PHYSICAL REVIEW E **82**, 056411 (2010)

Thermodynamic and transport properties of nonideal systems with isotropic pair potentials

O. S. Vaulina,[1] X. G. Koss,[1,2,*] Yu. V. Khrustalyov,[1,2] O. F. Petrov,[1,2] and V. E. Fortov[1,2]
[1] *Institution of Russian Academy of Sciences, Joint Institute for High Temperatures RAS,*
Izhorskaya Street, 13 Boulevard 2, Moscow 125412, Russia
[2] *Moscow Institute of Physics and Technology (State University), Institutskiy Lane, 9, Dolgoprudnyj 141700, Russia*

(Received 16 April 2010; revised manuscript received 21 September 2010; published 22 November 2010)

The equations of state and the structural, thermodynamic, and transport properties of the two- and three-dimensional nonideal dissipative systems consisting of particles interacting with different isotropic pair potentials are studied in a wide range of parameters typical for laboratory dusty plasma. Simple semiempirical expression for the energy density in liquid systems is considered. Comparison of the theoretical and numerical results is presented.

DOI: 10.1103/PhysRevE.82.056411 PACS number(s): 52.27.Lw, 52.27.Gr, 52.35.Fp

I. INTRODUCTION

The study of thermodynamic and transport properties of the systems of interacting particles is of significant interest in various fields of science and technology (plasma physics, medical industry, physics of polymers, etc.). The main problem involved in the studies of these systems is associated with the absence of analytically justified theory of liquid which could provide simple parametrical expressions for its equations of state, thermodynamic characteristics, and kinetic coefficients (e.g., constants of diffusion, thermal conductivity, or viscosity). To predict the physical properties of nonideal systems, various semiempirical approaches and computer simulations of particles' dynamics involving different models for their interaction potentials are widely used [1–11].

Dusty plasma (consisting of electrons, ions, neutral gas, and solid macroparticles of micron sizes) is a good experimental model for studying the nonideal systems including the verification of existing analytical approaches and the development of new models in theory of liquid. Dusty plasma is ubiquitous in nature and often appears in a number of technological processes. Most of the experimental investigations of dusty plasma are performed in weakly ionized plasma of gas discharges where a dissipation of dust energy due to dust-neutral collisions can considerably influence the physical properties of the system. In gas discharge plasma, the nonemitting micron-size grains acquire a significant negative charge eZ (where e is the electron charge) and can form the three-dimensional (3D) or the two-dimensional (2D) structures similar to liquids or solids. The quasi-2D structures—which consist of one to approximately ten layers of grains—are typical for plasma of radio-frequency (RF) discharge [8–12].

At present the problem about the form of interaction potential between dust particles in plasma has no satisfactory solution. The best-known model for description of pair interaction of repelling dust particles is based on the screened potential of the Yukawa type [8–10],

$$\phi = A\exp(-r/\lambda)/r. \tag{1}$$

Here, r is the distance between particles, λ is the screening length, and A is a parameter equal to $(eZ)^2$ for two similar charged particles. It should be mentioned that simple Yukawa model (1) agrees with numerical and experimental results in complex plasma only for short distances $r<4\lambda_D$ between two isolated macroparticles in plasma; here, λ_D is the Debye length [13–16]. With increasing distance r the screening effect weakens and the asymptotic character of the potential ϕ for large distances $r \gg \lambda_D$ can follow the power-law dependence: $\phi \propto r^{-2}$ [17] or $\phi \propto r^{-3}$ [18]. The Yukawa model may also be incorrect under conditions of dense grain cloud and in the sheath region of laboratory gas discharges. Furthermore, this model does not take into account the ionization or recombination processes, the collisions of plasma electrons, ions with neutrals, and many other factors [10,19].

Here we introduce two dimensionless parameters (by analogy with the parameters found in [12,20–22]), which are responsible for mass transfer and phase state in nonideal dissipative systems within wide range of the isotropic pair potentials, namely, the effective coupling parameter,

$$\Gamma^* = c_1 r_p^2 \phi''/2T, \tag{2}$$

and the scaling parameter,

$$\xi = \omega^*/\nu_{fr} = (c_2\phi''/2\pi M)^{1/2}/\nu_{fr}. \tag{3}$$

Here M is the particle mass, ν_{fr} is the friction coefficient of particles due to their collisions with the neutrals of surrounding gas, ϕ'' is the second derivative of a pair potential $\phi(r)$ at the point of the mean interparticle distance $r=r_p$, and c_1 and c_2 are the coefficients: $c_1=c_2\equiv 1$ for 3D systems and $c_1=1.5$ and $c_2=2$ for the 2D case. Note that the transport processes and spatial correlation of particles are defined by these two parameters $(\Gamma^*;\xi)$ for a wide range of $\phi(r)$ functions satisfying the empirical condition [12,20],

$$2\pi > |\phi'' r_p/\phi'|. \tag{4}$$

Here ϕ' is the value of the first derivative of $\phi(r)$ at the point of mean interparticle distance. In this case the spatial correlation of particles is independent of the friction (ν_{fr}) and is defined by the Γ^* value within the range between $\Gamma^* \sim 10$ and the crystallization point Γ^*_c (i.e., the point of formation of

---

[*] Formerly X. G. Adamovich.

the "perfect" crystal where no migration of particles occurs and their diffusion coefficient $D=0$). For the nonideal dissipative 2D systems forming the hexagonal primitive (hp) lattice in their crystal state, the value of $\Gamma_c^*=\Gamma_{2D}^*\cong 154\pm 4$ [12,22]; for 3D systems forming the body-center-cubic (bcc) lattice, the Γ_c^* value is equal to $\Gamma_{3D}^*\cong 102\pm 3$ [12,20].

Here we study thermodynamic properties in nonideal dissipative systems of particles interacting with the different isotropic pair potentials commonly used for simulation of repulsion in kinetics of interacting particles. Semiempirical approach for calculations of the energy density in strongly coupled systems is proposed. Analytical relations between the basic transport constants and the energy density are considered. The basic attention is given to the screened Coulomb potential of Yukawa type (1) that is of particular interest in the context of investigation of dusty plasma [8–10] and for colloid systems (including medical and biological systems and polymer structures) [2–7]. For these Yukawa systems the effective coupling parameter [see Eq. (2)] may be rewritten as

$$\Gamma^* = c_1\Gamma(1+\kappa+\kappa^2/2)\exp(-\kappa), \tag{5}$$

where $\Gamma=(Ze)^2/(Tr_p)$ is the Coulomb coupling parameter and $\kappa=r_p/\lambda$ is the screening factor. Then, the characteristic frequency ω^* in Eq. (3) may be presented as

$$\omega^* = \left[c_2(eZ)^2\left(1+\kappa+\frac{\kappa^2}{2}\right)\frac{\exp(-\kappa)}{r_p^3\pi M}\right]^{1/2}. \tag{6}$$

To conveniently compare the results of various works with our data, we introduce the normalized values of the Coulomb coupling parameter and the screening factor, which take into account the Wigner-Seitz radius, namely, $\Gamma_2=\Gamma(\pi)^{1/2}$, $\kappa_2=\kappa(\pi)^{-1/2}$ and $\Gamma_3=\Gamma(4\pi/3)^{1/3}$, $\kappa_3=\kappa(4\pi/3)^{-1/3}$ for the 2D and 3D Yukawa systems, respectively.

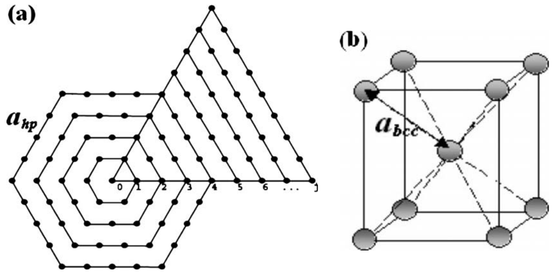

FIG. 1. Illustration of arrangement of particles in (a) hp and (b) bcc lattices. The step of hp lattice: $a_{hp}\equiv(\sqrt{3}/2)^{1/2}r_p$ and the minimal interparticle distance in bcc lattice $a_{bcc}\equiv 2^{1/3}r_p$.

II. BASIC EQUATIONS AND THEORETICAL APPROACHES

A. Equations of state for nonideal fluid systems

It is necessary to note that at present time the theoretically proved forms of the equations of state exist only for some solid crystal structures (for example, in the model of Mi and Grjunejzen) and for gases (the virial equation). In case of isotropic pair interactions [with the known interaction energy $\phi\equiv\phi(r)$] the physical properties of nonideal systems, such as the energy density U and the pressure P, are determined by the temperature T, the concentration n, and the pair-correlation function $g(r)$, which can be measured experimentally or may be found from the computer simulations [4–6],

$$U = \frac{m}{2}T + (m-1)\pi n\int_0^\infty \phi(r)g(r)r^{m-1}dr, \tag{7}$$

$$P = nT - \frac{(m-1)\pi n^2}{m}\int_0^\infty \frac{\partial\phi(r)}{\partial r}g(r)r^m dr, \tag{8}$$

where $m=2,3$ is the number of dimensions in the system and $n=r_p^{-m}$. Since both equations of state [*thermal* $P(T,n,\phi,g)$ and *calorific* $U(T,n,\phi,g)$] are known, any thermodynamic function may be found by means of basic formulas of thermodynamics. For example, the normalized thermal coefficient of pressure $\beta_V=n^{-1}(\partial P/\partial T)_V$, the heat capacity $C_V=(\partial U/\partial T)_V$ at constant volume V, and the normalized isothermal compressibility $\chi_T=T/(\partial P/\partial n)_T$. Isothermal compressibility χ_T can be also defined from a known relation of statistical physics, $S(0)=\chi_T$, where the structure factor $S(k)$ is related to the function $g(r)$ by the Fourier transform,

$$S(k) = 1 + 2\pi n(m-1)\int_0^\infty [g(r)-1]r^{m-1}\Psi(kr)dr. \tag{9}$$

The $\Psi(kr)$ function is determined by the dimension of the Fourier transform: $\Psi(kr)=\sin(kr)/(kr)$ for $m=3$ and $\Psi(kr)=J_0(kr)$ for $m=2$, where $J_0(k)$ is the zero-order Bessel function of the first kind. Note that the majority of experimental methods for studying the physical properties of real molecular liquids are based on measurements of structural factor $S(k)$ by various methods of spectroscopy [2]. Taking into consideration Eq. (9) at $k\to 0$, the value of isothermal compressibility may be presented as

$$\chi_T = T\left(\frac{\partial n}{\partial P}\right)_T \equiv 1 + 2\pi n(m-1)\int_0^\infty [g(r)-1]r^{m-1}dr. \tag{10}$$

In case of $T\to 0$ the values of $U\to U_0$, $P\to P_0$, and $\chi_T/T\to\chi_T^0/T=[(\partial P_0/\partial n)_T]^{-1}$, where U_0 and P_0 are the energy density and the pressure for the crystal lattice at $T=0$, respectively. For any lattice of known type, e.g., for classical triangular lattice (hp crystal) or for the bcc lattice, the values of U_0 and P_0 may be easily computed. The illustration of an arrangement of particles in two mentioned types of lattices is presented in Fig. 1. In Table I the normalized values of energy $U_0(\Gamma T)^{-1}$, pressure $P_0(n\Gamma T)^{-1}$, and compressibility $\chi_T^0\Gamma$ calculated in the Yukawa systems with different screening parameters κ are shown for hp and bcc lattices. Procedure of definition of U_0 and P_0 for isotropic pair potentials of any form is briefly described in the Appendix.

To avoid repeated computer calculations of the $U(T,n,\phi,g)$ and $P(T,n,\phi,g)$ functions with a change of the system parameters (T,n,ϕ,g), the various approximations for both equations of state (7) and (8) are widely used [4,5,23–30]. Some of them are complicated polynomials obtained by the best fitting of numerical data by the various

TABLE I. The energy $U_0(\Gamma T)^{-1}$ pressure $P_0(n\Gamma T)^{-1}$ and $\chi_T^0\Gamma$ in the Yukawa systems with different screening parameters, κ, for hp and bcc lattices.

κ	$\frac{U_0}{\Gamma T}$ (hp)	$\frac{P_0}{n\Gamma T}$ (hp)	$\chi_T^0\Gamma$ (hp)	$\frac{U_0}{\Gamma T}$ (bcc)	$\frac{P_0}{n\Gamma T}$ (bcc)	$\chi_T^0\Gamma$ (bcc)
1	1.62532	2.18866	0.20716	5.27533	5.82251	0.08376
1.5	7.59943×10^{-1}	1.17343	0.36339	1.95710	2.35588	0.20100
2	3.93543×10^{-1}	6.90916×10^{-1}	0.57723	8.80191×10^{-1}	1.16464	0.39121
2.5	2.14259×10^{-1}	4.24073×10^{-1}	0.87662	4.34854×10^{-1}	6.33702×10^{-1}	0.68704
3	1.19909×10^{-1}	2.65362×10^{-1}	1.30390	2.26360×10^{-1}	3.62802×10^{-1}	1.14122
3.5	6.82001×10^{-2}	1.67435×10^{-1}	1.92353	1.21584×10^{-1}	2.13634×10^{-1}	1.83764
4	3.91733×10^{-2}	1.05911×10^{-1}	2.83392	6.66133×10^{-2}	1.27778×10^{-1}	2.90901
4.5	2.26391×10^{-2}	6.69524×10^{-2}	4.18603	3.69740×10^{-2}	7.70731×10^{-2}	4.56518
5	1.31346×10^{-2}	4.22279×10^{-2}	6.21252	2.07047×10^{-2}	4.66832×10^{-2}	7.13853
5.5	7.63929×10^{-3}	2.65513×10^{-2}	9.27356	1.16661×10^{-2}	2.83228×10^{-2}	11.15676

approximating curves [23–30], while the others are based on Mayer's cluster expansion for weakly nonideal systems [23]. In both cases the form of approximating curves (for U and/or P) can vary depending on a range of system parameters (T, n, ϕ, g). Accuracy of such approaches often does not allow the correct calculation of other thermodynamic characteristics on the base of known formulas of thermodynamics (which include the integrals and/or differentials of U and/or P) without the use of additional fitting procedures.

B. Approximations for the energy density in the Yukawa systems

The energy density U may be represented as sum of the simple thermal part ($U_{th}=mT/2$) and the potential part [$U_p=U-U_{th}$, i.e., second term in Eq. (7)]. Owing to this, the existing approaches of U are commonly restricted by choosing a suitable U_p function. Proposed approximations usually describe the thermal component U_p^{th} of the potential energy,

$$U_p^{th} = (U_p - U_0) \equiv \left(U - U_0 - \frac{mT}{2}\right), \qquad (11)$$

or its negative correlation (or "cohesive") component,

$$U_c = U_p - U_H \equiv (m-1)\pi n \int_0^\infty \phi(r)[g(r)-1]r^{m-1}dr. \qquad (12)$$

Here, U_H is the positive Hartree part of the potential energy,

$$U_H = (m-1)\pi n \int_0^\infty \phi(r) r^{m-1}dr. \qquad (13)$$

In the Yukawa systems $U_H/T=\Gamma_2/\kappa_2\equiv\pi\Gamma/\kappa$ for 2D case and $U_H/T=3\Gamma_3/(2\kappa_3)\equiv2\pi\Gamma/\kappa$ for 3D case. When Γ increases ($\Gamma\to\infty$), the U_c value approaches the value of the Madelung energy E_M (for an appropriate lattice): $U_c\to E_M=U_0-U_H$. Sometimes the contributions of background plasma in the correlation part of energy are considered, so, for example, for the 3D Yukawa systems we have $U_c^0=U_c-T\Gamma_3$ and $\kappa_3\equiv U_c-T\Gamma\kappa$ [27–30]. Thus, the expression $E_M^0=U_0-U_H-T\Gamma\kappa$ is used to estimate the value of the Madelung energy. Thus, in terms of E_M and U_c, the thermal component of the potential energy can be presented as $U_p^{th}=U_c-E_M$. Without dependence on the form of representation (11) or (12), in the majority of existing works, the choice of the approximating factors in the proposed approaches of U is carried out using the numerical data for the $U_c/(T\Gamma)$ function [23–30].

For convenience of comparison of various approximations we will use the normalized value for the thermal component U_p^{th} of the potential energy,

$$\delta U = (U - U_0 - mT/2)/T. \qquad (14)$$

Some approximations for the energy density in the Yukawa systems [23,24,28,29] are given below. So, the calculations for fluid 3D systems were performed in the works of Hamaguchi and co-workers [28,29] and the following approximation expression for the δU value was proposed:

$$\delta U \cong \delta U_3^{H\text{-}F} = A_1\Gamma_3 + A_2\Gamma_3^{1/3} + A_3 + A_4\Gamma_3^{-1/3}. \qquad (15)$$

Here, for $\kappa_3\leq1$ [28], the coefficients A_i may be represented by the polynomials

$$A_1 \cong -0.003\,256 - 0.000\,482\kappa_3 - 0.000\,964\kappa_3^2,$$

$$A_2 \cong 0.559\,934 + 0.026\,341\kappa_3 + 0.050\,644\kappa_3^2,$$

$$A_3 \cong -0.192\,006 - 0.082\,556\kappa_3,$$

$$A_4 \cong -0.040\,346 - 0.044\,115\kappa_3. \qquad (16)$$

For the case of $\kappa_3\geq1.2$ Hamaguchi *et al.* [29] proposed the other values A_i; some of them are tabulated in Table II.

The calculations for the fluid 2D Yukawa systems were presented in the work of Totsuji *et al.* [23] together with an approximate expression for δU in the range of $0.05\leq\Gamma_2\leq100$ and $0.5\leq\kappa_2\leq2$,

TABLE II. Fluid fitting parameters A_i ($i=1,2,3,4$) defined by Eq. (13) for $\kappa_3 \geq 1.2$ [29].

κ_3 (κ)	A_1	A_3	A_2	A_4
1.2 ($\sim$1.934)	−0.002524	0.522733	−0.305649	0.026740
1.4 ($\sim$2.257)	−0.002451	0.514325	−0.344195	0.049258
2.0 ($\sim$3.224)	−0.001545	0.442193	−0.382900	0.100506
2.6 ($\sim$4.191)	−0.000865	0.366308	−0.411566	0.159826
3.0 ($\sim$4.836)	−0.000559	0.312503	−0.394913	0.173963
3.6 ($\sim$5.803)	−0.000253	0.239251	−0.362000	0.195448
4.0 ($\sim$6.448)	−0.000080	0.182517	−0.257154	0.131096

$$\delta U \cong \delta U_2^{TLTT} = (B_1\Gamma_2 + B_2)\exp[-2.55(\Gamma_2^{0.18} - 0.05^{0.18})]. \tag{17}$$

Here $B_1=\pi^{-1/2}(-1.9605+0.8930\kappa_2-0.1959\kappa_2^2+0.017\,15\kappa_2^3) \cong U_0/(\Gamma T)-\pi/\kappa$ describes the Madelung energy E_M for triangular lattice and $B_2=\Gamma_2^2\{\ln(2\Gamma_2\kappa_2)+2\gamma-1\}$, where $\gamma=0.5772\ldots$ is the Euler constant. It was confirmed that the relative error in a determination of $U_c/(T\Gamma_2)$ from Eq. (17) is less than 1% for $10 \leq \Gamma_2 \leq 100$, less than 3% for $1 \leq \Gamma_2 \leq 10$, and less than 10% for $0.05 \leq \Gamma_2 \leq 1$.

Another approximation for δU was proposed in the work of Hartmann *et al.* [24] for the 2D Yukawa systems with $0.05 \leq \Gamma_2 \leq 120$ and $0 \leq \kappa_2 \leq 3$,

$$\delta U \cong \delta U_2^{HKDK} = \Gamma_2(C_1 + C_2 C_3^{-2/3}) - C_0, \tag{18}$$

where $C_0=U_0/(\Gamma T)-\pi/\kappa$ and the coefficients C_i ($i=1,2,3$) may be represented by the polynomials

$$C_1 = -1.113 + 0.505\kappa_2 - 0.107\kappa_2^2 + 0.006\,86\kappa_2^3 + 0.0005\kappa_2^4,$$

$$C_2 = 0.384 - 0.036\kappa_2 - 0.052\kappa_2^2 + 0.0176\kappa_2^3 + 0.001\,65\kappa_2^4,$$

$$C_3 = \Gamma_2(1 - 0.388\kappa_2^2 + 0.138\kappa_2^3 - 0.0138\kappa_2^4). \tag{19}$$

Note that the value of $C_3 \propto \Gamma^*$ determines the form of pair-correlation function, $g(r)$ [25].

C. New analytical approaches for the thermodynamic function in the fluid systems

Here we present the simple analytical approximation for the energy density of the 2D nonideal systems that was obtained by means of the semiempirical "jumps" theory based on the analogies between solid and liquid states of matter [1,3]. According to this theory, physical properties of the strongly nonideal systems may be characterized by a single average energy, namely, the energy of jump activation W_a (i.e., the energy which is necessary for a particle to pass from one "settled" condition to another). Note that this theory works well in determination of the transport constants (diffusion, viscosity, thermal conductivity, etc.) both for simulated systems and for real molecular liquids. Following the jump theory and a principle of detailed balance [1,3,31–34] let us consider a system consisting of $N=N_1+N_2$ particles, where $N\equiv$const, N_1 is the number of settled particles with the energy density U_1, and N_2 is the number of "free" migrating particles with the energy density U_2. Under equilibrium conditions for the system in a contact with "thermostat" we have

$$w_{12}N_1 = w_{21}N_2,$$

$$w_{12}/w_{21} = \exp[(\varepsilon_2 - \varepsilon_1)/T] \equiv \exp(\varepsilon_f/T), \tag{20}$$

where w_{12} and w_{21} are the probabilities of transition from a settled state ($i=1$) to a free state ($i=2$) and vice versa, respectively, and ε_i is the energy of corresponding state ($i=1,2$) per one degree of freedom. Further, assuming $U_1=(U_0+mT/2)$ and $(U_2-U_1)=a_1\varepsilon_f$, where the a_1 value is determined by the total number of degrees of freedom s ($a_1 \sim s$) [27], the energy density of the analyzed system may be written as

$$U = \frac{U_2 - U_1}{1+\exp(\varepsilon_f/T)} + U_1 \equiv \frac{a_1\varepsilon_f}{1+\exp(\varepsilon_f/T)} + U_0 + \frac{mT}{2}. \tag{21}$$

According to the absorption or adsorption theory, the ε_f value is determined by the energy of jump of deactivation [1,7,34,35] [$\varepsilon_f=W_a+Q_a$, where $W_a=a_2T_c$ and $Q_a=a_3(T-T_c)/2$ are the energy and the heat of jump activation, respectively; T_c is the crystallization temperature of the system (formation of the perfect crystal) and a_i ($i=2,3$) are some coefficients depending on the type of lattice in system's crystalline state ($s \geq a_i \geq 1$)],

$$\varepsilon_f = W_a + Q_a \equiv a_2T_c + a_3(T-T_c)/2. \tag{22}$$

Thus, under the assumption of $a_i \approx$const [$\neq f(T)$], the approximation for the energy density in fluids may be found by the choosing of appropriate coefficients (a_i, $i=1,2,3$) in Eqs. (21) and (22).

Under a simplified quasiclassical approach for these systems, $a_2=m$ and $a_3=1$, and we may rewrite the energy ε_f [Eq. (22)] as

$$\frac{\varepsilon_f}{T} = \frac{0.5(\Gamma_c^* - \Gamma^*) + m\Gamma^*}{\Gamma_c^*}. \tag{23}$$

After some transformations the energy density of systems considered may be presented in the form

$$U \cong U_a = U_0 + \frac{mT}{2} + \frac{a_1\varepsilon_f}{1+\exp(\varepsilon_f/T)}, \tag{24}$$

and normalized value for the thermal component of the potential energy can be written as

$$\delta U = \frac{U - U_0 - mT/2}{T} \cong \frac{a_1\varepsilon}{1+\exp(\varepsilon)}, \tag{25}$$

where $\varepsilon=\varepsilon_f/T\equiv 0.5+(m-0.5)\Gamma^*/\Gamma_c^*$, $\Gamma_c^*=\Gamma_{2D}^*$ for 2D systems and $\Gamma_c^*=\Gamma_{3D}^*$ for the 3D case.

The approximation of U_a [Eq. (24)] may be used for determination of various thermodynamic functions. So, the heat capacity $C_V \cong C_V^a=(\partial U_a/\partial T)_V$ may be presented as

$$C_V^a = \frac{m}{2} + \frac{0.5a_1 + (\varepsilon - 0.5)\delta U \exp(\varepsilon)}{1 + \exp(\varepsilon)}. \quad (26)$$

Approximate expressions for the pressure P_a may be obtained from a well-known relation

$$-n^2(\partial U_a/\partial n)_T = T(\partial P_a/\partial T)_n - P_a. \quad (27)$$

Further, after certain development,

$$n^2T^{-2}(\partial U_a/\partial n)_T = (\partial\{P_aT^{-1}\}/\partial T)_n,$$

$$(mr_pT)^{-1}\frac{d(U_aT^{-1})}{d\varepsilon}\left(\frac{\partial\varepsilon}{\partial r_p}\right)_T = \frac{d(P_aT^{-1})}{d\varepsilon}\left(\frac{\partial\varepsilon}{\partial r_p}\right)_n,$$

we have

$$P_a = P_0 + nT + \alpha n\delta UT/m, \quad (28)$$

where $\alpha=-(\partial\Gamma^*/\partial r_p)r_p/\Gamma^*$, i.e., $\alpha=(1+\kappa+\kappa^2/2+\kappa^3/2)/(1+\kappa+\kappa^2/2)$ for the Yukawa systems. Thus, approximate expressions for the thermal coefficient of pressure $\beta_V^a=n^{-1}(\partial P_a/\partial T)_V$ and the normalized isothermal compressibility $\chi_T^a=T/(\partial P_a/\partial n)_T$ may be written as

$$\beta_V^a = 1 + m^{-1}\alpha(C_V^a - m/2), \quad (29)$$

$$(\chi_T^a)^{-1} = 1 + \Gamma(\Gamma\chi_T^0)^{-1} + \alpha_0^2(\varepsilon - 0.5)\left(\frac{a_1 - \delta U}{1 + \exp(\varepsilon)} - \delta U\right) + \left(\frac{\alpha_0(m-1)}{m} + \alpha_0^2\alpha_1\right)\delta U, \quad (30)$$

where $\alpha_0=\alpha/m$ and $\alpha_1=\Gamma^*(\partial^2\Gamma^*/\partial r_p^2)/(\partial\Gamma^*/\partial r_p)^2-1$.

Finally, we note that the relation between heat capacities $C_V=(\partial U/\partial T)_V$ (at constant volume V) and $C_P=(\partial I/\partial T)_P$ (at constant pressure P, where I denotes enthalpy) may be written as

$$(C_P - C_V) = \beta_V^2\chi_T. \quad (31)$$

Bear in mind that the difference C_P-C_V is insignificant [5] for liquids in the majority of cases.

D. Theories of melting for two dimensions

Here we need some short remarks that may be useful for discussion of the below-mentioned numerical data. There are two main approaches in the melting theory for two dimensions that are based on unbinding of topological defects. The first of them is the Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) theory which predicts two phase transitions from the solid to liquid state via an intermediate state (so-called "hexatic" phase) [36–38]. In this hexatic phase the spatial reducing of peaks (g^k) for pair correlations function $g(r)$ is described by an exponential law [$g^k(r)\propto\exp(-\mu r)$, $\mu\equiv$const], and the bound orientation function $g_6(r)$ obeys power law [$g_6(r)\propto r^{-\psi}$, $\psi>0.25$]. The second melting theory, the theory of grain-boundary-induced (GBI) melting [39,40], predicts a single first-order transition from the solid to the liquid state without an intermediate phase for a certain range of values of the point-defect core energies. In this case, the mentioned spatial KTHNY—reducing of $g(r)$ and $g_6(r)$ functions—is not valid for both phase states of the system. (Note that the question of alternative two-stage melting is still open in GBI theory.)

Compelling evidence for KTHNY theory in the systems with different interparticle potentials has been presented in a set of experimental and numerical works [22,36,41–47]; e.g., a detailed study of validity of KTHNY theory for the simulated quasi-two-dimensional dissipative Yukawa systems is presented in [22,47]. The numerical simulations [22,47] have shown that the physical properties of these systems have two singular points. The first of them ($\Gamma^*=\Gamma_h^*\approx 98\pm 3$) may be related to the fluid-to-hexatic phase transition, the second point ($\Gamma^*=\Gamma_{2D}^*\cong 154\pm 4$) is the point of hexatic-to-perfect (without defects) crystal transition. Nevertheless, a comparison of existing experiments in dusty plasma [48,49] with the predictions of mentioned theories of 2D melting shows no strong evidence neither for KTHNY theory nor for GBI theory.

E. Transport coefficients in the liquid systems

The coefficients of diffusion D, thermal conductivity χ, and viscosity η reflect the thermodynamic state of a system. In the case of gases, the constants of diffusion, kinematical viscosity $\nu=\eta/\rho$, and thermal diffusivity $\theta=\chi/(\rho c_P)$ have close values and may be written in the form of known analytical relations [31] (here, $\rho=Mn$ and $c_P=C_Pk_B/M$ stand for specific-heat capacity at constant pressure P and k_B is the Boltzmann constant). Such relations for the liquid state of matter accept applying known hydrodynamic models for analysis of the wave propagation and the formation of vortices and various instabilities in nonideal media. When the deviations of the system from the statistical equilibrium are small, the kinetic coefficients of linear dissipative processes (constants of diffusion, viscosity, thermal conductivity, etc.) can be found from the well-known Green-Kubo formulas. However, in the general case of nonideal fluids, the analytical solutions of the Green-Kubo equations are unavailable.

Existing numerical study [11,21,22] shows that the diffusion coefficient for the strongly coupled (liquidlike) systems (with $100>\Gamma^*>50$) can be approximated as

$$D \approx \frac{T\Gamma^*}{12\pi(\xi+1)\nu_{fr}M}\exp\left(-3\frac{\Gamma^*}{\Gamma_a^*}\right). \quad (32)$$

Here Γ_a^* is the crystallization point ($\Gamma_a^*=\Gamma_{3D}^*\cong 102$) for the 3D problem [11,21] and $\Gamma_a^*=\Gamma_h^*\cong 98$ for the 2D case, where Γ_h^* is the Γ^* value in the point of formation of the hexatic phase of solid [22,47].

Relations between the energy density, heat capacity, and diffusion constants in the 3D and 2D Yukawa systems were studied in a recent paper [50] where it was found that the energy density for the 2D and 3D nonideal system may be presented as

$$U = U_0 + mT/2 + mT(1 - D^*) - (m-1)\Gamma^*T/\Gamma_c^*, \quad (33)$$

where $D^*=D(\nu_{fr}+\omega^*)M/T$ and $\Gamma_c^*=\Gamma_{3D}^*$ for the 3D case ($m=3$) and $\Gamma_c^*=\Gamma_{2D}^*$ for 2D case ($m=2$). Thus, the approximation of diffusion constants may be presented as (see Secs. II C and III B; $a_1=4$)

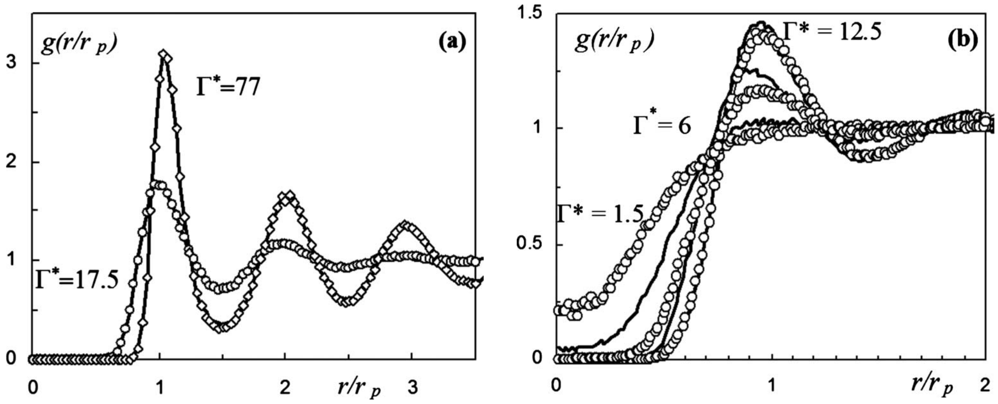

FIG. 2. Results of numerical calculations of $g(r/r_p)$ functions for 2D systems with Γ^* parameters (indicated in figures) and for different pair potentials—(a) (lines) $\phi/\phi_c=\exp(-4r/r_p)$ and $\xi\approx 3$; (○) $\phi/\phi_c=\exp(-3r/r_p)+0.05r_p/r$ and $\xi\approx 0.12$; (◇) $\phi/\phi_c=0.05(r_p/r)^3$ and $\xi\approx 0.5$; (b) (○) $\phi/\phi_c=\exp(-2r/r_p)$ and $\xi\approx 0.5$ and (lines) $\phi/\phi_c=\exp(-4r/r_p)$ and $\xi\approx 0.5$.

$$D^*\cong 1-\frac{1}{m}\left(\frac{4\varepsilon}{1+\exp(\varepsilon)}+(m-1)\frac{\Gamma^*}{\Gamma_c^*}\right). \tag{34}$$

Proposed relation (34) provides a better description of the numerical data (in the wide range of Γ^* values from ~ 10 to $\sim\Gamma_c^*$) than expression (32) [50]. The relative accuracy of Eq. (34) is within 5–10 % for $10<\Gamma^*<100$, which corresponds to the error of the numerical experiment.

We may also assume that presented approach (34) is valid for the various types of pair potentials which satisfy condition (4). This is due to the fact that for systems satisfying this condition both D^* and δU functions (as it is illustrated below) are determined by the Γ^* parameter only.

In addition, the values of constants of viscosity and thermal diffusivity may be easily estimated for the strongly coupled liquid systems ($50<\Gamma^*<\Gamma_c^*$) via Eq. (34) using the known Einstein-Stokes relations [5,22,51,52]. The numerical simulation of transfer processes in simple monatomic liquids with a wide scope of interaction potentials reveals that the relations between the transport coefficients may be approximated as [4]

$$\nu\cong\frac{0.12r_p^2T}{MD}, \tag{35}$$

$$\theta\cong 1.5\frac{r_pV_t}{C_P}\left(\frac{0.6r_pV_t}{D}\right)^{5/8}, \tag{36}$$

where $V_t=(T/M)^{1/2}$.

III. RESULTS OF NUMERICAL SIMULATION AND THEIR DISCUSSION

A. Parameters of numerical simulation

The simulation was carried out by the Langevin molecular-dynamics method based on the solution of the system of differential equations with a stochastic force that takes into account processes leading to the established equilibrium (stationary) temperature T of particles' system (i.e., the one considered when concerning temperature of a continuous media) which characterizes kinetic energy of their random (thermal) motion. The simulation technique is detailed in [11,21,22].

The calculations were carried out for various types of pair isotropic potentials $\phi(r)$ that represent various combinations of power-law and exponential functions commonly used for simulation of repulsion in physical kinetics [2,7],

$$\phi=\phi_c\left[b_1\exp\left(-\kappa\frac{r}{r_p}\right)+b_2\left(\frac{r_p}{r}\right)^s\right], \tag{37}$$

which satisfies empirical condition (4) under the additional limit: $|\phi'' r_p/\phi'|>1$. Here $b_{1(2)}$, $\kappa=r_p/\lambda$, and ζ are variable parameters; $\phi_c=(eZ)^2/r$ is the Coulomb potential energy. The calculations were performed for a uniform 3D system and for a quasi-2D system representing an extensive dusty layer. The scaling parameter was varied from $\xi\approx 0.04$ to $\xi\approx 4$, i.e., in the range typical for the laboratory dusty plasma in gas discharges. The Γ^* value was varied from ~ 1 to 120–250.

In the 3D case the external forces were considered to be absent since the periodical boundary conditions were used for all three directions, **x**, **y**, and **z**. The number of independent particles N_p in the central calculated cell was varied from 250 to 686; accordingly, the cutoff distance of potential was varied from $4r_p$ to $8r_p$ [here, $r_p=(N_p/V_c)^{-1/3}$, where V_c is the volume of simulated cell]. In the quasi-2D case the simulations were carried out for a monolayer of grains with periodical boundary conditions in the directions **x** and **y**. In **z** direction the gravitational force Mg compensated by the linear electrical field $E_z=\beta z$ was considered. Here β is the magnitude of gradient of electrical field. The number of independent particles N_p in the central calculated cell was varied from 256 to 1024; accordingly, the cutoff distance of potential was altered from $8r_p$ to $25r_p$ [here $r_p=(N_p/S_c)^{-1/2}$, where S_c is the area of simulated cell].

The β value was varied from $\sim 10^{-2}$ to ~ 100 V/cm^2, and for the simulated monolayers of grains the β value was in an agreement with the criterion proposed in [53],

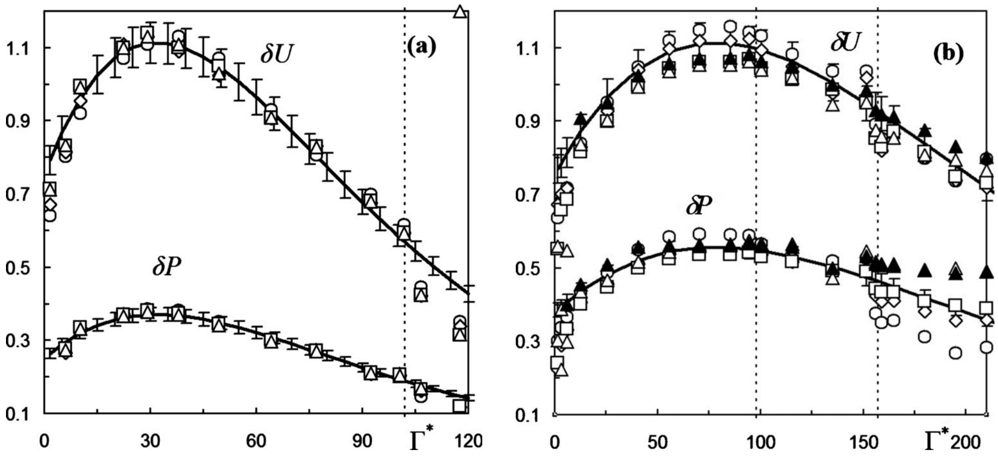

FIG. 3. The values of δU and $\delta P=(P-P_0-nT)/(\alpha nT)$ vs Γ^* for (a) 3D and (b) 2D with different potentials ϕ/ϕ_c: (○) $\exp(-2r/r_p)$; (△) $\exp(-5.5r/r_p)$; (◇) $\exp(-3r/r_p)+0.05r_p/r$; (□) $\exp(-4r/r_p)+0.01(r/r_p)^2$; and (▲) $0.05(r_p/r)^3$; solid lines are approximations (25) and (28) with $a_1=4$.

$$|eZ\beta| < 2\sum_{i=1}^{N_p} \phi'(r_i)/r_i. \tag{38}$$

Under this condition any considerable dependence of particles' dynamics on the values of β and N_p has not been detected in our simulations.

B. Results of numerical simulations of thermodynamic and transport properties

For all cases under study the form of obtained pair-correlation functions $g(r)$ was determined by the value of Γ^* parameter for the systems with $\Gamma^*>10-15$. For illustration, Fig. 2 shows the simulations of the pair-correlation functions for the 2D layer of particles interacting with various potentials and values of Γ^* parameter. Similar results for the 3D systems with isotropic pair potentials within wide ranges of values of their parameters were obtained in [21].

The numerical study of the 2D systems shows also that the physical properties of analyzed systems [such as extrema of pair-correlation functions $g(r)$ and the diffusion coefficients D] have two singular points. The first of them (the inflection point at $\Gamma^*=\Gamma^*_h\approx 98\pm 3$) may be related to the fluid-to-hexatic phase transition; the second one (the point of abrupt changes at $\Gamma^*=\Gamma^*_c\equiv\Gamma^*_{2D}\cong 154\pm 4$, where $D\to 0$) tends to be the point of hexatic-to-perfect crystal transition. The spatial reduction of peaks (g^k) for pair correlation function $g(r)$ subject to the exponential law $g^k(r)\propto\exp(-\mu r)$ for the liquid [$\mu=\mu(T)>\mu_h$ for $\Gamma^*<\Gamma^*_h$] and for the hexatic phase ($\mu=\mu_h\cong 0.6$ for $\Gamma^*_h<\Gamma^*<\Gamma^*_{2D}$) was described by the power law $g^k\propto(r/r_p)^{-\psi}$ with $\psi<1/3$ for all pikes of $g(r)$ excluding its first maximum in the case of perfect crystal ($\Gamma^*>\Gamma^*_{2D}$), where $D=0$. The disagreement between the results of the all calculations was within the limits of the numerical error and did not exceed $\pm 1-3$ %. The similar results were obtained earlier for simulated the quasi-2D dissipative Yukawa systems [22,47] (see Sec. II D).

The calculations of thermodynamic characteristics [U, P, $\beta_V=n^{-1}(\partial P/\partial T)_V$, $C_V=(\partial U/\partial T)_V$, and $\chi_T=T/(\partial P/\partial n)_T$] vs Γ^* using the obtained $g(r)$ functions and Eqs. (7) and (8) for the 2D and 3D systems are presented in Figs. 3–6 for various pair potentials $\phi(r)$ and scaling factors ξ. The error bars in these figures correspond to the relative error of 5%.

The illustrations of $U(\Gamma^*)$ and $P(\Gamma^*)$ are presented in Fig. 3 for the 2D and 3D systems with different potentials.

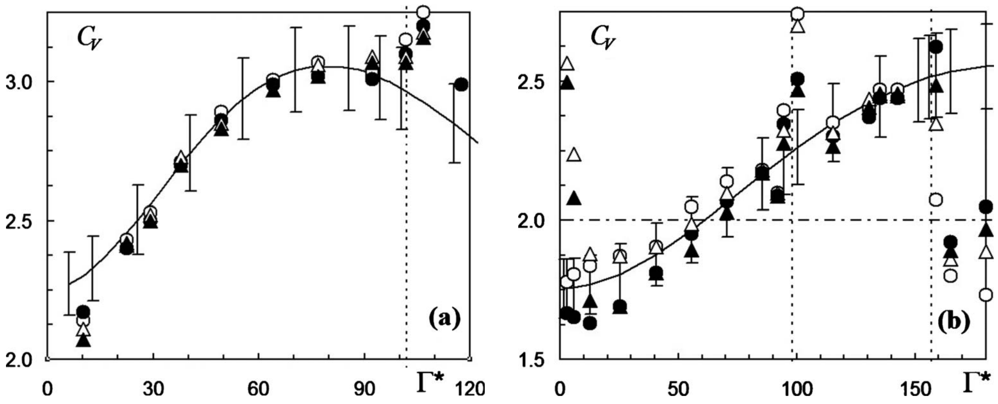

FIG. 4. The C_V values vs Γ^* for (a) 3D and(b) 2D Yukawa systems with different κ: (○;●)—2, (△;▲)—5.5, and ξ: (●;▲)—0.2, and (○;△)—2; solid lines correspond to approximation C_V^a [Eq. (26)].

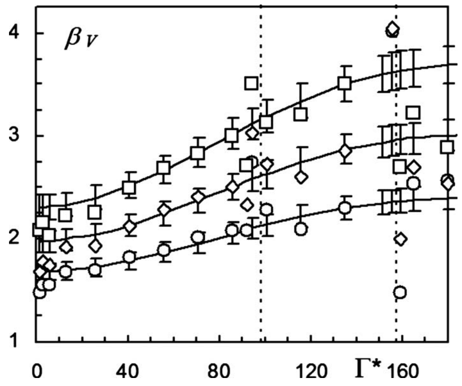

FIG. 5. Function β_V vs Γ^* for the 2D Yukawa systems with ξ=1.86 and different κ: (○)—2; (◇)—3; and (□)—4; solid lines correspond to approximation β_V^a [Eq. (29)].

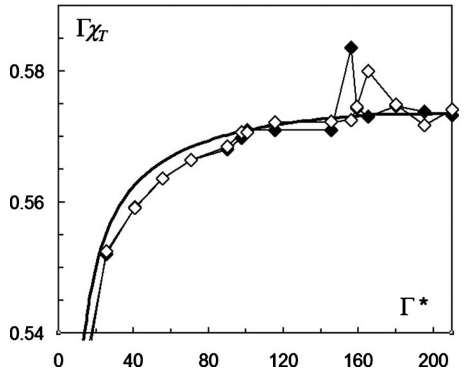

FIG. 6. Function of $\Gamma\chi_T$ vs Γ^* for the 2D Yukawa systems with κ=2 and different ξ: (-◇-)—0.23; (-◆-)—1.86; deep line is approximation (30).

It is easily seen that the obtained normalized values of $\delta U=(U-U_0-mT/2)/T$ and $\delta P=(P-P_0-nT)/(\alpha nT)$ are completely determined by the value of Γ^* parameter in accordance with the semiempirical approaches [Eqs. (25) and (28)]. Under the assumption of $a_i \approx \text{const}$ $[\neq f(T)]$ the expression for the energy density $U_a(\Gamma^*)$ may be found by the choosing the appropriate coefficients (a_i, $i=1,2,3$) in Eqs. (21) and (22) using the best fitting of the numerical calculations $U(\Gamma^*)$ by the analytical curve. The calculations have shown that these coefficients can be presented as $a_1 \cong 4$, $a_2 \cong m$, and $a_3 \cong 1$ for all cases under study. Thus, the energy density of analyzed systems may be written in form Eq. (24) with $a_1=4$. One can easily see that the relative deviations of δU values for proposed approximation (25) from numerical results are less than 5% in the range from $\Gamma^* \approx 10-15$ to the point of formation of the perfect lattice ($\Gamma^*=\Gamma_c^*$).

The heat capacity $C_V=(\partial U/\partial T)_V$, together with the approximation C_V^a [Eq. (26)], is shown in Fig. 4 for the Yukawa systems with various screening factors κ and scaling parameters ξ. Additionally, in Figs. 5 and 6 the results of numerical simulations of other thermodynamic coefficients (β_V, χ_T) and their analytical approximations [Eqs. (29) and (30)] for the 2D Yukawa systems are also shown.

The relative deviations of proposed approximation [Eqs. (26) and (28)–(30)] from numerical results are less than 5% in the range from $\Gamma^* \sim 15$ to $\Gamma^* \sim \Gamma_c^*$ (excluding the point of phase transition). Singularity (jumps) of the thermodynamic coefficients $[C_V(\Gamma^*), \beta_V(\Gamma^*), \chi_T(\Gamma^*)]$ close to the values of $\Gamma^* \approx \Gamma_{3D}^*$ (pointed in figures with a dotted line) corresponds to the point of crystallization of the analyzed 3D systems. In the 2D case, two singularities for the above-mentioned coefficients close to the values of $\Gamma^* \approx \Gamma_h^*$ and $\Gamma^* \approx \Gamma_{2D}^*$ are determined by the two-stage scenario of melting in the 2D systems (see Sec. II D).

C. Comparison with the existing numerical data

Comparison of new approximation for the energy density with the existing approaches for U functions for the 2D and 3D fluid Yukawa systems [23,24,28,29] is presented in Figs. 7–9. The error bars in these figures correspond to the relative error of 5%.

So, the approximation for δU [Eq. (25)] together with the expression $\delta U_3^{H\text{-}F}$ [Eq. (15)] [28,29] is illustrated in Fig. 7(a) and the $\delta C_V(\Gamma^*)=(C_V-m/2)$ functions are presented in Fig. 7(b). The deviations of the functions $\delta U_3^{H\text{-}F}(\Gamma^*)$ from the curve shown in Fig. 7(a) are less than 1% in the range of κ from 0 up to 5.5. Thus, we can conclude that the approximation of $\delta U_3^{H\text{-}F}$ [28,29] is also determined by the Γ^* value, as the new approximation δU [Eq. (25)]. Nevertheless, there is the difference between δU and $\delta U_3^{H\text{-}F}$, which is $\Delta^{H\text{-}F}=\delta U_3^{H\text{-}F}-\delta U \approx 1.78\Gamma^*/\Gamma_c^* \cong 0.0178\Gamma^*$. This difference

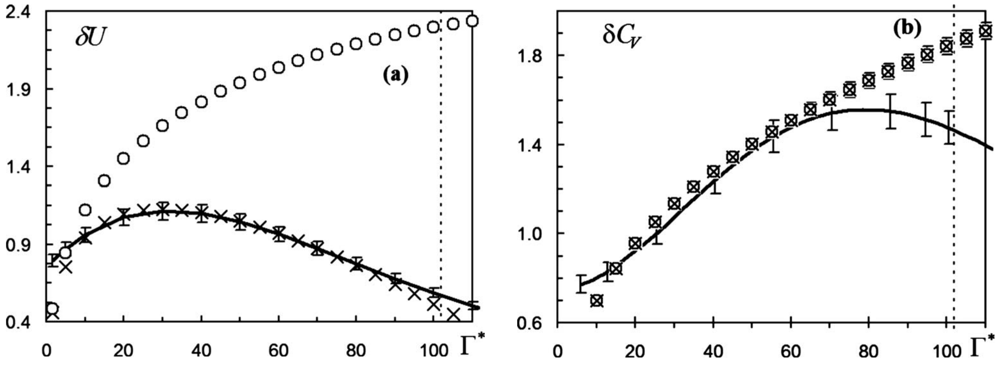

FIG. 7. The values of (a) δU and (b) $\delta C_V=(C_V-m/2)$ vs the 3D Yukawa systems obtained using the various approaches for the U function: (deep lines)—approximation (25), (symbols): (○)—Eq. (15) for κ from 0 up to 5.5; and (×)—corrected Eq. (15), i.e., $\delta U=\delta U_3^{H\text{-}F}-\Delta^{H\text{-}F}$.

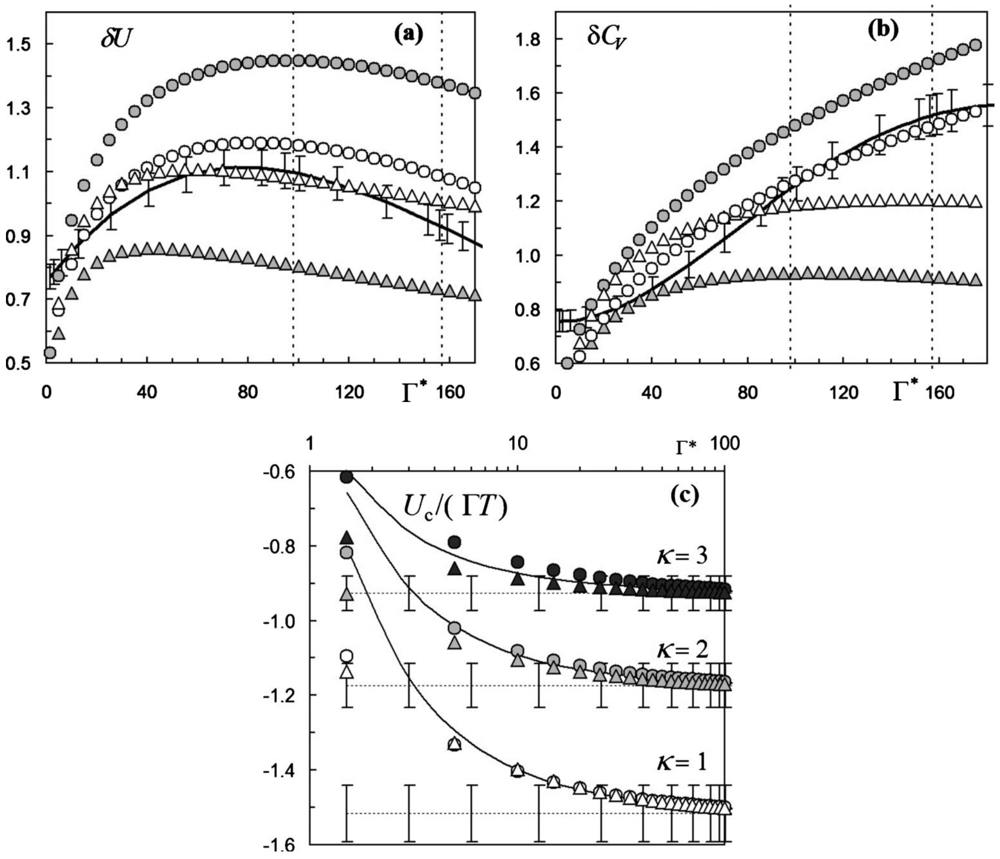

FIG. 8. The values of (a) δU, (b) $\delta C_V = (C_V - m/2)$, and (c) $U_c/(\Gamma T)$ vs Γ^* for the 2D Yukawa systems obtained using the various approaches for the U function: (lines)—approximation (25); (symbols): (○; ●; ●)—Eq. (18), (△; ▲; ▲)—Eq. (17); that is, (○; △)—for $\kappa=1$; (●; ▲)—for $\kappa=2$; and (●; ▲)—for $\kappa=3$.

$\Delta^{H\text{-}F}$ does not affect the $C_V(\Gamma^*)$ function [see Fig. 7(b)] due to the $(T\Delta^{H\text{-}F})$ value that is independent of the temperature T, i.e., $(T\Delta^{H\text{-}F}) \neq f(T)$.

It is necessary to remember that in the majority of existing works the choice of the approximating factors in the proposed approaches of U is based on the numerical data for the $U_c/(T\Gamma)$ function [23–30] (see Sec. II B). It is possible to estimate the deviation δ_Δ to the value of $U_c/(T\Gamma)$ [28,29] from the additional term $\Delta^{H\text{-}F}$ as

$$\delta_\Delta = \frac{\Delta^{H\text{-}F}/\Gamma}{U_c/(T\Gamma)} \approx 0.0178\left(1+\kappa+\frac{\kappa^2}{2}\right)\frac{\exp(-\kappa)}{\kappa+2\pi/\kappa},$$

i.e., it is less than 0.5% for all values of Γ and κ under consideration.

Let us consider δU_2^{TLTT} [Eq. (17)] and δU_2^{HKDK} [Eq. (18)] in case of the Yukawa fluids. Note that within domain of applicability, which is described for these approaches in [23,24], the values of δU_2^{TLTT} and δU_2^{HKDK} correspond to the proposed $\delta U(\Gamma^*)$ and $\delta C_V(\Gamma^*)$ functions (with deviation of less than 7%) only for the scaling parameters $0.5 \leq \kappa \leq 1$ [see Figs. 8(a) and 8(b)]. Nevertheless, the error in the definition of $U_c/(\Gamma T)$ for all three mentioned approximations is insignificant (i.e., it is within ~1–2 %) for all scaling parameters $\kappa \leq 5.5$ and $\Gamma^* > 10$ [see Fig. 8(c)]. With the decreasing of Γ^*, the difference between the mentioned approximations and numerical data grow depending on the ξ value (see Fig. 9). Note that calculations in Refs. [23,24] were performed for a case $\xi \to \infty$ ($\nu_{fr} \equiv 0$). Therefore, the considered approximations are not suitable for estimations of energy density in the real dissipative ($\nu_{fr} \neq 0$) systems with $\Gamma^* > 5$.

Finally, in this section we consider some illustration for possibility to use the presented results for the analysis of heat

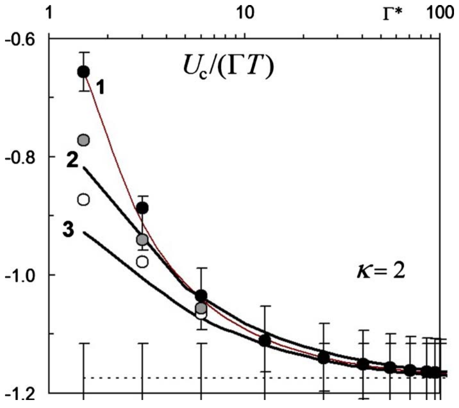

FIG. 9. (Color online) The values of $U_c/(\Gamma T)$ vs Γ^* for the 2D Yukawa systems ($\kappa=2$) obtained using various approaches for the U function: 1—Eq. (25); 2—Eq. (18); and 3—Eq. (17); symbols are the results of the numerical simulations for the various ξ: (○)—1.84; (●)—0.92; and (●)—0.23.

capacities C_V and C_P for dust component in experiments with laboratory complex (dusty) plasma of a RF discharge [51]. Estimations of the value of C_P may be performed from the coefficients of thermal conductivity χ and of thermal diffusivity θ, which were measured in [48] as $C_P \propto \chi/\theta$. So we can find that $C_P = 1.95 \pm 0.1$ in the range of Γ^* from 6 to 14. Neglecting the difference $(C_P - C_V)$ [Eq. (31)], which is less than 0.1 for $\Gamma^* > 5$ and $\kappa > 1$, we may assume $C_P \cong C_V \approx 1.95 \pm 0.1$. Note that in the Yukawa systems within Γ^* from 6 to 14 the heat capacities at constant volume are $C_V \approx 2.1 \pm 0.1$ for the 3D case and $C_V \approx 1.75 \pm 0.15$ in the 2D structures (see Fig. 4). Thus, the experimental results are in good accordance with our numerical data as the dust structures observed in mentioned experiments consisted of $\sim 13-15$ dust layers.

IV. CONCLUSIONS

To conclude, here we propose the analytical approximation for the energy densities in the 2D and 3D nonideal systems in a wide range of types of repulsive isotropic pair potentials. The parameters of proposed expression were obtained by the best fitting of the numerical and analytical data. In contrast to existing approaches the presented approximation can be used to formulate analytical expressions for the pressure, the thermal coefficient of pressure, the isothermal compressibility, and the heat capacities on base of the known thermodynamics formulas. The analytical relations between the basic transport constants and the energy density in strongly coupled systems are considered. The comparisons of obtained theoretical results with the numerical calculations have shown that the proposed approximations can be used for the description of thermodynamic properties in analyzed nonideal systems.

ACKNOWLEDGMENTS

This work was partially supported by the Russian Foundation for Fundamental Research (Grant No. 10-08-00389-a), by the CRDF (Grant No. RUP2-2891-MO-07), and by the Federal Agency for Science and Innovation (Grant No. MK-4112.2009.8), and by the Program of the Presidium of RAS.

APPENDIX

Procedure of definition of the U_0 and P_0 values for isotropic pair potentials is detailed below.

In the case of two-dimensional hexagonal primitive (hp) crystal lattice "zero" energy density and pressure can be presented as

$$U_{0,\mathrm{hp}} = \frac{1}{2}\sum_{i=1}\sum_{j=1}\phi(r_{ij}),$$

$$P_{0,\mathrm{hp}} = -\frac{1}{4r_p^2}\sum_{i=1}\sum_{j=1} r_{ij}\frac{\partial\phi(r_{ij})}{\partial r}.$$

Here $r_{ij} = a\sqrt{i^2 + j^2 + ij}$ and $a = a_{\mathrm{hp}} \equiv r_p(\sqrt{3}/2)^{1/2}$ is the step (the lattice spacing) of hp lattice.

For three-dimensional body-centered-cubic (bcc) crystal lattice zero energy density and pressure can be presented as

$$U_{0,\mathrm{bcc}} = \frac{1}{2}\sum_{i=0}\sum_{j=0}\sum_{k=0}[\phi(r_{1,ijk}) + \phi(r_{2,ijk})],$$

$$P_{0,\mathrm{bcc}} = -\frac{1}{6r_p^3}\sum r\frac{\partial\phi(r)}{\partial r}.$$

Here $r_{1,ijk} = a\sqrt{i^2 + j^2 + k^2}$ and $r_{2,ijk} = a/2\sqrt{4i^2 + 4j^2 + 4k^2 + 4i + 4j + 4k + 3}$, where we have $a = 2a_{\mathrm{bcc}}/\sqrt{3} \equiv 2^{1/3} r_p$ is the spacing of bcc lattice.

[1] Ya. I. Frenkel, *Kinetic Theory of Liquid* (Oxford University Press, Oxford, 1976).

[2] H. Z. Cummins and E. R. Pike, *Photon Correlation and Light Beating Spectroscopy* (Plenum, New York, 1974).

[3] R. Balescu, *Equilibrium and Nonequilibrium Statistical Mechanics* (Wiley Interscience, Chichester, 1975).

[4] N. K. Ailawadi, Phys. Rep. **57**, 241 (1980).

[5] N. H. March and M. P. Tosi, *Introduction to Liquid State Physics* (World Scientific, London, 1995).

[6] N. H. March, *Liquid Metals: Concepts and Theory* (Cambridge University Press, Cambridge, 1990).

[7] A. A. Ovchinnikov, S. F. Timashev, and A. A. Belyy, *Kinetics of Diffusion Controlled Chemical Processes* (Nova Science Publishers, Commack, New York, 1989).

[8] S. V. Vladimirov, K. Ostrikov, and A. A. Samarian, *Physics and Applications of Complex Plasmas* (Imperial College, London, 2005).

[9] V. E. Fortov *et al.*, Phys. Rep. **421**, 1 (2005).

[10] G. E. Morfill, V. N. Tsytovich, and H. Thomas, Plasma Phys. Rep. **29**, 1 (2003).

[11] O. S. Vaulina, X. G. Adamovich, O. F. Petrov, and V. E. Fortov, Phys. Rev. E **77**, 066404 (2008).

[12] O. S. Vaulina, X. G. Adamovich, O. F. Petrov, and V. E. Fortov, Phys. Rev. E **77**, 066403 (2008).

[13] U. Konopka, L. Ratke, and H. M. Thomas, Phys. Rev. Lett. **79**, 1269 (1997).

[14] J. E. Daugherty, R. K. Porteous, M. D. Kilgore, and D. B. Graves, J. Appl. Phys. **72**, 3934 (1992).

[15] S. A. Khrapak, B. A. Klumov, and G. E. Morfill, Phys. Rev. Lett. **100**, 225003 (2008).

[16] A. V. Filippov, A. F. Pal', A. N. Starostin, A. G. Zagorodny, and A. I. Momot, JETP Lett. **86**, 761 (2007).

[17] P. M. Chung, L. Talbot, and K. J. Touryan, *Electric Probes in Stationary and Flowing Plasmas: Theory and Application* (Springer, New York, 1975).

[18] D. Montgomery, G. Joyce, and R. Sugihara, Plasma Phys. **10**, 681 (1968).

[19] S. V. Vladimirov and M. Nambu, Phys. Rev. E **52**, R2172

(1995).
[20] O. S. Vaulina and S. V. Vladimirov, Phys. Plasmas **9**, 835 (2002).
[21] O. S. Vaulina *et al.*, Phys. Plasmas **11**, 3234 (2004).
[22] O. S. Vaulina and I. E. Drangevski, Phys. Scr. **73**, 577 (2006).
[23] H. Totsuji, M. S. Liman, C. Totsuji, and K. Tsuruta, Phys. Rev. E **70**, 016405 (2004).
[24] P. Hartmann, G. J. Kalman, Z. Donko, and K. Kutasi, Phys. Rev. E **72**, 026409 (2005).
[25] P. Hartmann, G. J. Kalman, and Z. Donko, J. Phys. A **39**, 4485 (2006).
[26] X. G. Adamovich, O. S. Vaulina, and I. E. Dranzhevsky, Czech. J. Phys. **56**, B591 (2006).
[27] S. Hamaguchi, R. T. Farouki, and D. H. E. Dubin, J. Chem. Phys. **105**, 7641 (1996).
[28] R. T. Farouki and S. Hamaguchi, J. Chem. Phys. **101**, 9885 (1994).
[29] S. Hamaguchi, R. T. Farouki, and D. H. E. Dubin, Phys. Rev. E **56**, 4671 (1997).
[30] R. T. Farouki and S. Hamaguchi, Appl. Phys. Lett. **61**, 2973 (1992).
[31] E. M. Lifshitz and L. P. Pitaevskii, *Physical Kinetics* (Pergamon Press, Oxford, 1981).
[32] W. Heitler, *The Quantum Theory of Radiation* (Clarendon Press, Oxford, 1954).
[33] F. Reif, *Statistical Physics, Berkeley Physics Course*, 2nd ed. (McGraw-Hill Book Co., New York, 1965), Vol. 5.
[34] L. D. Landau and E. M. Lifshitz, *Statistical Physics*, 3rd ed. (Butterworth-Heinemann, Oxford, 1980), Pt. 1.
[35] S. J. Gregg and K. S. W. Sing, *Adsorption, Surface Area and Porosity* (Academic Press, London, 1982).
[36] D. R. Nelson and B. I. Halperin, Phys. Rev. B **19**, 2457 (1979).
[37] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).
[38] A. P. Young, Phys. Rev. B **19**, 1855 (1979).
[39] S. T. Chui, Phys. Rev. B **28**, 178 (1983).
[40] K. Strandburg, Rev. Mod. Phys. **60**, 161 (1988).
[41] D. C. Glattli, E. Y. Andrei, G. Deville, J. Poitrenaud, and F. I. B. Williams, Phys. Rev. Lett. **54**, 1710 (1985).
[42] D. C. Glattli, E. Y. Andrei, and F. I. B. Williams, Phys. Rev. Lett. **60**, 420 (1988).
[43] C. A. Murray and R. A. Wenk, Phys. Rev. Lett. **62**, 1643 (1989).
[44] R. E. Kusner, J. A. Mann, J. Kerins, and A. J. Dahm, Phys. Rev. Lett. **73**, 3113 (1994).
[45] R. Seshadri and R. M. Westervelt, Phys. Rev. Lett. **66**, 2774 (1991).
[46] K. Zahn and G. Maret, Phys. Rev. Lett. **85**, 3656 (2000).
[47] O. S. Vaulina, I. E. Drangevski, X. G. Adamovich, O. F. Petrov, and V. E. Fortov, Phys. Rev. Lett. **97**, 195001 (2006).
[48] R. A. Quinn, C. Cui, J. Goree, J. B. Pieper, H. Thomas, and G. E. Morfill, Phys. Rev. E **53**, R2049 (1996).
[49] A. Melzer, A. Homann, and A. Piel, Phys. Rev. E **53**, 2757 (1996).
[50] O. S. Vaulina, Yu. V. Khrustalyov, O. F. Petrov, and V. E. Fortov, EPL **89**, 35001 (2010).
[51] V. E. Fortov, O. S. Vaulina, O. F. Petrov, M. N. Vasiliev, A. V. Gavrikov, I. A. Shakova, N. A. Vorona, Y. V. Khrustalyov, A. A. Manohin, and A. V. Chernyshev, Phys. Rev. E **75**, 026403 (2007).
[52] O. S. Vaulina *et al.*, Phys. Lett. A **372**, 1096 (2008).
[53] O. S. Vaulina, X. G. Adamovich, and S. V. Vladimirov, Phys. Scr. **79**, 035501 (2009).