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The combined energy distribution function of quantum, classical and fractal particles

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In the framework of statistical physics, the energy distribution functions for classical (Maxwell–Boltzmann distribution) and quantum (Fermi–Dirac and Bose–Einstein distributions) particles were established. The development of nanotechnology has led to the necessity to use the Tsallis energy distribution function for the ensemble of fractal particles. Distinctive features of the listed associations of particles are: the distinguishability of classical particles; the presence of spin (half-integer — fermions, whole — bosons) in quantum particles; geometrical differences of fractal particles. On the other hand, the interrelation of organizational levels of matter raises the question about the existence of a unified distribution function on energies of the mentioned objects. The type of distribution function is found by using the Boltzmann cell method, by calculating the large statistical sum, by using the variational method, etc. In this paper, the representation of the known distribution functions in the form of solutions of the corresponding Cauchy problems allowed us to establish the form of a unified expression to describe the average numbers of particles in quantum, classical and fractal ensembles. It is shown that at the „deformation“ index $q = 0.5$ the fractal ensemble is described by a function similar to the energy noise in the system. In systems with $q < 0$, fractal ensembles originate at a certain threshold negative value (the internal energy of a fractal particle is less than its chemical potential) of the dimensionless energy.

Keywords: energy state, particle ensemble, temperature, chemical potential, fractal dimensionality.

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Fabrication of the nanostructured composites dictates the need for finding not only the particles size distribution function [1,2], but also their energy state distribution function. This is due to the changes occurring in the mechanical, electrical, magnetic, thermodynamic and other properties of small particles compared to objects of quantum and classical physics. In addition, the hierarchical structure of the levels of organization of matter [3] indicates the existence of a unified energy distribution function.

Therefore, the purpose of this brief report is to find a positive definite energy distribution function f that describes, in extreme cases, the average numbers of quantum, classical, and fractal particles at parameter thresholds. For the first time this task was set in [4]. It should be noted that the main attention in this report is paid to the mathematical aspect of the problem being solved, since the physical essence of distribution functions is described in detail in textbooks on theoretical and statistical physics, as well as in scientific articles.

Let's consider a macro-canonical assembly of classical particles with an energy of ε at pressure P and temperature T . Let us introduce a dimensionless energy.

$$x = \beta(\varepsilon - \mu), \quad (1)$$

here $\beta = 1/\theta$, $\theta = k_B T$, k_B — Boltzmann constant, chemical potential μ [5]

$$\mu = \mu_0(P, T) + \theta \ln a, \quad (2)$$

$\mu_0(P, T)$ — value of chemical potential at atmospheric pressure and room temperature, $a = \gamma x$ — activity, γ — activity coefficient, x — concentration of particles. For an ensemble consisting of identical particles, the activity is $a = 1$, for an n-component assembly of ideal elements — $\gamma = 1$.

Classical statistics. The solution of Cauchy problem [6] of kind

$$df(x)/dx = -f(x), \quad f(0) = 1 \quad (3)$$

is the function

$$f(x) = \exp(-x), \quad (4)$$

corresponding to Maxwell–Boltzmann distribution [7].

Fermions and bosons. Depending on the spin value, quantum particles are divided into fermions (half-integer spin), which obey Fermi-Dirac statistics [7,8]

$$f(x) = 1/[\exp(x) + 1], \quad (5)$$

and bosons (whole spin) with Bose–Einstein statistics [7,8]

$$f(x) = 1/[\exp(x) - 1]. \quad (6)$$

Functions (5) and (6) are solutions of the Cauchy problems (7) and (8), respectively

$$df(x)/dx = -f(x)[1 - f(x)], \quad f(0) = 0.5, \quad (7)$$

$$df(x)/dx = -f(x)[1 + f(x)], \quad \lim_{x \rightarrow 0} f(x) = \infty. \quad (8)$$

The equations (3), (7), and (8) in [4] were limited to Cauchy problem

$$A df(x)/dx = -f(x)[A + Bf(x)], \quad f(0) = A/(1 - B) \tag{9}$$

with solution

$$f(x) = A/[\exp(x) - B]. \tag{10}$$

The coefficient A determines the degeneracy of the energy level, and the parameter B is related to the spin of the particle. The classical distinguishable particles form a non-degenerate assembly ($A = 1, B = 0$) and the distribution of (10) is transformed into (4). Quantum identical particles are combined into degenerate assemblies with different spins ($A = 1, B = \pm 1$), while equality (10) passes into distributions (5) at $B = -1$ and (6) at $B = 1$ respectively. If $A = 1$ and $\exp(x)$ reach values significantly higher than B , then (10) takes the form (4).

Fractal objects. The distribution of fractal particles can be described by equation (3) with a deformed right-hand side

$$df(x)/dx = -f^q(x), \quad f(0) = 1, \tag{11}$$

where $q \neq 1$ is the „deformation“ indicator, which takes into account the influence of the geometric structure of fractal particles on their average number in an energy cell and generates a non-integer number of particles in a non-extensive system. The solution of the differential equation (11) is the function

$$f(x) = [1 + (1 - q)(-x)]^{1/(1-q)}, \tag{12}$$

the asymptotics for which at $q \rightarrow 1$ is the function (4). The function (12) defines the Tsallis distribution [9], it describes scale-invariant objects with a fractal structure of the phase space [10,11]. For the mono-fractals the indicator of „deformation“ q is associated with the fractal size D of the object by formula [3]

$$q = 1 - D, \tag{13}$$

and for multi-fractals, it is determined by the minimum α_{\min} and maximum α_{\max} Helder-Lipschitz indices (indicators of smoothness of the distribution function) [12]

$$(1 - q)^{-1} = \alpha_{\min}^{-1} - \alpha_{\max}^{-1}. \tag{14}$$

Combined distribution function. The above material allows us to obtain a combined Cauchy problem

$$A df(x)/dx = -f^q(x)[A + Bf(x)], \tag{15}$$

that is solved by the antiderivative

$$F(f(x), q, A, B) + C = A \int df(x)/\{f^q(x)[A + Bf(x)]\} = -x, \tag{16}$$

where C is the integration constant.

Let's consider private cases of distribution (16). With „deformation“ $q = 0.5$ parameter, condition $f(0) = A/(1 - B)$ and $AB > 0$, the equality (16) is expressed as [13]

$$2 \operatorname{arctg} \left[\frac{\sqrt{Bf(x)/A}}{\sqrt{AB}} \right] - 2 \operatorname{arctg} \left[\frac{\sqrt{B/(1 - B)}}{\sqrt{AB}} \right] = -x. \tag{17}$$

For parameters $A = 1, B \rightarrow +1$ the anti-derivative is equal

$$f(x) = \operatorname{tg}^2[(\pi - x)/2] = \operatorname{ctg}^2(x/2). \tag{18}$$

It can be seen from (18) that at points $x = 2\pi n, n = 0, \mp 1, \mp 2, \dots$ „condensation“ of fractal particles ($f(x) \rightarrow +\infty$) occurs, while their energy

$$\varepsilon = \mu - 2\pi n k_B T, \quad n = 0, \mp 1, \mp 2, \dots \tag{19}$$

At $AB < 0$ the solution (16) takes the form [14]

$$\ln \left| \frac{(\sqrt{A} + \sqrt{|B|}f(x))/(\sqrt{A} - \sqrt{|B|}f(x))}{\sqrt{A|B|} - \ln(\sqrt{A} + \sqrt{|B|}A/(1 + |B|))} \right| - \left| \frac{(\sqrt{A} - \sqrt{|B|}A/(1 + |B|))}{\sqrt{A|B|}} \right| = -x. \tag{20}$$

For the parameters $A = 1, B = -1$, the equality (20) takes the form

$$\ln | [1 + f(x)] / [3(1 - f(x))] | = -x$$

or

$$f(x) = [3 \exp(-x) - 1] / [3 \exp(-x) + 1] \quad 0 \leq f(x) < 1, \tag{21}$$

if $x = 0$, then $f(x) = 1/2$. The results obtained show that for $AB > 0$ fractal particles have the properties of bosons, and for $AB < 0$ — fermions.

For mono-ractal flat objects (as per (13) fractal dimension $D = 2$), parameter $q = -1$, and for three-dimensional objects (as per (13) $D = 3$) — $q = -2$. In these cases, the solutions of (16) are given by formulas [13]

$$f(x)/B - (A/B^2) \ln[A + Bf(x)] + C = -x, \tag{22}$$

$$f^2(x)/(2B) - Af(x)/B^2 + (A^2/B^3) \ln[A + Bf(x)] + C = -x \tag{23}$$

respectively. Computer calculations show the formation of a fractal assembly at a negative threshold (the internal energy of a particle is less than its chemical potential) of a dimensionless energy (1).

Thus, special cases of the combined distribution function (16) are the distributions:

$$\begin{aligned} F(f(x), 1, A, 0) &= -x \text{ — Maxwell–Boltzmann;} \\ F(f(x), 1, 1, -1) &= -x \text{ — Fermi–Dirac;} \\ F(f(x), 1, 1, 1) &= -x \text{ — Bose–Einstein;} \\ F(f(x), q, A, 0) &= -x, \quad q \neq 1 \text{ — Tsallis.} \end{aligned}$$

Conflict of interest

The author declares that he has no conflict of interest.

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