In the Proceeding of Satellite Coll.Math.results in Stat.Mech.,Marseille, 1999.

High and Low Temperature Expansions in the Classical Statistical Mechanics of Continuouse Systems.

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Abstract: In the report two type of cluster expansions for the correlation functions of the Classical Statistical Mechanics are considered in the framework of Poisson measure integral representation of these functions. The convergence of these expansions for wide class of many-body interactions in the region of high temperatures is proved. For superstable type interactions with nonintegrable singularity at the origine a low temperature expansion in the space of configurations is constructed. As an example a new simple proof of Ruelle's superstability bounds is given.

Keywords: Cluster expansion, Poisson measure, superstable interaction,correlation functions.

1 Introduction

In the last two decades the claster expansion method has become one of the main tool in the investigation of quantum field theory and statistical mechanics models. It is impossible to enumerate all articles, which were devoted to an application of this method, but the main development started from the articles by Glimm, Jaffe and Spencer [1] for the investigating of quantum field theory models and Brydges, Federbush [2,3] for studing of screening effects in charged particle systems.

One of the main point of application of cluster expansion method was the representation of Green functions and correlation functions by Gaussian functional integrals. But the technique of the construction of cluster expansion was very complicated and the range of applicability of the method was restricted to the exponentially decreasing interactions. In 1993 a new representation for distribution functions of grand canonical ensemble by Poisson measure integrals was propoused in [4]. The main very useful property of this measure is an infinite divisible property, which gives an opportunity to simplify considerebly the construction of cluster expansion and proof of its convergence. The next advantage of this representation consists in the application of this method to many -body interaction (see [5]). And finally using this representation we can construct the cluster expansion for the correlation functions in classical statistical mechanics for super-stable systems which is converged for arbitrary values of activity $z \geq 0$ and inverse temperature $\beta \geq 0$ (see [6]).

The main goal of this talk is a short description of this method and announcing some new results, which can be obtained using Poisson measure representation.

2 Poisson measure on the configuration space

We define a configuration space $\Gamma = \Gamma_{I\!R^\nu}$ by the formula

$$\Gamma_{I\!R^\nu} = \big\{\gamma = (x_1, ..., x_n, ...), x_i \in I\!R^\nu \mid x_i \neq x_j \quad for \quad i \neq j, \quad and \quad |\gamma \cap \Lambda| < \infty \quad if \quad |\Lambda| < \infty\big\}$$

For any $\Lambda \subset I\!R^\nu$ ($|\Lambda| < \infty$) we define the configuration space Γ_Λ as a projection of $\Gamma_{I\!R^\nu}$ on Λ as

$$\Gamma_\Lambda^\beta = \bigsqcup_{n=0}^{\infty} \Gamma_{\Lambda,n}^\beta, \qquad \Gamma_{\Lambda,n}^\beta := \{\, \gamma \in \Gamma^\beta \mid |\gamma| = |\gamma \cap \Lambda| = n \,\},$$

The Poisson measure with intensity $zdx(z > 0)$ can be defined via the Laplace transformation

$$\int_\Gamma \pi_z(d\gamma) e^{<f,\gamma>} \;=\; \exp\left\{ z \int_{I\!R^\nu} (e^{f(x)} - 1) dx \right\}, \tag{2.1}$$

where

$$< f, \gamma > = \int_{I\!R^\nu} f(x)\gamma(dx) \;=\; \sum_{x\in\gamma} f(x).$$

To apply these formulas to grand canonical corrilation functions we define $\pi_z^\Lambda(d\gamma) = \pi_z(d\gamma_\Lambda)$ as a projection of the measure π_z on the configuration space Γ_Λ. Then from (2.1) we have for any $F \in L_1(\Gamma_\Lambda, \pi_z(d\gamma))$:

$$\int_{\Gamma_\Lambda} \pi_z(d\gamma_\Lambda) F[\gamma] = e^{-z|\Lambda|} \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_{\Lambda^n} (dx)_1^n F\left[\sum_{j=1}^{n} \delta_{x_j} \right], \tag{2.2}$$

where we use the following notations: $(a)_n^m = a_m, ..., a_n$ and $\delta_{x_j}(x) = \delta(x - x_j)$. From the def.(2.1) one can obtain one important property of the Poisson measure – the infinite divisible property, i.e., if we have two functions $F_1(\gamma_{X_1})$ and $F_2(\gamma_{X_2})$ and $X_1 \bigcap X_2 = \emptyset, X_1,\ X_2 \subset \Lambda$, then (see [4–6] for details):

$$\int_{\Gamma_\Lambda} \pi_z(d\gamma_\Lambda) F_1(\gamma_{X_1}) F_2(\gamma_{X_2}) \;=\; \int_{\Gamma_{X_1}} \pi_z(d\gamma_{X_1}) F_1(\gamma_{X_1}) \int_{\Gamma_{X_2}} \pi_z(d\gamma_{X_2}) F_2(\gamma_{X_2}) \tag{2.3}$$

Next, we define the Wick regularization of a product m Poisson fields by the following formula:

$$:\prod_{j=1}^{m} \gamma(x_j): \;=\; \prod_{j=1}^{m} (\gamma(x_j) - \sum_{i=1}^{j-1} \delta(x_i - x_j)). \tag{2.4}$$

To construct the integral representation for distribution functions we will also employ the following lemma:

Lemma 2.1 *For any $\Phi, F \in \mathbf{L}_2(\Gamma, \pi)$ the following formula is true:*

$$\int \pi_z(d\gamma) : \gamma(x)\Phi[\gamma] : F[\gamma] = z \int \pi_z(d\gamma) : \Phi[\gamma] : F[\gamma + \delta_x]. \tag{2.5}$$

Proof. See [7].

3 Poisson integral representation of the correlation functions.

Let us consider the system of classical identical particles contained in a certain finite volume $\Lambda \subset I\!R^\nu$ and interacting by M-particle ($M \geq 2$ and fixed) potential of general form:

$$V \equiv (V_2(x_1, x_2), \ldots, V_M(x_1, \ldots, x_M)) \tag{3.1}$$

Then the potential energy for n-particles located at points $x_1, \dots, x_n$ is:

$$U(x)_1^n = \sum_{k=2}^{M} \sum_{1 \le i_1 < \dots < i_k \le n} V_k\left(x_{i_1}, \dots, x_{i_k}\right), \tag{3.2}$$

We assume that our potential satisfy the following stability condition:

$$Exists \quad B \ge 0 : s.th. for \quad all (x)_n^1 \in \Lambda^n \quad U(x)_n^1 \ge -Bn; \tag{3.3}$$

The stability condition allows us to define correlation functions in the grand canonical ensemble as usual:

$$\rho^{\Lambda}(x)_m = Z_{\Lambda}^{-1} \sum_{n=0}^{\infty} \frac{z^{m+n}}{n!} \int_{\Lambda^n} (dx)_{m+n}^{m+1} \exp\left\{-\beta U(x)_{m+n}^1\right\} \tag{3.4}$$

where

$$Z_{\Lambda} = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_{\Lambda^n} (dx)_n^1 \exp\left\{-\beta U(x)_n^1\right\} \tag{3.5}$$

is the grand partition function, β is an inverse temperature and z is an activity. Let $\mathbf{V}$ satisfy stability condition (3.3) then using (2.2) and (2.5) (Lemma 2.1) we can write the following formula:

$$\rho^{\Lambda}(x)_m^1 = Z(\Lambda)^{-1} \int_{\Gamma_{\Lambda}} \pi_z(d\gamma_{\Lambda}) : \gamma(x_1) \dots \gamma(x_m) : e^{-\beta U[\gamma_{\Lambda}]}, \tag{3.6}$$

where

$$U[\gamma_{\Lambda}] = \sum_{p=2}^{M} \frac{1}{p!} \int_{\Lambda^p} (dy)_p^1 V_p(y_1, \dots, y_p) : \gamma(y_1) \dots \gamma(y_p) : \tag{3.7}$$

and

$$Z(\Lambda) = e^{-z|\Lambda|} Z_{\Lambda} = \int_{\Gamma_{\Lambda}} e^{-\beta U[\gamma_{\Lambda}]}. \tag{3.8}$$

4 High temperature cluster expansion.

Following Ruelle [8], let us fill $I\!R^{\nu}$ with unit cubes Δ with ribs λ,centered in $r \in Z\!\!Z^{\nu}$:

$$\Delta \equiv Q_r(\lambda) \ = \ \left\{x \in I\!R^{\nu} \mid \lambda(r^i - 1/2) \le x^i < \lambda(r^i + 1/2), i = 1, ..., \nu.\right\}, |\Delta| = \lambda^{\nu}.$$

Let $\bar{\Delta}$ the set of cubes Δ. All sets, we consider, are the union of cubes from $\bar{\Delta}$.

Just for simplicity we consider the construction of cluster expansion for two-body case (for many-body interaction see [5]). Let $X_1 = Y_1$ be a minimal union of lattice cubes Δ for which $(x)_m^1 \in X_1$ and all $Y_2, ..., Y_{n_{\Lambda}}, n_{\Lambda} = |\Lambda \setminus Y_1| + 1$ are from $\bar{\Delta}$. Then let $X_n = Y_n \cup X_{n-1}$ and we define:

$$V(X, s)_n^1 = 1/2 \sum_{1 \le j \le n} V(Y_j; Y_j) + \sum_{1 \le i < j \le n} s_i ... s_{j-1} V(Y_i; Y_j)$$

with

$$V(Y; Y') \ = \ \int_Y dx \int_{Y'} dy : \gamma(x) V(x - y) \gamma(y) : .$$

The interpolation parameters $0 \le s_i \le 1$ specify the intensity of interaction between the particles in X_i and $\Lambda \setminus X_i$. They are used for factorization of $\exp[-\beta U[\gamma_{\Lambda}]]$ in (3.6) at every step of expansion which can be obtained by applying the Newton-Leibniz formula and using the property (2.3). As a result, we get

$$\rho^{\Lambda}(x)^1_m \;=\; \sum_{1\le n\le n_\Lambda}\sum_{Y_2,\dots,Y_n} b_n(X_n) f_\Lambda(X_n), \tag{4.1}$$

$$b_n(X_n) = (-\beta)^{n-1}\int_0^1 (ds)^1_{n-1}\int_{\Gamma_{X_n}} \pi(d\gamma_\Lambda) : \gamma(x_1)\dots\gamma(x_m) :$$

$$\prod_{2\le j\le n}\sum_{k=1}^{j-1} s_k s_{k+1}\dots s_{j-2} V(Y_k; Y_j), \tag{4.2}$$

$$f_\Lambda(X_n) \;=\; \frac{Z(\Lambda\setminus X_n)}{Z(\Lambda)}.$$

In the case of two-body interaction,the convergence of the expansion (4.1) for small values of invers temperature β were proved in [4] for integrable type of interaction potentials. In the article [5] the same result were obtained for many-body interaction if M-body ($M \ge 3$) terms in the expression for interacting energy have exponential decay with the distances.

5 Low Temperature Expansions.

In this section we consider some kind of expansions, which are converged for arbitrary values of $\beta \ge 0$ and $z \ge 0$. For this purpose we consider super-stable system, i.e. the N-particle energy satisfies the following condition:

$$U(x)^1_N \;\ge\; \sum_{r\in\mathbb{Z}^\nu}(AN_r^2 - BN_r), N = \sum_{r\in\mathbb{Z}^\nu} N_r, \tag{5.1}$$

where N_r is the number of particles in an elementary cube Δ. If $A = 0, B \ge 0$, the condition (5.1) is called *stability condition*; if $A > 0, B \ge 0$, the eq.(5.1) is called *superstability condition*. But to simplify the technique we consider a slightly stronger assumptions on the interaction potential:

(A1) $\varphi(x) = \varphi_+(x) + \varphi_{st}(x) = \varphi_+(x) + \varphi^+_{st}(x) - \varphi^-_{st}(x)$,
$\varphi_+(x) \ge 0$ and $\varphi_+(0)$ is large (see (A3)),
$\varphi_{st}(x)$ satisfies the stability condition.

(A2) *diam supp* $\varphi(x) \;=\; R < \infty$.

(A3) $\frac{1}{4}b - v_1 - B \ge 0$, where $b = \inf_{|x|\le\lambda\sqrt{\nu}}\varphi_+(x)$,

$$v_1 \;=\; \lambda^{-\nu}\|\varphi^-_{st}\| \tag{5.2}$$

where $\|\cdot\|_1$ is $L_1(\mathbb{R}^\nu)$-norm and $b \sim c_\varphi\lambda^{-\mu}$ in the case when $\varphi_+(x) \sim |x|^{-\mu}$ at the origin. So if $\mu \ge \nu$ (and c_φ is large for $\mu = \nu$) the assumption (A3) is true.

It will be more conviniant for the following construction to rewrite the representation (3.6) in the following form

$$\rho^{\Lambda}(x)_m \;=\; Z_\Lambda^{-1}\int_{\Gamma_\Lambda}\pi_z(d\gamma_\Lambda)\exp\left\{-\beta U(x)_m - \beta U((x)_m;\gamma_\Lambda) - \frac{1}{2}\beta U(\gamma_\Lambda)\right\}, \tag{5.3}$$

where we again use (2.5)(Lemma 2.1).

The main idea of the construction consists in the use of the fact that if two or more particle are in one elementary cube then Gibbs factor $\exp[-\beta\varphi(x_i - x_j)] \sim \exp[-\beta b]$ and $b \to \infty$, when $\lambda \to 0$.

We call such configurations as *dense* configurations unlike so-called *dilute* configurations where at most one particle in one elementary cube is situated. The main technical idea consists in separation dilute configurations from dense configurations. To define this configurations we define indicator function for the configuration in elementary cube Δ:

$$\chi_n^{\Delta}(\gamma_\Lambda) \;=\; \chi_n^{\Delta}(\gamma_\Delta) \;=\begin{cases} 1, & \text{for } |\gamma_\Delta| = n; \\ 0, & \text{otherwise.} \end{cases}$$

Then the indicator for *dilute* configuration we define as

$$\chi_{-1}^{\Delta}(\gamma_\Delta) \;=\; \chi_0^{\Delta}(\gamma_\Delta) + \chi_1^{\Delta}(\gamma_\Delta) \tag{5.4}$$

and for *dense* configuration

$$\chi_{+1}^{\Delta}(\gamma_\Delta) \;=\; \sum_{n\geq 2} \chi_n^{\Delta}(\gamma_\Delta). \tag{5.5}$$

To obtain decomposition we use the partition of the unite in the following way

$$1 \;=\; \prod_{\Delta\in\Lambda} \left[\chi_{-1}^{\Delta}(\gamma_\Delta) + \chi_{+1}^{\Delta}(\gamma_\Delta)\right] \;=\; \sum_{\omega} \prod_{\Delta\in\Lambda} \chi_{\omega(\Delta)}^{\Delta}(\gamma_\Delta), \tag{5.6}$$

where ω is the map of every elementary cubes of Λ into the numbers $+1$ or -1, $\omega(\Delta) = \pm 1$. Inserting (5.6) into (5.3) we get

$$\rho^{\Lambda}(x)_m \;=\; \frac{z^m}{Z_\Lambda} e^{-\beta U_+(x)_m} \widetilde{\rho}^{\Lambda}(x)_m, \tag{5.7}$$

$$\begin{aligned} \widetilde{\rho}^{\Lambda}(x)_m \;=\; & \textstyle\sum_\omega \int \pi_z(d\gamma_\Lambda) \prod_{\Delta\in\Lambda} \chi_{\omega(\Delta)}^{\Delta}(\gamma_\Delta) \times \\ & \times \exp\left\{-\beta U_{st}(x)_m - \beta U((x)_m;\gamma_\Lambda) - \tfrac{1}{2}\beta U(\gamma_\Lambda)\right\} \end{aligned} \tag{5.8}$$

Now we define the set

$$X \equiv X_+ \;=\; \{\Delta \in \Lambda \mid \omega(\Delta) = +1\}$$

Then the sum over all possible ω one can rewrite as the sum over all possible sets $X \equiv X_+$ in Λ. So the eq.(5.7) is:

$$\begin{aligned} \widetilde{\rho}^{\Lambda}(x)_m \;=\; & \textstyle\sum_{\emptyset\subseteq X\subseteq\Lambda} \int \pi_z(d\gamma_\Lambda) \widetilde{\chi}_+^{X}(\gamma_X) \widetilde{\chi}_-^{X^c}(\gamma_{X^c}) \times \\ & \times \exp\left\{-\beta V_{st}(x)_m - \beta V((x)_m;\gamma_\Lambda) - \tfrac{1}{2}\beta V(\gamma_\Lambda)\right\} \end{aligned} \tag{5.9}$$

Here we use the following notation

$$\widetilde{\chi}_{\pm}^{X}(\gamma_X) \;=\; \prod_{\Delta\in X} \chi_{\pm 1}^{\Delta}(\gamma_\Delta) \tag{5.10}$$

Definition 5.1.
For any $X \equiv X_+$ define graph $G_R(X)$ with vertices in the centers of elementary cubes $\Delta \in X$ and lines $l(\Delta, \Delta')$ iff $dist(\Delta, \Delta') \leq R$.

Definition 5.2.
The set $X \equiv X_+$ is called R-connected if the correspondent graph $G_R(X)$ is connected in ordinary way.

Then every set $X \equiv X_+$ can be represented as some fixed partition $\{X\}_n^R$ (see notation 6^0.) and so the sum over all possible X in Λ we can change by all possible sets $\{X\}_n^R$ (for $n = 0, X = \emptyset$). Further we pass from the sum over all such sets to the sum over $X_1, ..., X_n$ independently and to remove the conditions $dist(X_i, X_j) > R$ we introduce *hard-cor* potential

$$\chi_R^{cor}(X)_n \;=\; \begin{cases} 0, & \text{if for any } X_i, X_j, i \neq j, \text{ dist } (X_i, X_j) \leq R, 1 \leq i, j \leq n, \\ 1, & \text{otherwise.} \end{cases}$$

Then we get

$$\begin{aligned} \widetilde{\rho}^{\Lambda}(x)_m \;=\; & \sum_{n\geq 0} \tfrac{1}{n!} \sum_{(X)_n} \chi_R^{cor}(X)_n \int \pi_z(d\gamma_\Lambda) \widetilde{\chi}_+^X(\gamma_X) \widetilde{\chi}_-^{X^c}(\gamma_{X^c}) \times \\ & \times \exp\left\{-\beta V_{st}(x)_m - \beta V((x)_m; \gamma_\Lambda) - \tfrac{1}{2}\beta V(\gamma_\Lambda)\right\} \end{aligned} \tag{5.11}$$

Now, the last step to arrange our decomposition is the following. Define the set

$$X_R^m \;=\; \{\Delta \in \Lambda \mid dist(\Delta, x_j) \leq R, j = 1, ..., m\} \tag{5.12}$$

This is fixed set (for fixed variables of correlation function $\rho_\Lambda(x)_m$). Now we split every sum over $X_j, j = 1, ..., n$ into two sums: the first sum over those X_j, which nonintersect region X_R^m and the second one (we note it by Y_l), which intersect X_R^m. There are $n!/k!(n-k)!$ possibilities when any k sets X_j nonintersect X_R^m and $(n-k)$ sets Y_l intersect X_R^m. So the final expansion is the following:

$$\begin{aligned} \widetilde{\rho}^{\Lambda}(x)_m \;=\; & \sum_{n\geq 0} \sum_{k=0}^{n} \tfrac{1}{k!(n-k)!} \sum_{(X)_k \cap X_R^m = \emptyset} \sum_{(Y)_{n-k} \cap X_R^m \neq \emptyset} \chi_R^{cor}((X)_k, (Y)_{n-k}) \times \\ & \times \int \pi_z(d\gamma_\Lambda) \widetilde{\chi}_+^X(\gamma_X) \widetilde{\chi}_-^{X^c}(\gamma_{X^c}) \times \\ & \times \exp\left\{-\beta U_{st}(x)_m - \beta U((x)_m; \gamma_\Lambda) - \tfrac{1}{2}\underline{\mathrm{U}}(\gamma_\Lambda)\right\} \end{aligned} \tag{5.13}$$

As an application of this expansion we formulate the following result, which is the new (considerebaly simpler) proof of the result by D.Ruelle [8].

Theorem 5.1 *For the classical systems, which satisfy the assumptions* (A1)–(A3) *the correlation functions are bounded from above by:*

$$\rho^{\Lambda}(x)_m \leq \xi^m e^{-\beta U_+(x)_m} \tag{5.14}$$

for any $\beta, z \geq 0$, where $\xi = \xi(\beta, z)$ and $U_+(x)_m$ is the energy, constructed by $\varphi_+(x)$.

The proof of the theorem was done in the article [6] and consisted in the estimation of Gibbs energy on an every given configuration.

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