TO THE STATISTICAL DESCRIPTION OF THE STRUCTURE FORMATION IN COULOMB-LIKE SYSTEMS

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A new solution to the problem of the calculation of the partition function for a Coulomb-like system is proposed. The quantum-field-theory approach is used to give a statistical description of a system of interacting particles with due regard to an arbitrary spatially inhomogeneous configuration. The formation of structures in a Coulomb-like system is analyzed and applied to the dusty plasma treatment. A necessary condition for the crystal formation in a three-dimensional system of dust particles is obtained. In the one-dimensional case, an exact solution for the spatial distribution of charged particles is presented.

The statistical description of Coulomb-like systems is one of the key problems of statistical physics. Such systems might be helpful in testing the ideas concerning the description of systems with long-range interactions in terms of statistical mechanics [1]. The interest in this problem is also generated by its application to the studies of a variety of peculiar phenomena in various fields of science [2–4]. Solving the problem under consideration is complicated by the fact that the standard methods of statistical physics cannot be used in the case of a system with Coulomb interaction. For a system with long-range interaction, the thermodynamical ensembles are not equivalent. The phase transition in a Coulomb-like system also cannot be described in terms of the mean-field thermodynamics approach [1]. The formation of a dust crystal may provide a typical example of dusty plasmas with interaction. Moreover, such systems may serve as perfect media for the experimental investigation of classical fluids and solids [6–9]. The formation of a spatial distribution in a system of interacting particles is a typical problem that occurs in the statistical description of condensed matter, plasma-like media, biological systems, *etc.* In order to solve it, one should apply specific methods that would allow for an arbitrary inhomogeneity of particle distributions. In particular, these methods should employ an appropriate procedure to find the dominant contribution to the partition function and to avoid the free-energy divergences as the volume of the system grows infinitely. Only few model systems of interacting particles are known for which the partition function can be evaluated exactly, at least to within the thermodynamical limit [20]. As for the description of equilibrium states, only few results have been obtained within the framework of "exact" equilibrium statistical mechanics.

One of the ways to describe the spatially inhomogeneous distribution of a system of interaction particles is to use the new nonconventional method proposed in [15, 16] that employs the Hubbard–Stratonovich representation of the partition function [18]. This method is now extended and applied to a system with Coulomb-like interaction to find the solution for the particle distribution. It is important that this solution has no divergences for the thermodynamical limits. We use the saddle-point approximation with regard for the conservation of the number of particles, which yields a nonlinear equation for the new field variable. In the three-dimensional case, this equation reduces to the sine-Gordon equation whose solution determines the state associated with the dominant contribution in the partition function. This method makes it possible to describe the conditions for the formation of a Wigner crystal in a system of dust particles in a plasma. There may exist various possibilities for different parameters corresponding to the interaction potential. In order to understand the behavior of a dusty plasma in complicated situations, however, the results for simple and basic cases are indispensable. We have analytically derived the necessary condition for the crystal formation in a system of dust particles in the three-dimensional case. In the one-dimensional case, we have found an exact solution for the spatial distribution of charged particles.

We now describe in brief the well-known result concerning the statistical description of a system of interacting particles [15,16]. The method makes it possible to

describe an equilibrium system of interacting particles, by taking the formation of a thermodynamically stable spatial particle distribution into account, and to consider the collective behavior of the structures thus formed. The statistical investigation of the classical particle interaction in condensed matter is based on the function of the canonical ensemble of particle sets $\{n\}$. We have

$$Z_N = \sum_{\{n\}} \exp\left(-\beta H(n)\right), \tag{1}$$

where $\sum\limits_{\{n\}}$ implies the summation over all probable distributions $\{n_s\}$, $\beta = \frac{1}{kT}$ is the inverse temperature, and $H(n)$ is the configuration Hamiltonian of the system. A system of interacting particles with regard for the type of statistics, but neglecting quantum correlations, can be treated in the classical manner with the model Hamiltonian (see, e.g., [22]):

$$H(n) = \sum_s \varepsilon_s n_s - \frac{1}{2}\sum_{s,s'} W_{ss'} n_s n_{s'}, \tag{2}$$

where ε_s is the additive part of the energy in the state s that in most cases is equal to the kinetic energy, and $W_{ss'}$ are the interaction energies for the particles in the states s and s'. In this model, the macroscopic states of the system are described by a set of occupation numbers n_s. Index s labels an individual particle state that can correspond to a fixed site of the Ising lattice [23]. It is clear that the calculation of the partition function is a rather complicated problem even in the case of the Ising model. The partition function for the canonical ensemble of a system of interacting particles is given by [16]:

$$Z_N = \sum_{\{n\}} \exp\left(-\beta H(n)\right) =$$

$$= \sum_{\{n\}} \exp\left\{-\beta\left[\sum_s \varepsilon_s n_s - \frac{1}{2}\sum_{s,s'} W_{ss'} n_s n_{s'}\right]\right\}. \tag{3}$$

In order to perform a formal summation in (2), the additional field variables can be introduced in terms of the theory of Gaussian integrals [18, 22]:

$$\exp\left\{\frac{1}{2\theta}\nu^2 \sum_{s,s'} \omega_{ss'} n_s n_{s'}\right\} =$$

$$= \int\limits_{-\infty}^{\infty} D\varphi \exp\left\{\nu \sum_s n_s \varphi_s - \frac{1}{2\beta}\sum_{s,s'} \omega^{-1}_{ss'} \varphi_s \varphi_{s'}\right\}, \tag{4}$$

where $D\varphi = \frac{\prod\limits_s d\varphi_s}{\sqrt{\det 2\pi\beta\omega_{ss'}}}$ depends on the character of the interaction energy, and $\omega^{-1}_{ss'}$ is the matrix that is inverse to the interaction one. The latter satisfies the condition $\omega^{-1}_{ss''}\omega_{s''s'} = \delta_{ss'}$. The partition function of a Coulomb-like system may be rewritten as

$$Z = \int\limits_{-\infty}^{\infty} D\varphi \sum_{\{n_s\}} \exp\left\{\sum_s \left(i\varphi_s - \beta\varepsilon_s\right) n_s -\right.$$

$$\left. -\frac{1}{2\beta}\sum_{s,s'} \left(W^{-1}_{ss'} \varphi_s \varphi_{s'}\right)\right\}. \tag{5}$$

In the above analysis, we did not restrict the number of particles. Now, let us fix the total number of particles in the system, $N = \sum\limits_s n_s$. To do this, we use the well-known Cauchy formula $\frac{1}{2\pi i}\oint d\xi \xi^{\sum\limits_s n_s - N - 1} = 1$ [23]. The partition function takes the form

$$Z_N = \frac{1}{2\pi}\oint d\xi \int\limits_{-\infty}^{\infty} D\varphi \times$$

$$\times \exp\left\{-\frac{1}{2\beta}\sum_{s,s'} \left(W^{-1}_{ss'} \varphi_s \varphi_{s'}\right) - (N+1)\ln\xi\right\} \times$$

$$\times \prod_s \sum_{\{n_s\}} \left[\xi \exp\left(i\varphi_s - \beta\varepsilon_s\right)\right]^{n_s}. \tag{6}$$

After the summation over the occupation numbers n_s, it finally reduces to

$$Z_N = \frac{1}{2\pi}\oint d\xi \int\limits_{-\infty}^{\infty} D\varphi \exp(-\beta F(\varphi, \xi)), \tag{7}$$

where the effective free energy is given by

$$\beta F(\varphi, \xi) = \frac{1}{2\beta}\sum_{s,s'} \left(W^{-1}_{ss'} \varphi_s \varphi_{s'}\right) +$$

$$+\delta \sum_s \ln\left(1 - \delta\xi e^{-\beta\varepsilon_s}\cos\varphi_s\right) + (N+1)\ln\xi, \tag{8}$$

where $\delta = +1$ for the Bose statistics and $\delta = -1$ for the Fermi statistics, and $\xi \equiv e^{\beta\mu}$ is the absolute chemical activity of the chemical potential μ. The partition

function makes it possible to use the efficient methods developed in the quantum field theory without imposing any additional restrictions on the integration over the field variables. The functional $\beta F(\varphi,\lambda)$ depends on the distribution of field variables φ and the absolute chemical activity ξ. The field variable φ contains the same information as the original partition function with the summation of over the occupation numbers, i.e., all the information about probable states of the system.

Now, we can employ the saddle-point method to find the asymptotic value of the partition function Z_N as $N\to\infty$; the dominant contribution is given by the states that satisfy the extremum condition for the functional. The particle distribution is determined by the saddle-point method of solution of the equations, i.e.,

$$\frac{\delta\beta F}{\delta\xi}=\frac{\delta\beta F}{\delta\varphi}=0, \tag{9}$$

which is valid in both cases of spatially homogeneous or inhomogeneous distributions. As the volume of the system tends to infinity, the solutions associated with the finite effective free energy $F(\varphi,\lambda)$ are thermodynamically stable. The spatially inhomogeneous solution of these equations describes the distribution of interacting particles. Such inhomogeneous behavior is determined by the intensity of interaction. In other words, the accumulation of particles in a finite spatial domain is related to the spatial distribution of the fields and the activity. The inverse matrix $\omega^{-1}_{ss'}$ of the interaction, $\omega_{ss'}=\omega(|r_s-r_{s'}|)=\frac{Q^2}{|r_s-r_{s'}|}\exp(-\lambda|r_s-r_{s'}|)$, should be treated in the continuum limiting case in the operator sense [22], i.e.,

$$\omega^{-1}_{rr'}=\delta_{rr'}\widehat{L_{r'}}=-\frac{1}{4\pi Q^2}(\triangle-\lambda^2), \tag{10}$$

where Q is the particle charge, and $\triangle$ is the Laplace operator. With the accuracy up to the surface term, the effective free energy in the continuum case is given by

$$\beta F(\varphi,\xi)=\int dV\left\{\frac{1}{8\pi Q^2\beta}((\nabla\varphi)^2+\lambda^2\varphi^2)+\right.$$

$$\left.+\delta\sum_p\ln\left(1-\delta\xi e^{-\beta\varepsilon_p}\cos\varphi\right)\right\}+(N+1)\ln\xi. \tag{11}$$

As has been shown [24] for classical statistics, $\xi\le 1$ and $\delta\sum_p\ln\left(1-\delta\xi e^{-\beta\sum_p\varepsilon_p}\cos\varphi\right)\approx -\xi e^{-\beta\varepsilon_p}\cos\varphi+....$ The integration over the momentum and coordinates should be performed over the cell volume $(2\pi\hbar)^3$ in the phase space of individual states. The effective free energy for the Boltzmann statistics can be rewritten in the form [16]

$$\beta F(\varphi,\xi)=\int dV\left\{\frac{1}{8\pi Q^2\beta}((\nabla\varphi)^2+\right.$$

$$\left.+\lambda^2\varphi^2)-\xi A\cos\varphi\right\}+(N+1)\ln\xi, \tag{12}$$

where $A=\left(\frac{2\pi m}{\beta\hbar^2}\right)^{3/2}$. This form of the partition function turns out to be suitable in the case of a spatially inhomogeneous distribution of particles.

We start from the case of a system of noninteracting particles, $\varphi=0$. The effective free energy in this case can be written in the following simple form:

$$\beta F(\varphi,\xi)=-\int d\mathbf{r}\xi\left(\frac{2\pi m}{\beta\hbar^2}\right)^{3/2}+(N+1)\ln\xi. \tag{13}$$

The normalization condition reduces to the equation

$$V\xi\left(\frac{2\pi m}{\beta\hbar^2}\right)^{3/2}=N+1, \tag{14}$$

which yields the absolute chemical activity $\xi=\frac{N}{V}\left(\frac{2\pi m}{\beta\hbar^2}\right)^{-3/2}$. Substituting this quantity in the expression for the effective free energy yields the effective free energy for a fixed number of particles and the energy, and the partition function of noninteracting particles is given by $Z_N=\exp(-\beta F_{\rm B})$, where

$$\beta F_{\rm B}=\frac{3N}{2}-\ln\frac{N!}{V}\left(\frac{\beta\hbar^2}{2\pi m}\right)^{3/2}, \tag{15}$$

which reproduces the well-known formula for the free energy of the ideal Boltzmann gas.

In the case of interacting particles, we propose a method that makes it possible to determine the states with the dominant contributions to the partition function. Namely, we use the saddle-point approximation which provides an efficient powerful technique in quantum field theory. This approach has been successfully applied to many problems. In particular, such an approach holds in the case of high-temperature many-body systems. The equation for the saddle-point states $\frac{\delta\beta F}{\delta\varphi}=0$ is given by

$$\frac{1}{r_e}\left\{\triangle\varphi+\lambda^2\varphi\right\}+\xi A\sin\varphi=0, \tag{16}$$

where we introduce the notation $r_e = 2\pi Q^2\beta$. The chemical activity can be obtained from the normalization condition $\frac{\delta\beta F}{\delta\xi} = 0$:

$$\int dV\xi A\cos\varphi = N+1. \tag{17}$$

It should be noted that this condition enables us to introduce the concentration of particles $\rho(\mathbf{r}) = \xi A\cos\varphi(\mathbf{r})$. The first integral of the equation for the field variable can be obtained from the first equation by multiplying this equation by $\nabla\varphi$ with regard for the relation $\triangle = \nabla^2$. The first integral of the equation for the field variable can be presented in the form

$$\frac{1}{r_e}\left\{(\nabla\varphi)^2 + \lambda^2\varphi^2\right\} + \xi A\cos\varphi = E^2, \tag{18}$$

where E is an unknown integration constant that should be found from the condition of existence of the solution. Though this equation cannot be solved in the general case, it provides a tool to study many interacting Coulomb-like systems under various external conditions.

Let us start from the case of a homogeneous distribution of interacting particles. In this case, we have to derive the condition of existence of the solution $\varphi = \varphi_0 = \text{const}$ from the equation for the field variable

$$\frac{\lambda^2}{r_e}\varphi_0 + \xi A\sin\varphi_0 = 0 \tag{19}$$

and to find the chemical activity from the normalization condition

$$\xi AV\cos\varphi_0 = N+1. \tag{20}$$

Within the context of the first integral and the equation for the chemical activity, the free energy can be written in the simple form

$$\beta F = F_{\mathrm{B}} + N\left\{\frac{\lambda^2}{r_e n} - \ln\cos\varphi_0\right\}, \tag{21}$$

where we have introduced the concentration of particles $n = \frac{N+1}{v}$. Obviously, the second term in the free energy is always positive since $\cos\varphi_0 \le 1$. Thus, the free energy of a homogeneous system of interacting particle is greater than the free energy of the Boltzmann gas.

In the general case, the particle distributions in Coulomb-like systems are inhomogeneous, which is caused by the long-range nature of the Coulomb interaction. In the case of an intensive interaction, the Coulomb-like system is unstable as a whole, so the minimum value of free energy is achieved in the case of an inhomogeneous distribution of particles.

Now, we employ the proposed approach to show how the states associated with a Wigner crystal can be found. Taking into account that the density function $\rho(\mathbf{r}) = \xi A\cos\varphi$ is only positive and assuming that the state of interest does exist, we take the periodic distribution function in the form

$$\rho(\mathbf{r}) = \xi A\cos\varphi =$$

$$= \xi A\left\{1 + \cos(k_x x) + \cos(k_y y) + \cos(k_z z)\right\} \tag{22}$$

that corresponds to the cubic lattice with the wave vector $\mathbf{k} = (k_x, k_y, k_z)$. If we assume that one charged particle is present at every lattice site and that the lattice is isotropic ($k_x = k_y = k_z = 2\pi n^{1/3}$, where $n = \frac{N+1}{V}$ is the particle density), then the normalization condition yields $\xi = \frac{n}{A}$ or $\xi = \frac{N+1}{AV}$. From the first integral for the field variable, one can conclude that $E^2 = \frac{\pi^2\lambda^2}{r_e}$. We substitute this relation into the free energy which is presented through the first integral, i.e.,

$$\beta F = \int dV\left\{E^2 - 2\xi A\cos\varphi\right\} + (N+1)\ln\xi, \tag{23}$$

and thus obtain the free energy of the system in the following simple form:

$$\beta F = \beta F_{\mathrm{B}} + (N+1)\left\{\frac{4\pi^2\lambda^2}{nr_e} - 1\right\}. \tag{24}$$

Introducing the coupling parameter $\Gamma_e \equiv r_e n^{1/3}$ (which is the ratio of the Coulomb energy to the kinetic one) provides a relation for the critical value of the coupling parameter, i.e.,

$$\Gamma_e \ge 4\pi^2\lambda^2 n^{\frac{2}{3}} \equiv \left(2\pi\frac{L}{r_D}\right)^2, \tag{25}$$

where L is the lattice period, and r_D is the Debye length. With this condition being satisfied, we can expect a crystal structure to be formed. Namely, such structures are observed in dusty plasmas [2] In terms of the structure lattice parameter used in [2] $k \equiv \frac{L}{r_d}$ -(the interparticle distance normalized by the effective screening length), the relation obtained is given by

$$\Gamma_e \ge (2\pi k)^2. \tag{26}$$

This relation gives the value of the same order as the result of computer simulations [2]. We cannot solve the problem of the crystal structure formation in dusty plasmas exactly, nevertheless we can analytically predict the

conditions for such a formation. The problem is that we do not know the three-dimensional solution of the sine-Gordon equation that determines the field variable.

It seems to be useful to consider a one-dimensional analogy of the system considered above. In this case, the problem can be solved exactly [16]. Physically, this corresponds to a one-dimensional molecular system with free charges distributed along it. Let us consider a cylindrical molecule of length L and radius $r \ll L$. Let the Coulomb repulsive charges lie on the cylinder axis. In this case, the free energy can be presented as

$$\beta F = \frac{V}{L} \int\limits_0^L dz \left\{ \frac{1}{r_e} \left(\frac{d\varphi}{dz} \right)^2 - \xi A \cos\varphi \right\} + (N+1) \ln \xi. \tag{27}$$

Then the saddle-point equation reduces to the sine-Gordon equation

$$\frac{1}{r_e} \left(\frac{d^2\varphi}{dz^2} \right) - \xi A \cos\varphi = 0. \tag{28}$$

The first integral of this equation is given by

$$\frac{1}{r_e} \left(\frac{d\varphi}{dz} \right)^2 + \xi A \cos\varphi = C. \tag{29}$$

It corresponds to the exact solution with a finite period, i.e.,

$$l = \frac{1}{\sqrt{2r_e}} \int \frac{d\varphi}{\sqrt{C - \xi A \cos\varphi}} = \frac{4K(p)}{\sqrt{2r_e(C+\xi A)}}, \tag{30}$$

where $K(p)$ is the full elliptic integral of the first kind with the argument $p = \sqrt{\frac{2\xi A}{C+\xi A}}$. Depending on the integration constant C, the different solutions can appear [25]. Substituting this solution into the free energy yields

$$\beta F = 2\xi AV \left\{ \frac{2E(p)}{p^2 K(p)} - \frac{1}{p^2} + 1 \right\} - \xi AV + (N+1) \ln \xi. \tag{31}$$

Here $E(p)$ is the full elliptic integral of the second kind with the same argument. The free energy extremum is achieved for $p = 1$, which corresponds to the soliton solution given by

$$\varphi = 4 \arctan \exp(z\sqrt{r_e \xi A}). \tag{32}$$

This solution determines the state associated with the dominant contribution to the partition function. Thus, the free energy takes the form

$$\beta F = 8 \frac{V}{L} \left(\frac{\xi A}{r_e} \right)^{1/2} - \xi AV + (N+1) \ln \xi. \tag{33}$$

We can find the chemical activity and substitute its value in the free energy, which leads to the following formula for the free energy of a one-dimensional Coulomb-like system:

$$\beta F = \beta F_{\rm B} + (N+1) \left\{ 1 - \frac{8}{\sqrt{n r_e L^2}} \right\}. \tag{34}$$

If the second term is greater than the first one, then charged particles can form a periodic structure. The above system is homogeneous on the macroscopic scale, but the particle distribution can be spatially periodic.

Moreover, this approach provides a description of spatially periodic distributions. The partition function has no singularities for any values of the Coulomb-like field. As is shown, the minimum of the free energy does not always correspond to a homogeneous particle distribution, but could indicate the formation of a crystal-like structure.

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СТАТИСТИЧНЕ ОПИСАННЯ ФОРМУВАННЯ СТРУКТУР У КУЛОНІВСЬКИХ СИСТЕМАХ

Б.І. Лев, А.Г. Загородній

Р е з ю м е

Запропоновано новий підхід до статистичного описання кулонівських систем. Підхід ґрунтується на представленні статистичної суми в вигляді континуального інтеграла по додатковому полі, що дозволяє використати добре розроблені методи квантової теорії поля. Запропонований метод відбору станів, що вносять найбільший внесок в статистичну суму, дозволяє описати формування як просторово однорідного, так і неоднорідного розподілу взаємодіючих частинок. Проаналізовано умови формування періодичного розподілу порошинок у слабо іонізованій плазмі, а також колоїдних частинок на поверхні рідини. В одновимірному випадку знайдено точний розв'язок для просторового розміщення заряджених частинок.