CANONICAL ENSEMBLE OF OPEN STRINGS

V.I.Alkhimov

Moscow State University of Psychology and Education, 29 Sretenka Street,
127051 Moscow, Russia
alvaliv@list.ru

Abstract

The integral equation has been received for the probability density of distance r between the ends of the string with the preset length L. This equation is invariant under the continuous group of renormalization transformations that initiated using the renormalization method to search out the required probability density asymptotic. The ensemble of such strings with any lengths is considered, and the canonical distribution probability density of distance r is established. The results presented can be used to determine the entropy of nanostructures, thereby their thermodynamics in condition monitoring is established.

Keywords: Open string, canonical ensemble, entropy.

The configuration of d-dimensional model of an individual open flexible string with non-self-crossing intersectings in Euclidean space $\mathbf{R}^d$ is characterized by two parameters: the distance r between the ends of the string and its contour length L. The probability density asymptotic $W_L(r)$ has been received in [1] for this string model, as $2 \le d < 4$, $r \to \infty$ and $L \to \infty$. Now we consider the ensemble of M string models which average length over all strings is equal to the preset value $\bar{L}$, and use the most probable distribution of strings over their lengths in the limit M→∞. Let's accept that the string length in the ensemble can have any of values $L_k = k\sigma$ $(k = 0, 1, 2, \dots)$, where admissible values of elementary length σ can be arbitrarily small. If in the ensemble m_k the strings have the length L_k $(k = 0, 1, 2, \dots)$, the set of integers $\{m_k\}$ describes any distribution of the length over strings. These numbers should satisfy the following conditions

$$\sum_{k=0}^{\infty} m_k = M, \qquad \sum_{k=0}^{\infty} m_k L_k = M \bar{L} \ , \tag{1}$$

where $(\bar{L} / \sigma)$ and M are integers. Let $W\{m_k\}$ denotes the number of various ways to distribute the lengths over the strings at which the conditions (1) are satisfied. It is obvious that

$$W\{m_k\} = \frac{M!}{m_0!\, m_1!\, m_2! \dots} \quad .$$

According to the postulate of a priori equal probabilities in this case, all distributions of the length between strings have identical probability if the conditions (1) are satisfied. Thus $\{\bar{m}_k\}$ is the set corresponding to the maximum value of $W\{m_k\}$.

As almost all possible sets $\{m_k\}$ should coincide with the set $\{\overline{m}_k\}$, the latter can be found by Darwin-Fowler method[2], calculating the average value m_k over all possible length distributions

$$\langle m_k \rangle \equiv \left[\sum_{\{m_j\}} W\{m_j\} \right]^{-1} \sum_{\{m_j\}} m_k W\{m_j\},$$

where the sum is over all sets $\{m_k\}$ satisfying (1). If in the limit $\langle m_k^2 \rangle \to \langle m_k \rangle^2$, as $M \to \infty$, then in this limit $\langle m_k \rangle \to \overline{m}_k$. It is possible to show that the last condition is fulfilled at the most probable distribution of strings over their lengths and the probability to find out the length L_k in the string ensemble is defined by the canonical distribution

$$\lim_{M\to\infty} \frac{\langle m_k \rangle}{M} \equiv \mathbf{P}(L_k) = \left[\sum_{k=0}^{\infty} \exp(-\varepsilon L_k) \right]^{-1} \exp(-\varepsilon L_k), \tag{2}$$

where the coefficient ε is derived from the equation

$$\overline{L} = \mathbf{E} L \equiv \lim_{\sigma\to 0} \sum_{k=0}^{\infty} L_k \mathbf{P}(L_k), \tag{3}$$

from which it follows that $\overline{L} = \varepsilon^{-1}$. In the paper[1], the probability density $W_L(r)$ of the distances r between the ends of a string with the contour length L is presented in the form

$$W_L(r) = \int_{C-i\infty}^{C+i\infty} \frac{dE}{2\pi i} \exp(LE)\, \psi(r,E), \tag{4}$$

where

$$\psi(r,E) = \int_{\mathbf{R}^d} \frac{d\mathbf{p}}{(2\pi)^d} \exp(i\mathbf{R}\cdot\mathbf{p})\, \varphi(p,E), \tag{5}$$

The required function $\varphi(p, E)$ under the condition

$$|\varphi(p,E)| \le \left(\lambda p^2 + \mathrm{Re}\, E\right)^{-1} \tag{6}$$

satisfies the equation

$$\varphi^{-1}(p,E) = \lambda p^2 + E - F(p,E;h;\varphi), \tag{7}$$

and

h are well-defined parameters of the string model, the functional $F(p,E;h;\varphi)$ defined by a series that is convenient to represent it in the symbolic form;

$$F(p,E;h;\varphi) = \sum_{n\ge 1} N_n (-h)^n \int \{\varphi(\mathbf{p}-\mathbf{p}', E)\}^{2n-1} \{d\mathbf{p}'\}^n,$$

and N_n formally denotes the total number of non-equivalent n order terms of the series. Using the equation (3), we average the equality (4) over the canonical distribution (2):

$$\mathbf{E}W_L(r) = \lim_{\sigma\to 0} \sum_{k=0}^{\infty} \mathbf{P}(L_k) \int_{C-i\infty}^{C+i\infty} \frac{dE}{2\pi i} \exp(EL_k)\psi(r,E).$$

Interchanging the order of summation and integration in the last equality and taking the formula $\sum_{k=0}^{\infty} \mathbf{P}(L_k)\exp(E L_k) = [\exp(\sigma\varepsilon)-1][\exp(\sigma\varepsilon) - \exp(\sigma E)]^{-1}$ into account when $\varepsilon > ReE$, we receive the following result after integration over E and the subsequent transition to the limit at $\sigma \to 0$:

$$\mathbf{E}\, W_L(r) = \varepsilon\, \psi(r,\varepsilon)\,. \tag{8}$$

Further, we define the normalized distribution

$$\overline{W}(r,\overline{L}) = \left[\int_{\mathbf{R}^d} d\mathbf{r}\; \mathbf{E}W_L(r)\right]^{-1} \mathbf{E}W_L(r)\;. \tag{9}$$

Then, from the formulas (5), (8) and (9) it follows that

$$\overline{W}(r,\overline{L}) = \varphi^{-1}(0,\varepsilon)\,\psi(r,\varepsilon)\,. \tag{10}$$

Thus, the search for the function $\overline{W}(r,\overline{L})$ is reduced to solving the nonlinear integral equation (7). This equation is very difficult, therefore it is more realistic to find the asymptotic of the function $\overline{W}(r,\overline{L})$ for large values of r and $\overline{L}$.

From the formulas (4) and (5) it follows that to describe the asymptotic behavior of this function, it is necessary to know the properties of function $\varphi(p,\varepsilon)$ for small values of p and $|\varepsilon-\varepsilon_0|$, where ε_0 is farthest to the right on the real axis of the variable ε singularity of function $\varphi(0,\varepsilon)$ defined according to (7) by the equation $\varphi^{-1}(0,\varepsilon_0)\equiv 0$. But from the last equation by the inequality (6) it follows that $\varepsilon_0 = 0$. In the paper[1], the following expression for the required function $\varphi(p,\varepsilon)$ was accepted as the initial "trial" solution to the equation (7)

$$\widetilde{\varphi}(p,\eta) = \alpha\left(\frac{\xi}{\chi}\right)^{1-\mu} K_{1-\mu}(\xi\chi), \tag{11}$$

where $\chi^2 = p^2+\eta^2$, $p_\pm = \pm i\eta$ are roots of the equation $\varphi^{-1}(p,\varepsilon) = 0$ that are closest to the origin $p=0$, where the values of ε lie in the neighborhood of the point $\varepsilon = 0$, $K_k(z)$ is Macdonald function, values of the parameters α, ξ, $\mu = \mu(d)$, $(0<\mu<1)$ are determined by the equation properties (7).

Then the corresponding expression (11) formula for $\psi(r,\eta)$ in accordance with (5) is

$$\widetilde{\psi}(r,\eta) = (2\pi)^{-d/2}\alpha\,\eta\, R^{1-2\nu} K_\nu(\eta R), \tag{12}$$

where $R^2 = r^2+\xi^2$, $\nu = \mu + s$, $s = (d-2)/2$ [3].

The relationship between values ε and η is established by the equality

$$\varepsilon = \lambda\eta^2 + F(i\eta,\varepsilon;h;\widetilde{\varphi}),$$

in which the functional $F(i\eta,\varepsilon;h;\widetilde{\varphi})$ behavior for $0 \le s < 1$ $(2 \le d < 4)$ and small values η are described by

$$F(i\eta,\varepsilon;h;\widetilde{\varphi}) = \widetilde{h}\,\eta^{2\nu} + O(\lambda\eta^2), \qquad \eta \to 0,$$

where $0 < 2\nu < 1$, $\widetilde{h} = \widetilde{\alpha}\,h$, $\widetilde{\alpha}$ is some constant that is proportional to α. Thus, for small values ε we have

$$\eta \cong \left(\varepsilon/\widetilde{h}\right)^{1/2\nu}, \qquad \varepsilon \to 0.$$

Finally, from the condition of positivity of $\overline{W}(r,\overline{L})$ it follows that

$$\mu = \frac{2}{3}(1-s), \quad \left(\mu = \frac{4-d}{3}\right), \quad \nu = \frac{s+2}{3}, \quad \left(\nu = \frac{d+2}{6}\right).$$

Thus, when $\eta \to 0$ and $0 \le s < 1$ $(2 \le d < 4)$, the functions $\widetilde{\varphi}(0,\eta)$ and $\widetilde{\psi}(0,\eta)$ are determined, $\widetilde{L} = \widetilde{h}\,\overline{L}$ is denoted, and the following result is obtained:

$$\widetilde{W}(r,\widetilde{L}) \cong \widetilde{\varphi}^{-1}(0,\eta)\,\widetilde{\psi}(r,\eta) = C_d\, R^{-\alpha}\, \widetilde{L}^{-\beta}\, K_\nu\left(R/\widetilde{L}^{\gamma}\right) \qquad (13),$$

where $C_d = 2^{(d-4)/6}\,\Gamma\left(\frac{d-1}{3}\right)\Gamma^{-1}\left(\frac{5d+4}{12}\right)$, $\quad \alpha = \frac{d-1}{3}$, $\quad \beta = \frac{2d+1}{d+2}$, $\quad \gamma = \frac{3}{d+2}$.

Hence, for the even moments of the distribution function, we obtain

$$\left\langle r^{2n}\right\rangle_{\mathbf{R}^d} = \int\limits_{\mathbf{R}^d} d\mathbf{r}\, r^{2n}\,\widetilde{W}(r,\widetilde{L}) \cong C_d^{(n)}\,\widetilde{L}^{6n/(d+2)},$$

where

$$C_d^{(n)} = 2^{2n}\,\Gamma\left(n + \frac{5d+4}{12}\right)\Gamma\left(n+\frac{d}{4}\right)\Gamma^{-1}\left(\frac{5d+4}{12}\right)\Gamma^{-1}\left(\frac{d}{4}\right).$$

$\Gamma(z)$ is Euler gamma-function. If $d = 2$, it follows that

$$\widetilde{W}(r,\widetilde{L}) \cong \begin{cases} c_2^{<}\, R^{-1}\,\widetilde{L}^{-2}, & \textit{where} \quad R << \widetilde{L}^{3/4}, \\[2ex] c_2^{>}\, R^{-5/6}\,\widetilde{L}^{-7/8}\exp\left(-R/\widetilde{L}^{3/4}\right), & \textit{where} \quad R >> \widetilde{L}^{3/4}, \end{cases}$$

and respectively $\left\langle r^{2n}\right\rangle_{\mathbf{R}^2} \cong C_2^{(n)}\,\widetilde{L}^{3n/2}$, while for $d = 3$ we have

$$\widetilde{W}(r,\widetilde{L}) \cong \begin{cases} c_3^{<}\, R^{-3/2}\,\widetilde{L}^{-2}, & \textit{where} \quad R << \widetilde{L}^{3/5}, \\[2ex] c_3^{>}\, R^{-7/6}\,\widetilde{L}^{-11/10}\exp\left(-R/\widetilde{L}^{3/5}\right), & \textit{where} \quad R >> \widetilde{L}^{3/5}, \end{cases}$$

and respectively $\left\langle r^{2n}\right\rangle_{\mathbf{R}^3} \cong C_3^{(n)}\,\widetilde{L}^{6n/5}$, where $c_2^{<}$, $c_2^{>}$ and $c_3^{<}$, $c_3^{>}$ are determinate constants.

Thus, the formula (13) describes a desired canonical ensemble distribution of d-dimensional open strings with non-self-crossing intersectings when $2 \le d < 4$. The $d = 4$ case is special and requires a separate investigation. It is necessary to notice that the value of $\overline{L}$ may depend on parameters characterizing a physical state of environment (for example, its temperature).

The result obtained can be used as a purely theoretical study of various systems as well as in technical applications. In particular, by using the formula (13), the entropy of nanostructures can be determined, thereby their thermodynamics in condition monitoring is established. This result allows to establish criterion for the strength of chain systems, depending on the physical state of their environment.

REFERENCES

1. Alkhimov V.I., “Configuration statistics of the open string d-dimensional model”, Modelling and data analysis, 2011, No 1, pp 41 -54 (in Russian).
2. Huang K., “Statistical mechanics”, John Wiley & Sons, Inc.: N.Y.–London, 1963.
3. Bateman H., Erdelyi A., “Higher transcendental functions”, Vol 2, Mc Graw-Hill Book Comp. Inc.: N.Y.–London, 1953.

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