy $S(T)$ for temperature T in range from 0 to $2\varepsilon/k_B$. The reliability of the method is confirmed by excellent agreement of the obtained results with known wide-range analytics [2].

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1. F. Wang, D. P. Landau *Phys. Rev. Lett.*, 86, 2021.
2. S. Pieprzyk, D.M. Heyes, and A.C. Branca,*Phys. Rev. E*, 90,2014.