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Geometry of the equilibrium distribution of interacting particles

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ABSTRACT

The formations of structures in all systems of interacting particles at different temperatures and particle concentrations have the same physical nature and therefore they could be described geometrically the same way. We propose a geometric description of a thermodynamically stable distribution of interacting particles. The character and intensity of interaction between particles determine the effective geometry of the medium which is provided by the minimum of the total free energy with non-linearity. A realization of spaces with possible particle distributions of arbitrary-order symmetries (including fifth, seventh etc. orders) which cannot occur in the ordinary Euclidean space, is described.

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Any physical theory is based on the postulated geometric properties of the space. The problem of the geometry as a whole is equivalent to the problem of the behavior of the fields which form the space [1–5]. We think that in the problem formulated in a such way, the geometric aspect is important not only for the description of the Universe but also for study of the physical phenomena.

For the last years the big interest has been growing to the application of the methods of differential geometry in statistical physics and thermodynamics. The geometric approach is represented by two main ways of investigation. One of them is connected with the metric but another one considers the contact structure of the thermodynamic phase space. Using the metric tensor we can calculate the scalar curvature for some statistic and thermodynamic models and study the consequences that appear from the connection between metric and physical quantities. The another idea is that the curvature is proportional to the inverse free energy of the system. The scalar curvature is divergent near the critical point and due to its connection with the second moments of fluctuation the stability of the systems can be measured [6,7].

The average degree of instability of Hamiltonian dynamics can be given in terms of curvature-related quantities integrated over the whole mechanical (Riemannian) manifold. This fact establishes a link between dynamical aspect of a given system, the stability or instability of its trajectories and some global geometric properties of its associated mechanical manifold [8].

In the light of Riemann geometrization of Hamiltonian dynamics, where Lyapunov exponents are related to the average curvature properties of submanifolds of configuration space [9], the temperature dependence of abstract geometric observables, such as for e.g. the averages of curvature fluctuations, has been investigated [10].

Deformations of submanifolds of thermodynamic equilibrium states introduced by continuous contact maps on a phase-space manifold have been considered in terms of the geometrical formulation of thermodynamics [11].

In Riemannian geometric approach to thermodynamics the theory of fluctuations is also considered [12]. In such approach for the case of two independent thermodynamic variables the Riemann curvature is postulated to be inversely proportional to the free energy near the critical point [13]. That leads to a partial differential geometric equation for the free energy. Following [13], the solution is a generalized homogeneous function of its arguments and specifying the values of the critical exponents results in a full scaled equation of state. Latter this postulate was generalized for a case with more than two independent thermodynamic variables [14].

In condensed matter physics the attempts have already been made to use the geometric approach for the description of the phase space [6–9,15–17] to find the criteria of phase transitions [6,7,16,18] to study the formation of the phase boundary [19] and the membrane [20]. The geometric aspect of the physical phenomena occurring in condensed matter can be important for study of structural phase transitions which accompanied by the formation of nonuniform distributions of interacting particles [21,22]. A nonuniform particle distribution can induce an individual effective space which reflects the character and intensity of interaction in the system. In Euclidean space we observe the particle distribution determined either by the structure of the crystal in which redistribution of spins, dipoles, atoms, molecules occurs or by the geometry of the sample with fixed boundaries in which

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the macroscopic structures are formed. But the effective geometry of the particle distribution can be another than Euclidean. This observation is especially important for soft systems with particle distributions governed only by the character and intensity of the intrinsic interaction. Even in the crystal structures formed by the interaction between atoms, an effective non-Euclidean geometry can occur and be manifested in the existence of quasicrystals, fullerenes etc. [23].

There is some approach to use the geometric aspects for the description of physical problems of condensed matter. First of all it is the usage of the direct analogue with the general theory of relativity. Other approach is based on the definition of interacting particle distribution in the curved space. In biophysics and the theory of liquid crystals we have solved the problem of definition of the form of new formation obtained from a minimum of the free energy. Nevertheless the very important questions remain unsolved about the possible internal reasons induced the change of internal geometry in the system of interacting particles and how the character and magnitude of interaction between particles change this geometry. The pure gravitational interaction in the system of self-gravitating particles leads to the fractal distribution of particles in the space [24].

Many physical and chemical systems (e.g., membranes, vesicles, type I superconductor films) displaying macroscopic patterns and textures in equilibrium have been analyzed within the framework of competing interactions. The related phenomena of structure formation in colloidal suspensions and superlattice formation in adsorbate films on crystalline substrates have also been investigated [25]. In condensed matter physics the phase transitions with the formation of spatially inhomogeneous distribution of particles, clusters or cellular structures are of the great interest. It was shown earlier that the formations of structures in all systems of interacting particles have the same physical nature [26] and thereby allowing us to describe them geometrically the same way.

The purpose of this paper is to find the effective space of a thermodynamically stable distribution of interacting particles and to give a geometrical description of the structural phase transitions induced by the character and intensity of the interaction in the system.

Thus we consider the system of many particles. The free energy in self-consistent field and in many-body approximation can be written as

$$F = F_p + F_s + F_n. \tag{1}$$

Here

$$F_p = \int U(\mathbf{r}-\mathbf{r}')f(\mathbf{r})f(\mathbf{r}')d\mathbf{r}d\mathbf{r}' + \ldots \tag{2}$$

is the free energy in terms of particle distribution function $f(\mathbf{r})$, $U(\mathbf{r}-\mathbf{r}')$ is the sum of all energies of particle interactions,

$$F_s = kT\int \left(f(\mathbf{r})\ln f(\mathbf{r}) + [1-f(\mathbf{r})]\ln[1-f(\mathbf{r})]\right)d\mathbf{r} \tag{3}$$

is the entropy part of the free energy,

$$F_n = \int f(\mathbf{r})\sum_i W(\mathbf{r}_i-\mathbf{r})d\mathbf{r} \tag{4}$$

is the free energy resulting from the coupling between particles and matter where $W(r)$ gives the microscopical information about wetting properties of the surface of particle location in spatial point $\mathbf{r}_i$.

The minimum of the free energy (1) corresponds to the self-consistent field solution for $f(\mathbf{r})$. If distribution of particles in the system is homogeneous in every spatial point $\mathbf{r}_i$ then $f(\mathbf{r}_i) = c$ where $c = const$ is the particle concentration. In the case of inhomogeneous particle distribution $f(\mathbf{r}) = c + \varphi(\mathbf{r})$ where $\varphi(\mathbf{r})$ is the deviation of particle concentration from equilibrium in different spatial points. In continuum description (when the deviations of c are smooth on the scale much longer than the distance between particles) we can write $\varphi(\mathbf{r})$ as power series expansion

$$\varphi(\mathbf{r}') = \varphi((\mathbf{r}) + \rho_i\partial_i\varphi(\mathbf{r}) + \frac{1}{2}\rho_i\rho_j\partial_j\partial_i\varphi(\mathbf{r}) + \ldots \tag{5}$$

where $\rho = \mathbf{r}-\mathbf{r}'$ is the distance between two particles. In long-wavelength approximation, using the expansion (5) and taking into account that $\int f(\mathbf{r})d\mathbf{r} = N$, $\int \varphi(\mathbf{r})d\mathbf{r} = 0$, we can rewrite the free energy (1) as

$$\triangle F(\varphi) = \int d\mathbf{r}\left\{\frac{1}{2}l^2(\nabla\varphi)^2 - \frac{1}{2}\mu^2\varphi^2 + \frac{1}{4}\lambda\varphi^4 - \varepsilon\varphi\right\} \tag{6}$$

where the coefficients

$$\mu^2 = V - \frac{kT}{c(1-c)}, \quad V = \int U(\rho)d\rho, \quad l^2 = \int U(\rho)\rho^2 d\rho \tag{7}$$

are determined through the energy of interaction between the particles in the system.

The coefficient λ is responsible for the non-linearity of the system which is induced by the many-body interaction. As example $\lambda \propto \int U(\rho)U(\rho')d\rho d\rho'$ where ρ is the distance between two different particles and ρ' is the distance between other different particles. From non-linearity one can define the geometry of the effective space distribution of interacting particles.

The last coefficient $\varepsilon = N4\pi R_0^2 W$ represents the energy which includes every particle of size R_0 through the wetting effect.

The most important contribution to the concentration is associated with the field configuration for which the value of the free energy (6) is minimum, i.e.,

$$\triangle\varphi - \frac{d\Phi}{d\varphi} = 0 \tag{8}$$

where the potential Φ is

$$\Phi = -\frac{1}{2}\mu^2\varphi^2 + \frac{1}{4}\lambda\varphi^4 - \varepsilon\varphi. \tag{9}$$

When the difference of the minimum of the effective potential values is greater than the barrier height, the free energy can be written as

$$\Delta F = 2\pi\int_0^\infty r^2 dr\left\{\frac{1}{2}\left(\frac{d\varphi}{dr}\right)^2 + \Phi(\varphi)\right\} = -\frac{4\pi}{3}r^3\varepsilon + 4\pi r^2\sigma \tag{10}$$

where σ is the surface energy of the cluster boundary that is equal to the free energy corresponded to the solution of the one-dimensional problem [18,27], i.e.,

$$\sigma = \int_0^\infty dr\left\{\frac{3}{2}\left(\frac{d\varphi}{dr}\right)^2 + \Phi(\varphi)\right\} = \int_0^\infty d\varphi\sqrt{2\Phi(\varphi)}. \tag{11}$$

The formation of each particle distribution in condensed matter induces an individual effective space which does not occur in the Euclidean case. The effective space can be observed through the curvature, torsion and probable realization of the topologies with arbitrary-order symmetries (including fifth, seventh etc.). Symmetry and topological properties of the effective space are determined first of all by the peculiarities of the interaction in the system. It is clear that the problem becomes much more complicated, nevertheless the way to solve it still exists. The idea is associated with

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