

THERMODYNAMIC PROPERTIES OF TWO-DIMENSIONAL SYSTEMS WITH ISOTROPIC PAIR INTERACTION POTENTIALS

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Recently the investigations of physical properties in two- and quasi two-dimensional (2d-) non-ideal systems attracted particular interest [1-3]. In this work we present the simple analytical approximation for the energy densities of the two-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 the solid and the liquid state of matter [4]. This theory gives good results in the determination of transport constants (diffusion, viscosity, thermal conductivity etc.) for simulated systems and for real non-ideal media both for simple monatomic fluids and for a number of complex molecules. 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

$$(U_p - U_0) = a_0 T + a_1 \epsilon_f / \{1 + a_2 \exp(\epsilon_f / T)\}, \quad (1)$$

where a_0, a_1, a_2 are some coefficients dependent on a type of lattice and a spectrum of realized oscillations, and ϵ_f is the characteristic energy of particle in one degree of freedom. (In case of $a_0 = a_1 = a_2 = -1$, and $\epsilon_f = h \nu$, the Eq.(1) is the well-known Einstein’s formula for the system of one-dimensional oscillators.) In the limits of Einstein’s and “jump” theories, the lattice energy may be characterized by a single oscillation frequency ν_c only. Under the assumption of $\nu_c \approx const$, the approximation for the energy density of fluids may be found by the choosing of appropriate coefficients (a_0, a_1, a_2), and ϵ_f value in Eq.(1).

Here we present the results of numerical study of thermodynamic properties (the energy densities, U , the pressures, P , the normalized thermal coefficient of pressure, $\nu = n^{-1} (\partial P / \partial T)_V$, and the heat capacities $C_V = (\partial U / \partial T)_V$) for non-ideal dissipative systems of particles forming a monolayer for parameters close to the conditions in dusty plasma experiments in RF- discharges. The simulation technique is detailed in [3, 5].

The calculations were carried out for various types of pair isotropic potentials $\phi(r)$ that represented different combinations of power-law and exponential functions, commonly used for simulation of repulsion in kinetics of interacting particles in various fields of science and

technology (plasma physics, biology, medical industry, physics and chemistry of polymers, etc.) [2, 4, 6]:

$$= c [b_1 \exp(-r/l_p) + b_2 (l_p/r)^m \exp(-r/l_p)].$$

Here $b_{1(2)}$, $c = (Q)^2/r$ is the Coulomb potential energy for the particle with the charge Q .

The parameters of proposed approximation, Eq.(1), were obtained using the best fitting of the direct numerical calculations of U_p by analytical curves. These calculations have shown that the coefficients in Eq.(1) can be presented as $a_0 = 0$, $a_1 = 4$, $a_2 = 1$ for all cases under study; the characteristic energy of particles ϵ_f is determined by the relation: $\epsilon_f/T = (0.5 + \Gamma^*/\Gamma_c^*)$, where $\Gamma^* = 1.5 l_p^2 \epsilon_f / (2T)$ is the effective coupling parameter, $\Gamma_c^* \cong 100$ is the coupling parameter at the point of crystallization of system (at the point of formation of the hexatic phase of solid [7]).

One can easily see that the value of ϵ_f in the crystallization point is in accordance to the full energy of 2d- systems of harmonic oscillators in one degree of freedom. (Recall that the full energy E_f for 2d- systems of oscillators is equal to $E_f \cong 2 \epsilon_f = 3T$, in accordance with virial theorem.) Thus, the energy density of analyzed systems, and also its derivative ($C_V = (\partial U / \partial T)_V$) may be presented as

$$U_a = U_0 + T + 4 \epsilon_f / \{1 + \exp(\epsilon_f/T)\}, \text{ где } \epsilon_f/T = (0.5 + \Gamma^*/\Gamma_c^*); \tag{2a}$$

$$C_V^a = 1 + \frac{0.5\Gamma_c^* + U_a \Gamma^* \exp(\epsilon_f/T)}{\Gamma_c^* \{1 + \exp(\epsilon_f/T)\}}. \tag{2b}$$

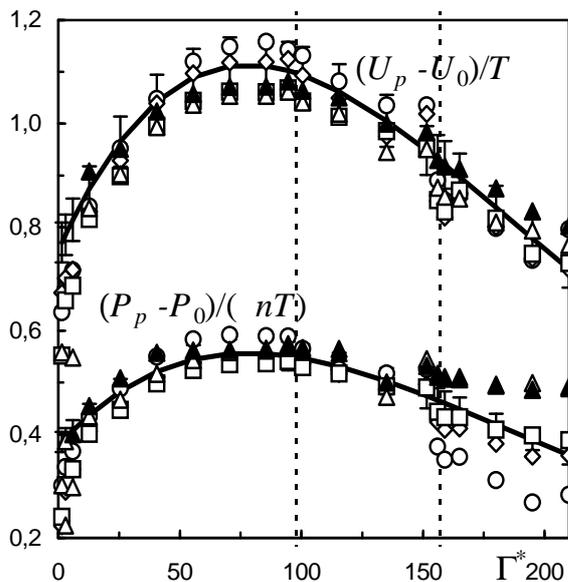


FIGURE 1. Potential components of U_p , and P_p vs. Γ^* for different potentials ϵ_c : (○) – $\exp(-2r/l_p)$; (△) – $\exp(-6r/l_p)$; (◇) – $\exp(-3r/l_p) + 0.05 l_p/r$; (□) – $0.1\exp(-2r/l_p) + \exp(-4r/l_p)$; (▲) – $0.05(l_p/r)^3$. Solid lines are the approximations $(U_a - U_0 - T)/T$, and, $(P_a - P_0 - T)/T$, respectively (see Eqs. (2a),(3a)).

The results of numerical calculations of energy for analyzed systems together with its approximation U_a , Eq.(2a), are presented in Fig.1 for various pair potentials (used here for the illustrations of our calculations). The heat capacity C_V together with its approximation C_V^a , Eq.(2b), are shown in Fig. 2a. One can easily see that the relative deviations of proposed approximations from numerical results are less than 5% (pointed in the figures) in the range from $\Gamma^* \sim 10$ to the point of formation of the “perfect” lattice ($\Gamma^* \approx 160$). Singularities (the “jumps”) for the heat capacities, C_V , about $\Gamma^* \approx 100$ and $\Gamma^* \approx 160$ (pointed in Fig. 2a by the dashed lines) are determined by the two-stage scenario of the melting in 2-d systems (see Kosterlitz-Thouless-Halperin-Nelson-Young theory of 2-d melting, [8, 9]). We’d also like to point out two additional features. It is that the 5% deviation of $(U_a - U_0 - T)/T$ presented in Fig. 1 provides the errors for full approximation U_a (2a) well below than 0.5% for all mentioned range of Γ^* . Also, the relative high errors for the C_V approximation are determined significantly by the procedure of differentiation of numerical data.

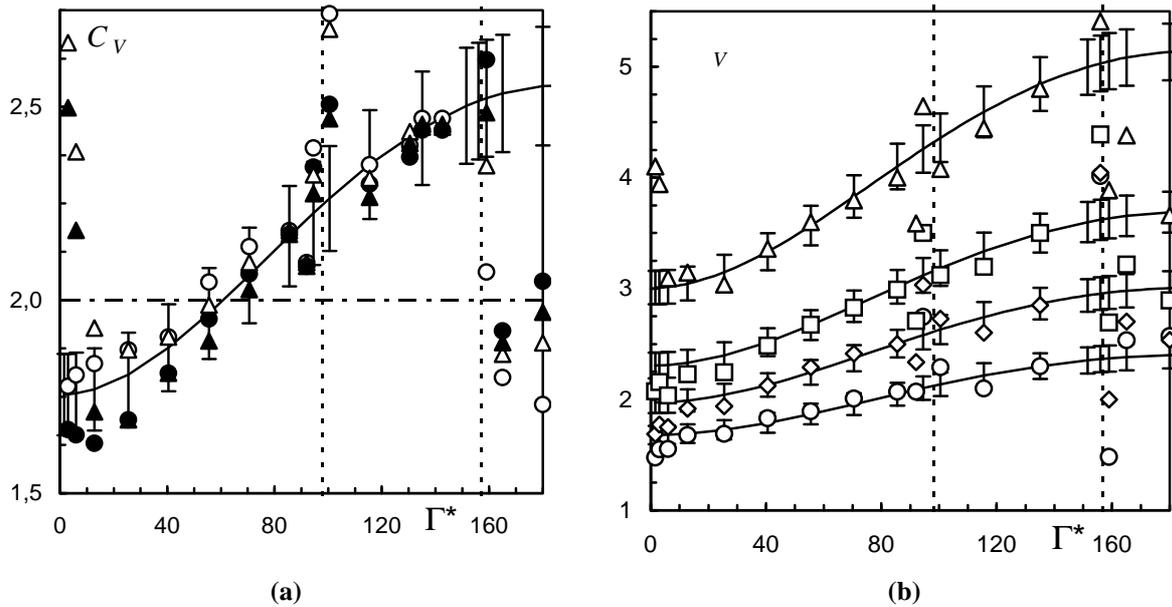


FIGURE 2. Function of C_V (a) and v (b) vs. Γ^* for the Yukawa potentials with different α :
 (○;●) – 2; ◇ – 3; □ – 4; (▲;△) – 6. Dark symbols – $\alpha = 0.23$; transparent symbols – $\alpha = 1.86$ ($\alpha = \epsilon^*/v_{fr}$, where $\epsilon^* = |2 \pi \epsilon_0 l_p|^{1/2} (2 M)^{-1/2}$). Solid lines are the approximations, C_V^a , and, v^a , respectively (see Eqs. (2b),(3b)).

Appropriate expression for the pressure, P (including the thermal coefficient of pressure, $\alpha_P = n^{-1} (\partial P/\partial T)_V$), in analyzed systems may be obtained from the known formula of thermodynamics ($(\partial U/\partial V)_T = T(\partial P/\partial T)_V - P$), using Eq. (2a)

$$P_a = P_0 + nT + 2 \pi n \epsilon^* / \{1 + \exp(\epsilon^*/T)\}, \tag{3a}$$

$$v^a = 1 + C_V^a / 2, \tag{3b}$$

where $\alpha = (\partial\Gamma^*/\partial l_p) l_p/\Gamma^*$. Illustrations of direct numerical calculations of P together with its approximation, P_a Eq.(3a), are presented in Fig.1; and the value of α_v together with its approximation α_v^a , Eq.(3b), is shown in Fig. 2 b. Here we can see also that the proposed approximations are in a good accordance (within 5%) with the numerical data for the range of Γ^* from ~ 10 to ~ 160 , excluding the range close to points of the phase transitions.

To conclude, here we proposed the suitable analytical approximation for the energy densities of the two-dimensional non-ideal systems with the wide range of types of repulsive isotropic pair potentials. The parameters of proposed relationship were obtained by the best fitting of the numerical and analytical data. 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. The comparisons of obtained results with the numerical calculations have shown that the proposed approximations can be used for the description of thermodynamical properties in analyzed non-ideal systems. Finally, we 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.

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