Thermodynamic properties of two- and three-dimensional systems with Yukawa pair interaction potential

O.S. Vaulina, X.G. Koss, O.F. Petrov, V.E. Fortov

JIHT RAS, Moscow, Russia

Here we present the results of numerical study of thermodynamic characteristics (such as energy densities, U, and the heat capacities $C_V = (\partial U/\partial T)_V$) for non-ideal dissipative systems with Yukawa interaction potential. We considered two- and three-dimensional systems of the particles interacting with the screened Coulomb potential in a wide range of parameters typical for the laboratory dusty plasma experiments. The calculations were performed by Langevin molecular dynamic method.

In this work, the simple analytical approximation is presented for the energy densities of the two- and three-dimensional non-ideal systems, that was obtained with a help of the semi-empirical "jumps" theory developed for molecular fluids, and based on the analogies between solid and liquid state of matter. Following the "jump" theory, a difference between the potential part U_p of the energy of fluid and the lattice energy, U_0, may be presented as

$$(U_p - U_0) = mT/2 + a_1\, \varepsilon_f/\{1 + \exp(\varepsilon_f/T)\}, \qquad (1)$$

where a_0, a_1 are some coefficients dependent on a type of lattice and a spectrum of realized oscillations, m is the number of dimensions in the system, and ε_f is the characteristic energy of particle in one degree of freedom. The parameters of proposed approximation, Eq.(1), were obtained using the best fitting of the numerical calculations of U_p by analytical curves.

The presented approximation was used for the determination of analytical expressions for the pressures, the thermal coefficient of pressure, and the heat capacities on base of the thermodynamics relations. To test a suitability of proposed approximation of U_a for a correct determination of C_V, the calculation of the heat capacity, $C_V^a = (\partial U_a/\partial T)_V$, was performed both in numerical experiment and from Eq.(1)

$$C_V \cong C_V^a = 1 + \frac{2\Gamma^*_c + (U_a - U_0 - T)\Gamma^* T^{-1} \exp(\varepsilon_f / T)}{\Gamma^*_c\{1 + \exp(\varepsilon_f / T)\}}. \qquad (2)$$

The comparisons of obtained results with the numerical calculations have shown that the proposed approximations can be used for the description of thermodynamic properties in analyzed non-ideal dissipative systems. We also note that results of the present study may be adapted to obtain the suitable approximations for the thermodynamic functions of the non-ideal systems with other types of pair interactions.