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# «Phase transitions in 2D-Coulomb gas»
# «Фазові переходи у 2D-кулонівському газі»

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# CONTENT

## INTRODUCTION

The present Diploma Project is devoted to study of the simplest phase transitions in the two dimensional Coulomb gas: 1) vapor-liquid phase transition and 2) Dielectric-Conductor transition. These problems are solved on the base of cluster representations generating by strong Coulomb interaction between positive and negative discs.

In rare Coulomb gas such discs, colliding between themselves, form the dipole pairs which are electro-neutral particles having dipole moments. In fact the rare Coulomb gas can be considered as an ensemble of dipole pairs. To describe the thermodynamic properties of such a gas we can apply to the standard virial expansion, often using for usual electro-neutral gases. With its help we can construct the van der Waals equation of state (vdW EoS). It is well known that vdW EoS allows us to predict the coexistence curve separating the vapor phase from liquid one, each of which is consistent from dipole pairs. They differ from each other by essentially different densities of dipole pairs. In such a way we can determine the binodal and spinodal for the Coulomb gas, as well as the critical point, which is unique general point of these curves.

It is also necessary remember that the size of dipole pairs is not constant, it increases with temperature. It leads to the increase of dipole moments and stronger interaction between dipole pairs. This circumstance influences on the character of the coexistence curve and the location of the critical point. Moreover, at some temperature the average size of a dipole pair becomes equal to the average distance between neighboring dipole pairs. In this case the thermal motion of charged discs becomes independent from each other. As a consequence a Coulomb gas becomes conductive and we can speak about the Dielectric-Conductor transition. This is a new property lacking for usual molecular systems. It is clear that the Dielectric-Conductor transition occurs at the temperature depending on density. The characteristic temperature corresponding to negligibly small density is named by the Kosterlitz-Thouless one. The curve outgoing from this temperature is named by

the Dielectric-Conductor line transition. Its description is one of the important problems for solution of which our Diploma Project is devoted.

# 1. The most important properties of the 2D-Coulomb gas

## 1.1. Electrostatic interaction between charged discs in 2D-Coulomb gas

We will name by the Coulomb gas an electro-neutral system, consisting from 2D-discs, the half of which is positively charged and the half – by negatively charged. We suppose that discs have the diameter $\sigma$ and charged by $\pm q$.

As the first step let us consider the electric field created by a charged disc.

### The potential of positively charged disc

The electrostatic potential of a charged disc depends only on the distance $r$ between the center of disc and the observation point: $\varphi = \varphi(r)$. Outside a disc potential $\varphi(r)$ of electric field satisfies the Laplace equation [1]:

$$\Delta_r \varphi = 0, \quad r > \sigma/2, \tag{1.1}$$

where

$$\Delta_r = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)$$

is the radial part of the Laplace operator.

The solution of the equation (1) has the structure:

$$\varphi(r) = C_1 \ln r + C_2 .$$

The dependence of the potential on distance will be correct if under the symbol $\ln$ will be dimensionless variable. It can be carried out if $C_2 = -C_1 \ln\sigma$. Then the potential reduces to

$$\varphi(r) = C_1 \ln\frac{r}{\sigma}.$$

The constant $C_1$ should be identified with the charge of disc. At that the potential should decrease if the distance $r$ between center of disc and the observation point increases. This effect can be reached if the charge $q$ will be taken with the minus sign:

$$\varphi(r) = -q \ln\frac{r}{\sigma}. \tag{1.2}$$

The interaction energy of two charges $q_1$ and $q_2$, placed in points $\vec{r}_1$ and $\vec{r}_2$, is equal to

$$U_{12}(r_{12}) = q_2\varphi_1(r_{12}) = -q_1q_2 \ln\frac{r_{12}}{\sigma}, \quad \vec{r}_{12} = \vec{r}_2 - \vec{r}_1, \tag{1.3}$$

and $r_{12} = |\vec{r}_{12}|$.

Coulomb law takes the view:

$$\vec{F}_{1\to 2} = \frac{q_1q_2}{r_{12}}\frac{\vec{r}_{12}}{r_{12}}. \tag{1.4}$$

From the dimensionless reasons ($[F_{1\to 2}r_{12}] = [q_1q_2]$) it follows that the physical dimensionality of the charge and temperature are connected by the relation [2,3]:

$$[q^2] = [k_BT]. \tag{1.5}$$

Thus, the dimensionless temperature is determined according to

$$\tilde{T} = T/T_*, \quad T_* = q^2/k_B. \tag{1.6}$$

It is necessary to note that in $3D-$space the analogous behavior of the potential is characteristic for infinity charged filament:

$$\varphi(r) = -2\chi \ln\frac{r}{\sigma}, \tag{1.7}$$

where $\chi$ is the charge on the length unity.

The interaction energy of the infinity charged filament with the length unity of the second one oriented parallel to the first is equal to

$$U_{12}(r_{12}) = \chi_2\varphi_1(r_{12}) = \chi_1\chi_2 \ln\frac{r_{12}}{\sigma}. \tag{1.8}$$

### 1.2. Phase diagram for the electro-neutral system of charged discs: dielectric-conductor phase transition and the coexistence curve for vapor-liquid transition in a system

Since $2D-$Coulomb systems are absent in the nature, they can be investigated in computer experiments. In works [4,5] the main attention is focused on the study of the phase diagram of the Coulomb gas. At that, it is assumed in them that the interaction energy is equal to

$$U_{\text{int}} = \sum_{1<i<j<N} U_{ij}(r_{ij})$$

where

$$U_{ij}(r) = \begin{cases} -\dfrac{q_i q_j}{\varepsilon_0} \ln\left(\dfrac{r_{ij}}{\sigma}\right), & r_{ij} > \sigma \\ \infty, & r_{ij} < \sigma \end{cases}, \qquad (1.6)$$

and $\varepsilon_0$ is the dielectric permittivity for two-dimensional medium in which positive and negative discs are situated. The structure of $U_{\text{int}}$ allows us to introduce the following dimensionless density $\tilde{n}$ and temperature $\tilde{T} = T/T_*$:

$$\tilde{n} = n\sigma^2, \quad T_* = \frac{q^2}{k_B \varepsilon_0}, \qquad (1.7)$$

where $n$ - is the density of discs. The corresponding phase diagram, constructed in [4], has the following view (Fig.1.)

Let us note the most important elements of the phase diagram:

1) the vapor-liquid coexistence curve presented by open circles;

2) dielectric-conductor transition line presented by squares;

3) the vapor-liquid critical point;

4) KT (Kosterlitz-Thowless) point [7] giving the beginning of the dielectric-conductor transition line;

5) the conjugation point of the coexistence curve and dielectric-conductor transition line.

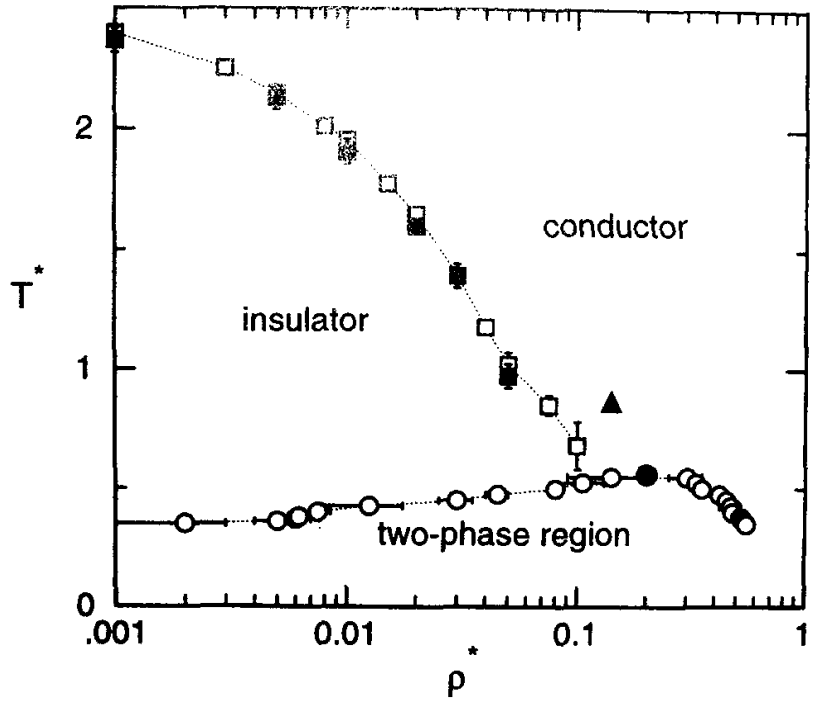


*Fig.1.1. Phase diagram of* $2D-$ *Coulomb gas according [4]. Open circles designate the coexistence curve, dark circle –the position of the critical point, light and dark squares – dielectric-conductor transition line (squares of different coloring correspond to different number of particles in computer experiments), dark triangle notes the critical point location in the computer experiments [6].*

According to [4] the following coordinates for the critical point were established:

$$\tilde{T}_c = 0.056, \quad \tilde{n}_c = 0.21. \tag{1.8}$$

The critical temperature and density, determined in [6], are noticeably different from (3):

$$\tilde{T}_c = 0.085, \quad \tilde{n}_c = 0.16. \tag{1.9}$$

The conjugation point of the coexistence curve and dielectric-conductor transition line is close to the critical point;

The characteristic temperature $T_{KT}$ practically coincides with the value obtained in [7].

The very important value for the correct description of physical properties of Coulomb gas has the screenshot for the spatial distribution of discs presented in Fig.2.

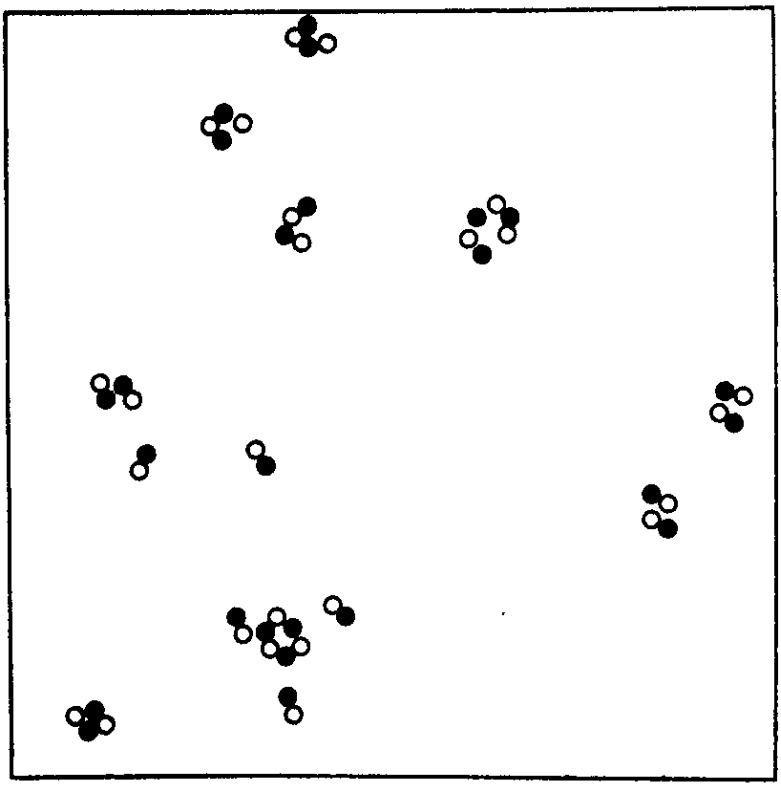

*Fig.1.2. Space distribution of positively and negatively charged discs in some moment of time in the computer experiment [4]. Circles of different color correspond to charges of opposite sign.*

As we can see from Fig.2, the most characteristic peculiarity in the spatial discs distribution is their clusterization and formation of electro-neutral clusters. Among clusters the following dominate:

a) dipole pairs;

b) quadrupole clusters;

c) hexamers and higher order.

As it should be all clusters are electro-neutral, but their shapes are not regular. It means that they transform to excited states. The excitation of clusters is caused by collisions between them and electrostatic multipole interactions. The

most essential role belongs to quadrupole clusters as playing the dominating role in the screenshot (Fig.2).

Thus, our approach to the creation of theoretical basis for the Coulomb gas should start from the mixture of particles reflecting properties of clusters enumerated above. It will be very important also the taking into account rotations and excitations of clusters.

### 1.3. Clusterization processes in 2D-Coulomb gas: properties of dipole and quadrupole clusters

Due to electrostatic interaction positively and negatively charged discs tend to form the dipole pairs:

$$q_+ + q_- \Leftrightarrow d\,, \tag{1.10}$$

where $d$ denotes a dipole pair having the dipole moment:

$$\vec{d} = q_+(\vec{r}_+ - \vec{r}_-)\,, \tag{1.11}$$

$\vec{r}_+, \vec{r}_-$ are the radius vectors of these charges. It as also possible the opposite process: the disintegration of a dipole pair on charges. The minimal energy of a dipole pair corresponds to contacting discs $|\vec{r}_+ - \vec{r}_-| = \sigma$ (Fig.3.1), which rotates and can be considered as an effective disc with the diameter: $r_d = 2\sigma$,

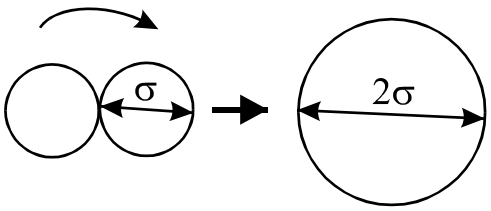


*Fig.1.3. The transformation of rotating dipole pair to a effective disc, having the diameter* $2\sigma$ *and the dipole moment such as a initial dipole pair.*

The averaged potentials of interaction between dipole pairs ant the effective discs are the same therefore the EoS for them will be equivalent.

If the dipole pair is excited the distance between charged discs becomes more than for contacting discs: $r_d = \sigma + r'$.

Due to collisions between dipole pairs their can form a quadrupole cluster $Q$ (see [8,9]):

$$d + d \Leftrightarrow Q. \tag{1.12}$$

It is supposed that this process can be also going in the opposite direction: a quadrupole cluster dissociates on two dipole pairs. The simplest quadrupoles having the minimal energies are presented in Fig.3.2

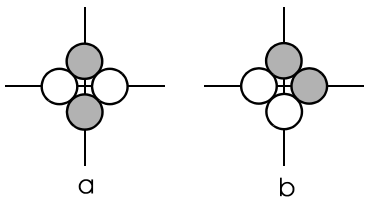


*Fig.1.4. The simplest configurations of quadrupole clusters. Different colors correspond to charges of opposite sign.*

The presented configurations have values of energy:

$$E_4^{(a)} = -q^2 \ln 2, \quad E_4^{(b)} = q^2 \ln 2. \tag{1.13}$$

Since contacting dipole pairs have energy: $E_2^{(c)} = 0$, we conclude that the formation of symmetrical quadrupole configuration $a$ is the most advantageous.

Considering the reaction (3.3) we get the following values of the stoichiometric coefficients;

$$\nu_d = \nu_d = -\nu_Q = 1,$$

and increments of quadrupoles and dipole pairs are connected by the equation:

$$\Delta N_Q = -\frac{1}{2}\Delta N_d. \tag{1.14}$$

In the equilibrium state the thermodynamic potential of the system $\Phi(N_d, N_Q)$ takes the minimal value (see [2]):

$$\frac{\partial \Phi}{\partial N_d} + \frac{\partial \Phi}{\partial N_Q}\frac{\partial N_Q}{\partial N_d} = 0. \qquad (1.15)$$

Since $\frac{\partial \Phi}{\partial N_i} = \mu_i$, and $\mu_i$ have meaning of the chemical potentials for components of the reaction, $i = d, Q$, then (3.5) and (3.6) lead to the equation:

$$\mu_Q - 2\mu_d = 0, \qquad (1.16)$$

connecting the chemical potentials of components. As a result, it plays the key role for determination of concentration for different component.

### 1.4. Methods of chemical kinetics

The free energy for ideal gas of spherical particles is determined by the general expression [2]:

$$F_{id} = -NT \ln\left[ e\upsilon \left( \frac{2\pi mT}{h^2} \right)^{3/2} \zeta \right], \qquad (1.17)$$

where $N$, $T$ are the number of particles and temperature in the system, $\upsilon = V/N$ is the specific volume per particle, $m$ is its mass, $h$ is the Planck constant, $\zeta$ is the statistical sum of its internal states (here and in the following we use the rule: ( $k_B T \to T$ ). Taking into account that $\upsilon = 1/n$, and $h^2/mT = \Lambda_B^2$ is the square for the de Broglie thermal wave length, we can rewrite (4.1) in the view:

$$F_{id} = -NT\left[ 1 + \ln\upsilon - \frac{1}{T} f(T) \right], \qquad (1.18)$$

where

$$f(T) = T \ln\left(\Lambda_B^3(T)/\zeta\right)). \qquad (1.19)$$

The thermodynamic potential $\Phi = F - \upsilon \frac{\partial F}{\partial \upsilon}$, in accordance with (1.18) i (1.19), is equal to:

$$\Phi_{id} = N\mu_{id}, \tag{1.20}$$

where

$$\mu_{id} = \begin{cases} -T\ln\upsilon + f(T) \\ T\ln n + f(T) \end{cases} \Rightarrow T\ln P + \chi(T) - \tag{1.21}$$

is the chemical potential in the ideal gas approximation and

$$\chi(T) = -T\ln T + f(T).$$

In order to take into account the interaction between particles let us apply to the van der Waals equation of state:

$$P = \frac{T}{\upsilon - \upsilon_0} - \frac{a}{\upsilon^2}.$$

The free energy, leading to this equation according to $P = -\frac{1}{N}\frac{\partial F}{\partial \upsilon}$, takes the structure:

$$F = F_{id} - N\left[T\ln\frac{(\upsilon - \upsilon_0)}{\upsilon} + \frac{a}{\upsilon}\right]. \tag{1.22}$$

As we can see, additionally to $F_{id}$, we take into account 1) the proper volume $\upsilon_0$ of molecules ($\upsilon \to \upsilon,\ \upsilon_0$), та 2) the interaction between particles ($-a/\upsilon$). Thus, the expression:

$$\mu^{(ex)} = T\ln\frac{(\upsilon - \upsilon_0)}{\upsilon} + \frac{a}{\upsilon}, \tag{1.23}$$

has meaning that part of the chemical potential, which is caused by the interaction between particles.

### 1.5. Formulation of the diploma problems

The following problems are planned to study in the Diploma Project:

- to discuss the formation of dipole pairs and to calculate the temperature dependence of their spatial size;
- to describe the distribution of the dipole pairs and quadrupole clusters in the plane temperature-density;
- to construct the curve separating the Dielectric and Conductive states of the rare Coulomb gas;
- using the virial expansion for the free energy to construct the van der Waals equation of state for the Coulomb gas considering as an ensemble of dipole pairs and quadrupole clusters;
- to determine the positions of binodal and spinodal for the system described in the previous task as well as the location of the critical point in which the vapor and liquid branches diverges;
- to discuss the agreement between the results obtained on the base of theoretical model, developed in our work, and with the help of computer methods.

# 2. THE MOST IMPORTANT CONSTRUCTIVE ELEMENTS IN THE DIPLOMA PROJECT

## 2.1. Mean square value of the dipole moment for a dipole pair as function of temperature and density

The configurational integral $Q$ for the 2D-Coulomb gas is determined by the expression (see [2,3]):

$$Q_N = \int_S d\vec{s}_1 ... d\vec{s}_N \exp\left( -\frac{U_{\text{int}}(\vec{r}_1,...,\vec{r}_N)}{k_B T} \right), \tag{2.1}$$

where $d\vec{s}_i$ is the volume element for i-$th$ particle in the plane, $U_{\text{int}}$ is the interaction energy:

$$U_{\text{int}} = \sum_{1<i<j<N} U_{ij}(r_{ij})$$

and

$$U_{ij}(r) = \begin{cases} -\frac{q_i q_j}{\varepsilon_0} \ln\left(\frac{r_{ij}}{\sigma}\right), & r_{ij} > \sigma \\ \infty, & r_{ij} < \sigma \end{cases} \tag{2.2}$$

and $\varepsilon_0$ is the dielectric permittivity of medium. The structure of $U_{\text{int}}$ allows us to introduce the following dimensionless density $\tilde{n}$ and temperature $\tilde{T}$:

$$\tilde{n} = n\sigma^2, \quad \tilde{T} = T / T_*, \quad T_* = \frac{q^2}{k_B \varepsilon_0}, \tag{2.3}$$

where $n$ - is the total density of discs.

In two-particle approximation we only have positive and negative discs and

$$Q_2 = \int_S d\vec{s}_1 d\vec{s}_2 \exp\left( -\frac{U_{\text{int}}(\vec{r}_1,\vec{r}_2)}{k_B T} \right). \tag{2.4}$$

From the homogeneity reasons the expression (4) is written in the view:

$$Q_2 = S\int_S d\vec{s}_2 \exp\left(-\frac{U_{\text{int}}(|\vec{r}_2 - \vec{r}_1|)}{k_B T}\right),$$

which passes to the following expression:

$$\exp\left(-\frac{U_{\text{int}}(|\vec{r}_2 - \vec{r}_1|)}{k_B T}\right) = \exp\left(-\frac{q^2}{\varepsilon_0 k_B T}\ln\frac{r_{12}}{\sigma}\right) \Rightarrow \exp\left(\ln\frac{r_{12}}{\sigma}\right)^{-1/\tilde{T}} \Rightarrow \left(\frac{r_{12}}{\sigma}\right)^{-1/\tilde{T}},$$

due to identical transformations. Here $\tilde{T} = T/T_*$, and also $\tilde{\beta} = 1/\tilde{T}$.

The pair distribution function takes view:

$$\rho(\vec{r}) = C\exp\left(-\frac{q^2}{\varepsilon_0 k_B T}\ln\frac{r}{\sigma}\right) \Rightarrow C\left(\frac{r}{\sigma}\right)^{-1/\tilde{T}}.$$

The normalization constant is determined by the equation:

$$C = 1/\int_\sigma^\infty d\vec{r}\,\rho(\vec{r}).$$

Since

$$\int_\sigma^\infty d\vec{r}\,\rho(\vec{r}) \Rightarrow 2\pi\sigma^2\int_1^\infty x^{1-\tilde{\beta}}dx = 2\pi\sigma^2\frac{x^{2-\tilde{\beta}}}{2-\tilde{\beta}}\Bigg|_1^\infty = \frac{2\pi\sigma^2}{2-\tilde{\beta}}, \quad \tilde{\beta} = T_*/T$$

then

$$C = \frac{2-\tilde{\beta}}{2\pi\sigma^2}.$$

The applicability region of these expressions is determined by the convergence of integral taking place at

$$2-\tilde{\beta} < 0 \quad or \quad 2 < \tilde{\beta} \quad or \quad \tilde{T} < 1/2.$$

The mean square value of the dipole moment is determined by the integral:

$$<\vec{d}^{\,2}> = q^2 <r^2> \Rightarrow q^2\int_S d\vec{r}\,\rho(\vec{r})r^2 = (q\sigma)^2\frac{\tilde{\beta}-2}{\tilde{\beta}-4}. \qquad (2.5)$$

In another view

$$<\vec{d}^{\,2}> = d_0^2\zeta(\tilde{T}), \quad d_0^2 = q^2\sigma^2, \quad \zeta(\tilde{T}) = \frac{1-2\tilde{T}}{1-4\tilde{T}}, \quad \tilde{T} < 1/4. \qquad (2.6)$$

In order to guarantee $<\vec{d}^{\,2}(T)> > 0$ we should take: $\tilde{T} = 1/4 - \delta$. Then

$$< \vec{d}^{\,2}(T) >= d_0^2 \frac{0.125}{\delta} + ..., \quad \delta > 0. \tag{2.7}$$

As it should be at $\tilde{T} \to \tilde{T} = 1/4 - \delta$ we get $< \vec{d}^{\,2}(T) > \to \infty$ i.e. the temperature $\tilde{T} = 1/4 - \delta$ coincides with the Kosterlitz-Thowless one at $\delta = 0$ [7, 10-12].

## 2.2.The distribution of the dipole pairs and quadrupole clusters on the density-temperature phase diagram;

If the Coulomb gas is not too dense it consists from dipole pairs and quadrupole clusters. The collision of dipole pair is accompanied by the formation of the quadrupole cluster:

$$d + d \Leftrightarrow Q.$$

The process can go from the left to right and vice versa. The concentrations of dipole pairs and quadrupole clusters can be determined with the help of method of chemical equilibrium in a system of reacting components. At that the concentration of dipole pairs

$$c = \frac{n_d}{n_d + n_Q} \equiv n_d / n$$

is determined by the equation:

$$\frac{1-c}{c^2} = P \exp\left( \frac{2\chi_d - \chi_Q}{T} \right). \tag{2.8}$$

The combination $K(T) = \exp\left( -\frac{2\chi_d - \chi_Q}{T} \right)$ is accepted to name by the constant of chemical equilibrium.

Indeed, we start from the equation (3.7):

$$\mu_Q = 2\mu_d$$

and the expressions (4.5) for the chemical potentials:

$$\mu_i = T \ln P_i + \chi_i, \quad i = d, Q,$$

and (1.23) for

$$\chi_i = -T \ln T + f_i(T).$$

Here $P_i$ are the partial pressures $P_d$ and $P_Q$ of dipole pairs and quadrupole clusters. In ideal gas approximation we have

$$P_d = cP, \quad P_Q = (1-c)P,$$

and

$$\chi_d = T \ln \frac{\Lambda_d^2}{\zeta_d T}, \quad \chi_Q = T \ln \frac{\Lambda_Q^2}{\zeta_Q T},$$

where $\Lambda_d$ and $\Lambda_Q$ are the lengths for de Broglie waves [13] corresponding to dipole pairs and quadrupole clusters, $\zeta_i$, $i = d, Q,$ are the statistical sums of their internal states (see the Section 4 in Chapter 1).

Since the mass of quadrupole cluster is twice more than that for dipole pair, we get:

$$\Lambda_d^2 / \Lambda_Q^2 = 2.$$

Additionally we assume that the classical character of thermal motion is observed at $T > T_0$, where the quantum degeneracy temperature $T_0$ is estimated as: $\Lambda_d^2(T_0)/\sigma^2 = 0.1$. Then,

$$\Lambda_d^2(T)/\sigma^2 = 0.1 \cdot (T_0/T)^{1/2}. \tag{2.9}$$

As consequence, the equation (2.2.1) transforms to

$$\frac{(1-c)(2-c)}{c^2} = 0.1\tilde{n}\left(\frac{T_0}{T}\right)^{1/2} \frac{\zeta_Q}{\zeta_d^2}, \tag{2.10}$$

where $\tilde{n} = n_0\sigma^2$, and the equation

$$n_0 = 2(2-c)(n_d + n_Q)$$

establishes the interconnection between numbers of clusters and positive and negative discs.

If $T << T_*$ the internal degrees of freedom of dipole pairs and quadrupole clusters can be considered as unexcited, therefore $\zeta_i$, $i = d, Q$, will be determined by the energy $E_i^{(0)}$ of their ground states: $\zeta_i = \exp(-E_i^{(0)}/T)$. Since,

$$E_d^{(0)} = 0, \quad E_Q^{(0)} = -q^2 \ln 2 \equiv -T_* \ln 2,$$

then

$$\zeta_d = 1, \qquad \zeta_Q = \exp\left(\ln 2 \cdot \frac{T_*}{T}\right) = 2^{T_*/T}. \tag{2.11}$$

Using these expressions we get:

$$\frac{(1-c)(2-c)}{c^2} = 2^{T_*/T}\tilde{n}\frac{\Lambda_d^2}{\sigma^2}. \tag{2.12}$$

For temperatures $T > T_0$, corresponding to classical effects, we can use (2.9) and the concentration of dipole pair is described by the equation:

$$\frac{(1-c)(2-c)}{c^2} = 0.1 \cdot 2^{T_*/T}\tilde{n}\left(\frac{T_0}{T}\right)^{1/2}. \tag{2.13}$$

In limit case, corresponding to $2^{T_*/T}\tilde{n} \to 0$, the concentration of dipole pairs changes according to:

$$c = 1 - 0.1 \cdot 2^{T_*/T}\tilde{n} + 0.03\left(2^{T_*/T}\tilde{n}\right)^2 + \ldots, \tag{2.14}$$

i.e. dipole pairs dominate in a system. In opposite case, when $2^{T_*/T}\tilde{n} >> 1$, the concentration tends to zero:

$$c \approx 3.16 \cdot 2^{-1/2(1+T_*/T)}\tilde{n}^{-1/2} \to 0, \tag{2.15}$$

i.e. a system is consisting from quadrupole clusters.

Let us use the formula (2.2.6) for the estimate $c$ at the Kosterlits-Thowless temperature ($t_{KT} = 0.25$ [7]). Accepting that $T_0 / T_* = 0.1$, we get:

$$\frac{(1-c)(2-c)}{c^2} = 1.01 \cdot \tilde{n}.$$

For a rarefied Coulombic gas, for which $\tilde{n} << 1$, the concentration of dipole pairs changes according to:

$$c(t = t_{KT}) \approx 1 - \tilde{n} + 3\tilde{n}^2 + \ldots \tag{2.16}$$

Let us describe the distribution of dipole pairs and quadruopole clusters with the help of iso-concentration curves, determined by the equations: $c(\tilde{n}, t) = c_0$. The iso-concentration curves at different values of $c_0$ are presented in Fig.2.1.

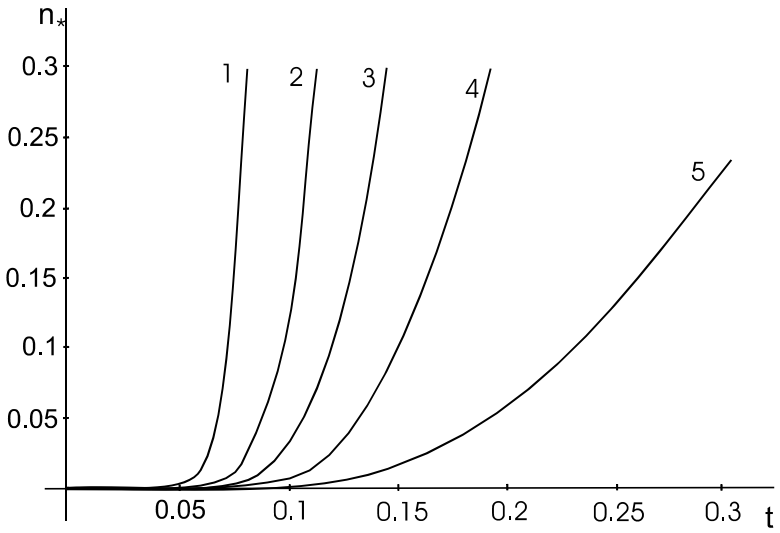


*Fig.2.1. The family of iso-concentration curves* $c(\tilde{n},t)=c_0$*, corresponding to the formula (2.2.6) at* $T_0=0.1T_*$*. The curves 1,…,5 are constructed for* $c_0=0.1,0.3,0.5,0.7,0.9$.

In particular, we can use the Fig.2.3. to get the temperature dependence of the concentration of dipole pairs on some isochore. In this case the corresponding values $c(\tilde{n},t)$ are determined by the iso-concentration curves in points of their intersections with straight lines coming from $n_*$ on the ordinate axis.

## 2.3. Dielectric-conductor transition line

We had been established that at low temperatures the electro-neutral rarefied system, consisting from positively and negatively charged discs, tends to be dimerized. The discs with opposite charges form dipole pairs, having dipole moments. Such a system has no free charges and cannot to conduct electric current.

If temperature increases the averaged distance between discs, forming dipole pairs, also increases and for some temperature it becomes exceeding the averaged distance $n^{-1/2}$ between any discs (where $n$ is the numerical density). In this case dipole pairs become instable and the system can be considered as consisting from

free charge discs. Thus, the temperature $\tilde{T}_{DC}$, corresponding the transition dielectric-conductor, is determined by the equation:

$$r_d^2(\tilde{T}_{DC}) \geq 1/n\,.$$

Substituting here the expression $r_d^2(\tilde{T})$ from (2.1.5) we obtain the following equation for $\tilde{T}_{DC}$.

$$\frac{1-2\tilde{T}_{DC}}{1-4\tilde{T}_{DC}} = 1/\tilde{n}\,. \qquad (2.17)$$

From here we find

$$\tilde{T}_{DC} = \frac{1}{2}\frac{1-\tilde{n}}{2-\tilde{n}}$$

or

$$\tilde{T}_{DC} = \frac{1}{2}\left(1-\frac{1}{2-\tilde{n}}\right). \qquad (2.18)$$

If density of a system $\tilde{n} \to 0$ the temperature of the dielectric-conductor tends to the Kosterlits-Thouless value [7]:

$$\tilde{T}_{DC} \to T_{KT} = 1/4\,.$$

The first asymptotic terms:

$$\tilde{T}_{DC} = 1/4\left(1-\tilde{n}/2-\tilde{n}^2/4+....\right) \qquad (2.19)$$

allows us to compare this theoretical result with experimental dependence on density.

If $\tilde{n} \to 1$, i.e. for dense system we get:

$$\tilde{T}_{DC}(\tilde{n}=1) = 0\,, \qquad (2.20)$$

that is quite understood. The last estimate for $\tilde{T}_{DC}$ is not agreed with computer calculations (see Fig.I.2.1). In order to improve this agreement let us consider the influence of quadrupole clusters.

***Influence of the quadrupole clusters on the conductivity of*** $2D$ ***– Coulomb gas***

As it had been shown in the previous Section the rarefied Coulomb gas is the mixture of dipole pairs and quadrupole clusters. Here it is necessary to note that the sizes of quadrupole clusters remain practically invariable. Indeed, the bounding energy of a quadrupole clusters in its ground state is equal to

$$E_Q = -q^2 \ln 2,$$

or in temperature units

$$E_Q = -k_B T_Q, \quad T_Q = T_* \ln 2.$$

The value of the dimensionless quadrupole temperature

$$\tilde{T}_Q = \ln 2 > \tilde{T}_{KT}$$

is higher then the Kosterlits-Thouless temperature. Therefore, until $T < \tilde{T}_{KT}$ we can use the quadrupole clusters in their ground states.

The concentrations of clusters are determined by the expressions:

$$c_d = \frac{n_d}{n_d + n_Q} \equiv n_d / n_{cl}, \quad c_Q = \frac{n_Q}{n_d + n_Q} \equiv n_Q / n_{cl}, \tag{2.21}$$

where $n_d$ and $n_Q$ are the densities of dipole pairs and quadrupole clusters, $n_{cl}$ is the density of clusters independent on their type. In accordance with definition, these concentrations satisfy the normalization condition:

$$c_d + c_Q = 1. \tag{2.22}$$

From here it follows $c_Q = 1 - c_d$.

Let us establish the interconnection between the density of clusters and the discs density $2n$. The last satisfies the equation:

$$2n_d + 4n_Q = 2n. \tag{2.23}$$

Combining (2.3.7) with $n_d + n_Q = n_{cl}$ we get:

$$n_{cl} = \frac{n}{2 - c_d} \tag{2.24}$$

and

$$n_d = \frac{c_d}{2-c_d} n, \quad n_Q = \frac{1-c_d}{2-c_d} n. \tag{2.5}$$

The averaged distance between dipole pairs equals to $R_{dd}^2 = n_d^{-1}$. Equaling it to the size of a dipole pair: $r_d^2 = \sigma^2 \zeta(T)$, we get the equation:

$$\frac{1-2\tilde{T}_{DC}}{1-4\tilde{T}_{DC}} = \frac{1}{\tilde{n}} \frac{2-c_d}{c_d} ,$$

determining the dimensionless temperature $\tilde{T}_{DC}$ of the dielectric-conductor transition for mixture of dipole pairs and quadrupole clusters. Since $c_d$ is the function of density $\tilde{n} = n\sigma^2$ according to Fig.2.3, we find:

$$\tilde{T}_{DC}(\tilde{n}) = \frac{1}{4} \frac{1-\frac{\tilde{n}+1}{2} c_d(\tilde{n})}{1-\frac{\tilde{n}+2}{4} c_d(\tilde{n})}. \tag{2.6}$$

At small dipole pair concentrations

$$\tilde{T}_{DC}(\tilde{n}) = \frac{1}{4}\left(1-\frac{1}{4} n c_d(\tilde{n}) + ...\right). \tag{2.7}$$

## 2.4. Dielectric permittivity for rarefied 2D-Coulomb gas

In general the induction $\vec{D}$ of the electric field in medium is connected with the Maxwell strength $\vec{E}$ of it by the relation [14]:

$$\vec{D} = \varepsilon \vec{E} ,$$

where $\varepsilon$ is the dielectric permittivity. There is also the equation [14-16]:

$\vec{D} = \vec{E} + 2\pi \vec{P}$,

connecting $\vec{D}$ and $\vec{E}$ with the polarization vector $\vec{P}$. Combining both these expressions we get:

$$\varepsilon - \varepsilon_0 = 2\pi \frac{P}{E}. \tag{2.8}$$

Here we take into account that in homogeneous and isotropic system the vectors $\vec{P}$ and $\vec{E}$ are codirectional. Thus, in order to calculate the dielectric

permittivity it is necessary to find the polarization vector as a function of Maxwell strength.

In the case of 3D-space the dielectric permittivity is determined by the similar equation, differing by the value of the coefficient [14-16]:

$$\varepsilon - \varepsilon_0 = 4\pi \frac{P}{E}. \tag{2.29}$$

In both cases the situation is simplified if 1) the system takes the sphere-like shape and 2) it is placed to the external field of the strength $\vec{E}_0$. The values of $\vec{E}$ and $\vec{E}_0$ satisfy to the boundary conditions which lead to the relation:

$$\vec{E} = \frac{2\varepsilon_0}{\varepsilon + \varepsilon_0} \vec{E}_0. \tag{2.30}$$

The polarization vector is also some function of $\vec{E}_0$. Therefore the equation (4.2) can be rewritten in the view:

$$\frac{\tilde{\varepsilon} - 1}{\tilde{\varepsilon} + 1} = \pi \frac{P(E_0)}{E_0}, \quad \tilde{\varepsilon} = \varepsilon / \varepsilon_0. \tag{2.31}$$

In 3D-space the corresponding formula for the dielectric permittivity takes the similar structure:

$$\frac{\tilde{\varepsilon} - 1}{\tilde{\varepsilon} + 2} = \frac{4\pi}{3} \frac{P(E_0)}{E_0}. \tag{2.32}$$

Let us consider the polarization vector for a system consisting from dipole pairs. In this case

$$\vec{P} = \frac{< \vec{D}_N >}{S}, \tag{2.33}$$

where $\vec{D}_N$ is the dipole moment of $N-$dipole pairs and the angular brackets denote the average procedure according to Gibbs distribution:

$$< \vec{D}_N >= \frac{\int \vec{D}_N \exp[-\beta H_N] d\Omega_N}{\int \exp[-\beta H_N] d\Omega_N},$$

$\beta = 1/k_B T \Rightarrow 1/T$ is the inverse temperature, $d\Omega_N = d\Gamma_1 d\Gamma_2 ... d\Gamma_N$ is the element of phase volume for a system, $d\Gamma_i = \sin\theta_i d\theta_i d\varphi_i$ is the area element on the unit sphere (angles $\theta_i$ and $\varphi_i$ describe the spatial orientation of i-th dipole pair). Here it

is taken into account that the Hamiltonian of a system is reduced to the interaction of dipole pairs with external field [14]:

$$H_N = -\vec{D}_N \cdot \vec{E}_0 .$$

The dipole moment of a system, consisting from $N$ dipole pairs, is determined by the sum: $\tilde{T} = T / T_*$

$$\vec{D}_N = \sum_{i=1}^{N} d(\tilde{T})\vec{n}_i = \sum_{i=1}^{N} d(\tilde{T})\left(\vec{k}\cos\theta_i + \vec{i}\sin\theta_i\cos\varphi_i + \vec{j}\sin\theta_i\sin\varphi_i\right),$$

where the unit vector $\vec{k}$ is directed along the strength of external electric field $\vec{E}_0$, $d(\tilde{T})$ is the average value of the dipole moment corresponding to the dimensionless temperature $\tilde{T}$.

In linear with respect to $\vec{E}_0$ approximation:

$$< \vec{D}_N >= \beta < \vec{D}_N \left(\vec{D}_N \cdot \vec{E}_0\right) >_0 + .. ,$$

where $<>_0$ denotes the averaging with isotropic distribution function. In this case

$$< \left(\vec{D}_N\right)_\alpha \left(\vec{D}_N\right)_\beta >_0 = \frac{1}{2}\delta_{\alpha\beta} < \left(\vec{D}_N\right)^2 >_0, \quad \alpha,\beta = 1,2,$$

therefore

$$< \vec{D}_N >= \frac{1}{2}\beta < \left(\vec{D}_N\right)^2 >_0 \cdot \vec{E}_0 . \qquad (2.34)$$

Taking into account only autocorrelation effects, we get

$$< \left(\vec{D}_N\right)^2 >_0 = N d^2(\tilde{T}) + ...$$

In accordance with (2.4.6) the polarization vector takes the value:

$$\vec{P} = \frac{1}{2}\beta d^2(\tilde{T}) n \cdot \vec{E}_0 + ..., \qquad (2.35)$$

where $n = N / S$ is the density of dipole pairs.

$$\frac{\varepsilon - 1}{\varepsilon + 1} = \frac{1}{2}\pi\beta d^2(\tilde{T}) n \qquad (2.36)$$

In the Section 1 it had been shown that the dipole moment of a dipole pair takes the view:

$$d^2(\tilde{T}) = d_0^2 \frac{1-2\varepsilon\tilde{T}}{1-4\varepsilon\tilde{T}}, \quad \tilde{T} < 1/(4\varepsilon), \quad d_0 = q\sigma,$$

where

$$\tilde{T} = T/T_*, \quad T_* = \frac{q^2}{k_B}.$$

Combining these expressions with (2.4.9) we get:

$$\frac{\varepsilon-1}{\varepsilon+1} = \frac{1}{2}\pi \cdot \frac{\tilde{n}}{\tilde{T}} \frac{1-2\varepsilon\tilde{T}}{1-4\varepsilon\tilde{T}}, \tag{2.37}$$

where $\tilde{n} = n\sigma^2$.

It is necessary to stress that the dielectric permittivity, described by the formula (2.4.10), is only caused by dipole pairs. The contributions, similar to electronic polarizability, are absent, since we suppose that positive and negative discs are structureless.

## 2.5. The averaged interaction potential between dipole pairs

The interaction potential $U(r)$ between dipole pairs, forming in two-dimensional Coulomb gas, with satisfactory accuracy can be approximated by sum of two contributions $U_r(r)$ and $U_a(r)$, which describe the repulsion and attraction between discs correspondingly:

$$U(r) = U_r(r) + U_a(r). \tag{2.38}$$

The first of them is usually modeled by the potential of hard disks:

$$U_r(r) = \begin{cases} \infty, & r \le \sigma, \\ 0, & r > \sigma. \end{cases} \tag{2.39}$$

***Dipole-dipole interaction energy***

The potential of the first dipole pair, created by he first and second close charges at the point $\vec{r}$, equals to

$$\varphi(\vec{r}) = q\left(\chi_d(\vec{r}-\vec{r}_1) - \chi_d(\vec{r}-\vec{r}_2)\right).$$

A function takes values:

$$\chi_d(r) = \begin{cases} 1/r, & d = 3, \\ \ln r, & d = 2. \end{cases}$$

Rewriting it in the view:

$$\varphi(\vec{r}) = q\left(\chi_d(\vec{r} - \vec{r}_1) - \chi_d(\vec{r} - \vec{r}_1 + \vec{r}_1 - \vec{r}_2)\right) \Rightarrow$$
$$\Rightarrow q \frac{\partial \chi_d(r)}{\partial r_\alpha}\bigg|_{r=|\vec{r}-\vec{r}_1|} (\vec{r}_1 - \vec{r}_2)_\alpha + ...$$
$$\Rightarrow d_\alpha^{(1)} \frac{\partial \chi_d(r)}{\partial r_\alpha}\bigg|_{r=|\vec{r}-\vec{r}_1|} +,,,$$

where $\vec{d}_1 = q(\vec{r}_2 - \vec{r}_1)$ is the dipole moment for the first dipole pair.

The interaction energy between the field of first dipole pair and charges 3 and 4 is equal to: $\varphi(\vec{r}_3)q - \varphi(\vec{r}_4)q = d_\alpha^{(1)} q \left( \frac{\partial \chi_d(r)}{\partial r_\alpha}\bigg|_{r=|\vec{r}_3-\vec{r}_1|} - \frac{\partial \chi_d(r)}{\partial r_\alpha}\bigg|_{r=|\vec{r}_4-\vec{r}_1|} \right)$

Since

$$\varphi(\vec{r}_3)q - \varphi(\vec{r}_4)q = d_\alpha^{(1)} q (\vec{r}_4 - \vec{r}_3)_\beta \frac{\partial^2 \chi_d(r)}{\partial r_\alpha \partial r_\beta}\bigg|_{\vec{r}=\vec{r}_3-\vec{r}_1} + ....$$

we finally obtain the energy of dipole-dipole interaction:

$$W_{\vec{d}_1\vec{d}_2} = \varphi(\vec{r}_3)q - \varphi(\vec{r}_4)q = d_\alpha^{(1)} d_\beta^{(2)} \frac{\partial^2 \chi_d(r)}{\partial r_\alpha \partial r_\beta}\bigg|_{r=|\vec{r}_3-\vec{r}_1|} + ....$$

Here $\vec{d}_2 = q(\vec{r}_4 - \vec{r}_3)$ is the dipole moment of the second dipole paior.

The attractive potential $U_a(r)$ can be described as an averaged expression for corresponding interaction of dipole pairs:

$$U_a(r) = < W_{el}(\vec{r}_1, \vec{r}_1) >, \qquad (2.40)$$

and symbol $< ... >$ designates the averaging on their directions of dipole moments.

In two-dimensional case for the interaction of dipole moments we get:

$$W_{dd}(\vec{r}_1, \vec{r}_2, \Omega) = -d_\alpha^{(1)} d_\beta^{(2)} \frac{\partial^2 \ln r}{\partial r_\alpha \partial r_\beta}, \qquad (2.41)$$

where $r = |\vec{r}_1 - \vec{r}_2|$, and $\Omega$ is the totality of angular coordinates describing directions of their dipole moments (here we changed $\vec{r}_3$ on $\vec{r}_2$).

The pair correlation function $g(\vec{r}_1,\vec{r}_2,\Omega)$, where $\vec{r}_1$ and $\vec{r}_2$ are the radius-vectors of dipole pairs, one can be approximated by the expression:

$$g(\vec{r}_1,\vec{r}_2,\Omega) \Rightarrow C\exp(-\beta W_{el}(\vec{r}_1,\vec{r}_2,\Omega)) \approx \frac{1}{(4\pi)^2}(1-\beta W_{el}(\vec{r}_1,\vec{r}_2,\Omega)).$$

In zeroth on the dipole-dipole interaction $< W_{ab} >_0 = 0$. In the first approximation:

$$U_a^{(dd)}(r) = -\beta < W_{dd}^2 >_0 \Rightarrow -\beta < d_\alpha^{(1)} d_\gamma^{(1)} >_0 < d_\beta^{(2)} d_\delta^{(2)} >_0 \frac{\partial^2 \ln r}{\partial r_\alpha \partial r_\beta}\frac{\partial^2 \ln r}{\partial r_\gamma \partial r_\delta}, \qquad (2.42)$$

Taking into account that

$$< d_\alpha^{(1)} d_\gamma^{(1)} >_0 = \frac{\vec{d}^2}{3}\delta_{b\gamma}, \quad < d_\beta^{(2)} d_\delta^{(2)} >_0 = \frac{\vec{d}^2}{3}\delta_{\beta\delta}, \qquad (2.43)$$

and also

$$\delta_{i_1 i_2}\frac{\partial^n \ln r}{\partial r_{i_1}\partial r_{i_2}} = \Delta \ln r = 0, \qquad (2.44)$$

we find: $U_a^{(dd)}(r) = -\frac{1}{4}\beta d^4\left(\frac{\partial^2 \ln r}{\partial r_\alpha \partial r_\beta}\right)^2$,

In accordance with our calculations in the Section 2.1 the dipole moment of a dipole pair is

$$\vec{d}^{\,2}(\tilde{T}) = (q\sigma)^2\zeta(\tilde{T}), \quad \zeta(\tilde{T}) = \frac{1-2\tilde{T}}{1-4\tilde{T}},$$

After simple calculations we get:

$$\tilde{U}_a^{(dd)}(r) = -\frac{1}{4}\left(\frac{\sigma}{r}\right)^4 \frac{1}{\tilde{T}}\zeta^2(\tilde{T}), \qquad (2.45)$$

where $\tilde{U}_a^{(dd)}(r) = U_a^{(dd)}(r)/(\varepsilon_0 k_B T_*)$ is the dimensionless energy.

As we can see, the interaction between two dipole pairs is determined by the attractive potential (the minus sign before the final expression).

## 2.6. The estimate of the critical point in dipole pair approximation

In this Section we will focus our attention on the equation of state (EoS) for a system consisting from dipole pairs. In more details we consider the positions a) the spinodal or the curve, separating the stable and absolutely unstable states of a system; b) the binodal, or the coexistence curve, describing the equilibrium between liquid and vapor phases in our system. Moreover, we study the position of the critical point, which is only joint point for the spinodal and bimodal.

For this aim we apply to the van der Waals EoS [2,3]:

$$P = \frac{T}{\upsilon - \upsilon_0} - \frac{a}{\upsilon^2}. \tag{2.46}$$

Here $P$ is pressure, $\upsilon$ is the specific volume per particle, i.e. on dipole pair, $\upsilon = 1/n$, $\upsilon_0$ is its own volume [2]. For the following we determine sequentially the position of the spinodal, critical point and binodal.

***Binodal, spinodal and the vapor-liquid critical point***

The spinodal is determined by the equation [2,3]:

$$\left.\frac{\partial p}{\partial \upsilon}\right|_t = 0, \tag{2.47}$$

and for the van der Waals equation it reduces to:

$$T = 2an(1 - n\upsilon_0)^2.$$

The position of the critical point is determined by the equations [2,3]:

$$\left.\frac{\partial p}{\partial \upsilon}\right|_t = 0, \quad \left.\frac{\partial^2 p}{\partial \upsilon^2}\right|_t = 0. \tag{2.48}$$

Together with the van der Waals equation (2.6.1) it leads to values of critical temperature, volume and pressure:

$$T_c = \frac{8}{27}\frac{a}{\upsilon_0}, \quad \upsilon_c = 3\upsilon_0, \quad p_c = \frac{1}{27}\frac{a}{\upsilon_0^2}. \tag{2.49}$$

The vapor-liquid coexistence curve or binodal is determined by the Maxwell rule of equal areas [2,3]:

$$\int_{\upsilon_l}^{\upsilon_g} \upsilon(p)dp = 0\,, \tag{2.50}$$

where $\upsilon_l$ and $\upsilon_g$ are the specific volumes for liquid and vapor correspondingly.

In dimensionless variables

$$t = T/T_c\,,\ \ \tilde{\upsilon} = \upsilon/\upsilon_c\,,\ \tilde{p} = p/p_c\,. \tag{2.51}$$

the van der Waals equation takes the view:.

$$\tilde{p} = \frac{8t}{3\tilde{\upsilon} - 1} - \frac{3}{\tilde{\upsilon}^2}\,. \tag{2.52}$$

or

$$\tilde{p} = \frac{8t}{3 - \tilde{n}} - 3\tilde{n}^2\,. \tag{2.53}$$

Near the critical point the equation (2.6.8) is approximated by the expansion:

$$\tilde{p} = 1 + 4\tau + 6\tau u + 3\tau u^2 + \frac{3}{2}u^3 + \frac{3}{4}u^4 + \ldots\,, \tag{2.54}$$

where $\tau = t - 1 \Rightarrow \frac{T - T_c}{T_c}$ and $u = \tilde{n} - 1 \Rightarrow \frac{n - n_c}{n_c}$. The solution of the equation: $\left.\frac{\partial\tilde{p}}{\partial u}\right|_\tau = 0$ , equivalent to (2.6.2) , determines the positions of liquid ($u_+$) and vaporous ($u_-$) spinodal branches:

$$u_\pm^{(s)} = \pm 2(-\tau)^{1/2} - \tau + \ldots\,, \tag{2.55}$$

The rule of equal areas: $\int_{n_g}^{n_l} \left.\frac{1}{\tilde{n}}\frac{\partial\tilde{p}}{\partial\tilde{n}}\right|_\tau d\tilde{n} = 0$ together with the expansion(2.6.9) reduces to the equation, determining the bimodal branches:

$$\tau \cdot u^2 + \frac{3}{8}(1+\tau)u^4 - \frac{1}{10}(1+\tau)u^5 + \ldots\Big|_{u_g}^{u_l} = 0\,. \tag{2.56}$$

From here we find the analog of the expansion (1.6.10) for the binodal:

$$u_\pm^{(b)} = \pm 2(-\tau)^{1/2} - \frac{16}{45}\tau + \ldots \tag{2.57}$$

The expressions (2.6.10) and (2.6.12) describe also the near-critical behavior of the

spinodal and binodal for the Coulomb gas. Its specificity is manifested in values of $T_c$ and $n_c$.

***Vapor-liquid critical point for the 2D-Coulomb gas***

Here we apply to virial expansions [2,3], connecting the parameters $\upsilon_0$ and $a$, entering to the van der Waals EoS (2.6.1), with the interparticle potentials [2].

At low temperatures, when the positive and negative discs contact with each other, $\upsilon_0 = 2\pi\sigma^2$ [8,9]. If temperature increases the radius of effective circle for a dipole pair equals to: $r_d(\tilde{T}) = \frac{1}{2}\sigma\left(1+\zeta^{1/2}(\tilde{T})\right)$, that leads to the

$$\upsilon_0(d) = 2\pi r_d^2 \Rightarrow \frac{\pi}{2}\sigma^2\left(1+\zeta^{1/2}(\tilde{T})\right)^2 \tag{2.58}$$

Within the limit $\tilde{T} \to 0$ the quantity $\zeta(\tilde{T}) \to 1$ and we return to initial value of $\upsilon_0(d)$. The constant $a$ is determined by the interparticle potential according to the formula:

$$a = \pi \int\limits_{(1/2)\sigma(1+\zeta^{1/2}(\tilde{T}))}^{\infty} |U(r)| r dr . \tag{2.59}$$

Let us substitute here the potential of the averaged interaction between two dipole pairs. It had been determined in the previous Section it had been shown that

$$U_a^{(dd)}(r) = -\frac{1}{32}\beta\left(\frac{d_0}{r}\right)^4 (1+\zeta^{1/2}(\tilde{T}))^4, \quad d_0 = q\sigma. \tag{2.60}$$

Substitution (2.6.15) to (2.6.14) leads to the result:

$$a_{dd} = \frac{\pi}{64}\beta q^4\sigma^2(1+\zeta^{1/2}(\tilde{T}))^2 . \tag{2.661}$$

Using the values of $a$ (2.6.16) and $\upsilon_0$ (2.6.2), as well as the first expression from (2.6.4) we get the following equation for the critical temperature

$$T_c = \frac{8}{27}\frac{a}{\upsilon_0} \to T_c^2 = \frac{1}{4\cdot 27}T_*^2 . \tag{2.62}$$

From here we find, that the dimensionless critical temperature for the Coulomb gas in the dipole pairs approximation equals to:

$$\tilde{T}_c \approx \frac{1}{6\sqrt{3}} \approx 0.096 . \tag{2.63}$$

The critical value of the specific volume takes view:

$$\tilde{\upsilon}_c = 3\upsilon_0/\sigma^2 \Rightarrow \frac{3\pi}{2}\left(1+\zeta^{1/2}(\tilde{T}_c)\right)^2. \qquad (2.64)$$

As we can see, 1) the vapor-liquid critical temperature, calculated for the 2D-Coulomb gas modeled by the ensemble of dipole pairs, is independent on their size; 2) the critical value of the specific volume is rather different for cases corresponding to contacting discs: $r_d = \sigma$ and non-contacting discs, when $r_d = (1/2)\sigma(1+\zeta^{1/2}(\tilde{T}_c))$.

The ratio of the specific volumes for these cases equals to:

$$\frac{\tilde{\upsilon}_c(\tilde{T}_c)}{\tilde{\upsilon}_c} = \frac{1}{4}\left(1+\zeta^{1/2}(\tilde{T}_c)\right)^2 \approx 1+\tilde{T}_c+... \qquad (2.65)$$

Thus, the changes of the critical temperature and specific volume due to the rotation effects within the dipole pairs ensemble are inessential.

## 2.7. The mixture of dipole pairs and quadrupole clusters

As we noted early, the dipole pairs during collisions can join to quadrupole clusters. It leads to the ensemble consisting from the dipole pairs and quadrupole clusters. In other words the $2D-$Coulomb gas can be considered as the mixture of two type clusters. In this case the parameters $\upsilon_0$ and $a$ for the van der Waalse EoS take the values (see [2], and [8,9]):

$$\upsilon_0(c) = c\upsilon_d + (1-c)\upsilon_Q$$

$$a(c) = c^2 a_{dd} + (1-c)^2 a_{QQ} + 2c(1-c)a_{dQ}.$$

where

$$c = \frac{n_d}{n_d + n_Q} \text{ -}$$

is the concentration of dipole pairs ($n_d$ and $n_Q$ are the densities of clusters). For contacting dipole pairs and quadrupole clusters:

$$\upsilon_d^{(c)} = 2\pi\sigma^2, \qquad \upsilon_Q^{(c)} = (3/2+\sqrt{2})\pi\sigma^2,$$

so

$$\upsilon_Q^{(c)} / \upsilon_d^{(c)} = (3/4 + 1/\sqrt{2}) \approx 1.$$

It means that the mixture of clusters can be considered as a system of particles having practically identical sizes.

Near the vapor-liquid critical point, calculated within the dipole pairs approximation, the $2D$-Coulomb gas is the mixture of dipole pairs and quadrupole aapproximation according to [8,9]:

$$a_{dd} = \frac{\pi}{16} \frac{q^4 \sigma^2}{T_*} \frac{1}{t},$$

$$a_{dQ} = \frac{16\pi}{(3+\sqrt{2})^4} \frac{q^4 \sigma^2}{T_*} \frac{1}{t},$$

$$a_{QQ} = \frac{3\pi}{(1+\sqrt{2})^6} \frac{q^4 \sigma^2}{T_*} \frac{1}{t}.$$

Their values are related to each other as:

$$a_{dd} : a_{dQ} : a_{QQ} = 1 : 0.67 : 0.24; \ ,$$

Taking into account that $c = 0.5$ with suitable accuracy we can get:

$$\upsilon_0(c) \approx \upsilon_d^{(c)}, \qquad a(c) \approx 0.645 a_{dd}.$$

From (2.6.17) it follows the following estimate for the critical temperature:

$$T_c = \frac{8}{27} \frac{a}{\upsilon_0} \rightarrow \ T_c^2 = \frac{0.645}{4 \cdot 27} T_*^2,$$

or

$$\tilde{T}_c \approx \frac{0.803}{6\sqrt{3}} \approx 0.077, \quad \tilde{\upsilon}_c \approx 6\pi.$$

These values, rewritten in the view:

$$\tilde{T}_c \approx 0.077, \quad \tilde{n}_c \approx \frac{1}{2\pi} \approx 0.16,$$

practically coincide with values obtained in computer experiments [4,6]. Here we take into account that each particle with probability $c$ consists from two discs (dipole pair) and with the probability $1-c$ it consists from four discs (quadrupole cluster), therefore

$$\tilde{n}_c = \left.\frac{2c + 4(1-c)}{\tilde{\upsilon}_c}\right|_{c=0.5} = \left.\frac{4-2c}{\tilde{\upsilon}_c}\right|_{c=0.5} \to \frac{1}{2\pi}.$$

## CONCLUSIONS

1. To describe the properties of the Coulomb gas in $2D-$space the approximations of dipole pairs and the mixture of dipole pairs and quadrupole clusters are used;
2. The temperature dependence of the dipole moments for the dipole pairs is studied;
3. The distribution of dipole pairs and quadrupole clusters in the plane density-temperature is considered in details;
4. The positions of the spinodal, binodal and the critical point for the Coulomb gas in the approximations of dipole pairs and the mixture of dipole pairs and quadrupole clusters are determined;
5. The dielectric permittivity of the $2D-$dimensional Coulomb gas in the approximation of dipole pairs is investigated;
6. The dielectric-conductor transition line is estimated within the dipole pairs approximation;
7. The applicability region for the dipole pairs approximation is discussed.

Author's signature _____

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## SUMMARY

***Wang Bin.*** «Phase transitions in 2D-Coulomb gas» - Thesis to obtain a master's degree in specialty 104 – physics and astronomy. Odesa I.I.Mechnicov National University. - Odesa, 2024

The research of the master's thesis is devoted to the study of the simplest phase transitions in the two dimensional Coulomb gas: 1) vapor-liquid phase transition and 2) Dielectric-Conductor transition. These problems are solved on the base of cluster representations generating by strong Coulomb interaction between positive and negative discs.

Such a system can be considered as an ensemble of dipole pairs, and its thermodynamic properties of such a gas are described in the paper using the standard virial expansion. It can be used to construct the van der Waals equation of state (vdW EoS). In this way, the binodal and spinodal for the Coulomb gas can be determined, as well as the critical point, which is the only common point of these curves.

It is taken into account that the size of dipole pairs is not constant with temperature, which affects the nature of the coexistence curve and as a result, the Coulomb gas becomes conductive and we can speak of a dielectric-conductor transition. This is a new property that is lacking in conventional molecular systems. The dielectric-conductor transition curve is one of the important problems, the solution of which is devoted to the qualification work.

*Keywords: Coulomb gas, binodal and spinodal, dielectric-conductor transition.*

# АНОТАЦІЯ

***Ван Бінь.*** «Фазові переходи у 2D-кулонівському газі» - Кваліфікаційна наукова робота на правах рукопису. Робота на здобуття наукового ступеня магістра за спеціальністю 104-фізика та астрономія. Одеський національний університет імені І .І. Мечникова. Одеса, 2024.

Дослідження магістерської роботи присвячено вивченню найпростіших фазових переходів у двовимірному кулонівському газі: 1) фазовий перехід пар-рідина та 2) перехід діелектрик-провідник. Ці проблеми вирішуються на основі представлень кластерів, породжених сильною кулонівською взаємодією між позитивним і негативним дисками.

Таку систему можна розглядати як ансамбль дипольних пар, а її термодинамічні властивості такого газу у роботі описано застосуваням стандартного віріального розкладу. З його допомогою можна побудувати рівняння стану Ван-дер-Ваальса (vdW EoS). Таким чином можна визначити бінодаль і спінодаль для кулонівського газу, а також критичну точку, яка є єдиною загальною точкою цих кривих.

Враховано,що розмір дипольних пар непостійний з температурою, що впливає на характер кривої співіснування і в результаті кулонівський газ стає провідним і можна говорити про перехід діелектрик-провідник. Це нова властивість, якої не вистачає звичайним молекулярним системам. Крива переходу діелектрик-провідник є однією з важливих задач, розв'язанню якої присвячена кваліфікаційна робота.

*Ключові слова: кулонівський газ, бінодаль і спінодаль, перехід діелектрик-провідник.*