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Poisson Measure Representation and Cluster Expansion in Classical Statistical Mechanics

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Abstract. A new representation for distribution functions of the grand canonical ensemble by the Poisson measure functional integral is obtained. Due to the ultralocal nature of the measure, the construction of the cluster expansion is very simple. For the convergence of the cluster expansion, the requirement of exponential decay of the interaction potential is not necessary.

1. Introduction

The cluster expansion method, proposed by Glimm, Jaffe, and Spencer [1] for the investigation of quantum field theory models, was greatly developed by Brydges and Federbush [2, 3] in statistical mechanics. It was especially fruitful in the classical statistical mechanics for the study of screening effects in charged particle systems [4–9]. However, the range of applicability of this method is restricted to exponentially decreasing interactions, and in addition, the technique of construction of cluster expansions is very complicated. The requirement of the exponential decay is needed to compensate the large powers of $N!$, where N is connected with the order of decomposition. These factorials appear especially due to variational derivatives over Gaussian fields (sine-Gordon variables). In turn, the variational derivatives arise on each step of decomposition in the formula of replacing the initial Gaussian measure by the new one which provides the factorization of Gaussian integrals (see [1, 4, 5, 10] for details).

In this paper, we propose a new representation for distribution functions of the grand canonical ensemble. This representation gives an opportunity to simplify considerably the construction of the cluster expansion and the proof of its convergence, and also extends the set of admissible potentials up to the class of integrable functions (or for slightly stronger condition). This representation is based on the fact that the expression which is obtained after the sine-Gordon transformation and summing up

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over the number of particles is again the characteristic functional of some Poisson process with independent values (infinitely divisible process). This allows to carry out the integration with respect to sine-Gordon variables and obtain the representation of distribution functions in terms of the ultralocal measure. Such a measure possesses the needed factorization property and enables us to get easily the cluster expansion which does not contain any derivatives over random fields. However, we should note that this construction is applicable when the total interaction potential (including short range forces) admits the approximation for which we can make the sine-Gordon transformation. This means that the initial potential can be represented as a pointwise limit of positive definite continuous functions, and then, after integration with respect to sine-Gordon variables, one can go back to the original potential. However, in this paper we consider only positive definite continuous potentials.

2. Functional Representation

Consider a system of identical particles interacting through a pair positive definite potential $V(x-y)$ with regularity condition

$$V(0) = v_0 < \infty .$$

We start from the ordinary definition of m-particle distribution functions in a finite volume box Λ for the grand canonical ensemble

$$\varrho^{\Lambda}(x)_m = Z_{\Lambda}^{-1} \sum_{n \geq m} \frac{z^n}{(n-m)!} \int\limits_{\Lambda^{n-m}} (dx)_{n\backslash m}\, e^{-\beta U(x)_n} , \tag{1}$$

where z is the fugacity of particles, Z_{Λ} is the grand partition function, and

$$U(x)_n = \sum_{1 \leq i < j \leq n} V(x_i - x_j) .$$

In (1) and below, we use the following abridged notations

$$(x)_m = (x_1, x_2, \ldots, x_m) ; \qquad (dx)_{n\backslash m} = dx_{m+1} \ldots dx_n .$$

The sine-Gordon transformation gives

$$e^{-\beta U(x)_n} = e^{1/2\beta n v_0} \int d\mu(\phi)\, e^{i\beta^{1/2} \sum\limits_{1 \leq j \leq n} \phi(x_j)} .$$

Then we directly obtain from (1) that

$$\varrho^{\Lambda}(x)_m = \tilde{z}^m Z_{\Lambda}^{-1} \int d\mu(\phi)\, e^{i\beta^{1/2} \sum\limits_{j} \phi(x_j)} \exp\left(\tilde{z} \int\limits_{\Lambda} e^{i\beta^{1/2}\phi(x)} dx \right) , \tag{2}$$

with

$$Z_{\Lambda} = \int d\mu(\phi) \exp\left(\tilde{z} \int\limits_{\Lambda} e^{i\beta^{1/2}\phi(x)} dx \right) ,$$

$$\tilde{z} = z\, e^{1/2\beta v_0} ,$$

and due to the condition $v_0 < \infty$ the Gaussian measure $d\mu(\phi)$ is defined on a measurable space of continuous functions $\phi(x)$, $x \in \Lambda$ with covariance V.

In the previous papers [4–9], Eq. (2) was the starting point for the cluster expansion. In this work, we want to carry out one more transformation which will allow to integrate over sine-Gordon variables. To do this we make the elementary renormalization and define

$$Z(\Lambda) = Z_\Lambda e^{-\tilde{z}|\Lambda|}.$$

Then

$$\varrho^\Lambda(x)_m = \tilde{z}^m Z^{-1}(\Lambda) \int d\mu(\phi) e^{i\beta^{1/2}\sum\limits_j \phi(x_j)} \exp\left[\tilde{z} \int\limits_\Lambda (e^{i\beta^{1/2}\phi(x)} - 1)dx\right]. \tag{3}$$

Now, one can easily find that the exponent in (3) is a characteristic functional of some generalized Poisson-type process with independent values at every point $x \in \Lambda$ [11, Chap. III], and by the Minlos theorem [11, Chap. IV], there exists a positive countably additive measure $dP(q)$ defined on the σ-algebra generated by cylindrical sets of $\mathscr{S}'(\mathbb{R}^3)$ such that

$$\exp\left[\tilde{z} \int\limits_\Lambda (e^{if(x)} - 1)dx\right] = \int\limits_{\mathscr{S}'} dP(q) e^{i\int\limits_\Lambda f(x)q(x)dx}. \tag{4}$$

We substitute (4) into the right-hand side of (3) and interchange integrals to obtain

$$\varrho^\Lambda(x)_m = z^m e^{-\beta U(x)_m} \tilde{\varrho}^\Lambda(x)_m, \tag{5}$$

$$\begin{aligned}\tilde{\varrho}^\Lambda(x)_m = Z^{-1}(\Lambda) \int dP(q) e^{-\beta\sum\limits_{1\le j\le m}\int\limits_\Lambda dx V(x_j - x)q(x)} \\ \times \exp\left[-\frac{\beta}{2}\int\limits_\Lambda\int\limits_\Lambda dx\,dy\, q(x)V(x-y)q(y)\right],\end{aligned} \tag{6}$$

$$Z^{-1}(\Lambda) = \int dP(q) \exp\left[-\frac{\beta}{2}\int\limits_\Lambda\int\limits_\Lambda dx\,dy\, q(x)V(x-y)q(y)\right]. \tag{7}$$

In fact, Eqs. (5)–(7) are the integral representation for the Poisson measure (1) which defines the initial Gibbs distribution. The ultralocal nature of the measure $dP(q)$ makes it possible to simplify the construction of a cluster expansion and proceed to $\Lambda \nearrow \mathbb{R}^3$ limit.

To conclude this section, we note that the transformations like (4) were used in [12] for construction of generalized random fields which satisfy Osterwalder-Schrader axioms.

3. Cluster Expansion

We fill $\mathbb{R}^3$ with a set of disjoint lattice unit cubes. All the subsets in $\mathbb{R}^3$ are given as a union of unit lattice cubes. Let $X_0 \equiv (x_1, \ldots, x_m)$ be some fixed variables of distribution functions $\tilde{\varrho}^{\Lambda}_{m}$, and let $X_1 = Y_1$ be a minimal union of lattice cubes which cover X_0. Let $Y_2, \ldots, Y_{n_\Lambda}$, $n_\Lambda = |\Lambda \backslash Y_1| + 1$ be disjoint unit cubes for which

$$\bigcup_{1 \le j \le n_\Lambda} Y_j = \Lambda .$$

The set $Y_1 = X_1$ is fixed, but the cubes Y_j, $j = 2, \ldots, n_\Lambda$ are the variables of corresponding series and can change their positions. We now define the sequence of these sets (see [4])

$$X_n = Y_n \cup X_{n-1}, \qquad X_{n_\Lambda} = \Lambda, \qquad X_n^c = \Lambda \backslash X_n .$$

To simplify the notation, we define

$$V_0(X) = V_0(X; q) = \sum_{1 \le j \le m} \int_X dx\, V(x_j - x) q(x), \tag{8}$$

$$V(X'; X'') = V(X'; X''; q) = \int_{X'} dx \int_{X''} dy\, q(x) V(x - y) q(y) \tag{9}$$

and, in addition, $Z(X)$ is the same expression as in (7) but with X instead of Λ. Then we have for Eq. (6) in the notations (8)–(9),

$$\tilde{\varrho}^{\Lambda}(x)_m = Z^{-1}(\Lambda) \int dP(q)\, e^{-\beta V_0(\Lambda) - 1/2 \beta V(\Lambda; \Lambda)} . \tag{10}$$

Now, let us introduce the sequences

$$V_0(X_n; (s)_{n-1}) = \sum_{1 \le j \le n} s_1 \ldots s_{j-1} V_0(Y_j), \tag{11}$$

$$V(X_n; (s)_{n-1}) = \frac{1}{2} \sum_{1 \le j \le n} V(Y_j; Y_j) + \sum_{1 \le i < j \le n} s_i \ldots s_{j-1} V(Y_i; Y_j) . \tag{12}$$

The interpolation parameters $1 \le s_i \le n - 1$ specify the intensity of interaction between the particles in X_i and in X_i^c. Equation (12) corresponds to the sequence of covariances of the sine-Gordon measure in [4]. In our case, it is used for the factorization of $\exp\left[-\frac{1}{2}\beta V(\Lambda; \Lambda)\right]$ in (19) at every step of the expansion and can be obtained by applying the Newton-Leibniz formula. We now use the property of dP:

$$\int dP\, F'_X(q) F''_{X^c}(q) = \int dP\, F'_X(q) \int dP\, F''_{X^c}(q), \tag{13}$$

where $F'_X(q)$ depends on fields $q(x)$ localized in X, and $F''_{X^c}(q)$ depends on fields $q(x)$ localized in X^c. As a result, we obtain the cluster expansion

$$\tilde{\varrho}^{\Lambda}(x)_m = \sum_{1 \le n \le n_\Lambda} \sum_{Y_2, \ldots, Y_n \subset \Lambda} b_n(X_n) F_\Lambda(X_n), \tag{14}$$

$$\begin{aligned} b_n(X_n) = (-\beta)^{n-1} \int_0^1 (ds)_{n-1} \int dP(q) \prod_{2 \le j \le n} &[s_1 \ldots s_{j-2} V_0(Y_j) \\ &+ s_1 \ldots s_{j-2} V(Y_1; Y_j) + s_2 \ldots s_{j-2} V(Y_2; Y_j) \\ &+ \ldots + s_{j-2} V(Y_{j-2}; Y_j) + V(Y_{j-1}; Y_j)] \\ &\times \exp(-\beta V_0(X_n; (s)_{n-1}) - \beta V(X_n; (s)_{n-1})), \end{aligned} \tag{15}$$

$$f_\Lambda(X_n) = \frac{Z(X_n^c)}{Z(\Lambda)} . \tag{16}$$

To obtain an ordinary tree-graph representation, we define

$$V_{1,j}(q) = V_0(Y_j) + V(Y_1; Y_j) , \tag{17}$$
$$V(Y_i; Y_j) = V_{i,j}(q) , \quad i > 1 . \tag{18}$$

Then we get for

$$b_n(X_n) = (-\beta)^{n-1} \sum_\eta \int_0^1 (ds)_{n-1} f_\eta(s)_{n-2} \int dP(q) \prod_{2\le j\le n} V_{\eta(j),j}(q) \times \exp(-\beta V_0(X_n; (s)_{n-1}) - \beta V(X_n; (s)_{n-1})) . \tag{19}$$

Recall that (see [3, 4, 10] for details)

$$f_\eta(s)_{n-2} = \prod_{2\le j\le n} s_{\eta(j)} \cdots s_{j-2} .$$

4. Thermodynamic Limit $\Lambda \nearrow \mathbb{R}$. Proof of Convergence

The main result of this section is formulated by the following

Theorem. *Let the interaction potential satisfy the following requirement*

$$\mathfrak{v} = \max_{Y'} \sum_{Y\subset\mathbb{R}^3} \tilde{V}_{Y',Y} < \infty ,$$
$$\tilde{V}_{Y',Y} = \max_{x\in Y'} \left(\int_Y dy |V(x-y)|^2 \right)^{1/2} , \tag{20}$$

where Y and Y' are unit lattice cubes in $\mathbb{R}^3$. Then there exists the constant $C(m, \beta, z)$ independent of Λ such that for sufficiently small β which satisfies the condition

$$64 C \beta \mathfrak{v} < 1 ;$$

the infinite volume limit $\tilde{\varrho}(x)_m$ exists for $\tilde{\varrho}^\Lambda(x)_m$ and can be represented by the series (14) *with $\Lambda = \mathbb{R}^3$, $n_\Lambda = \infty$, and $f(X_n) = \lim f_\Lambda(X_n)$ instead of $f_\Lambda(X_n)$.*

The Proof of the Theorem. We start from the estimation of $b_n(X_n)$. To estimate $b_n(X_n)$, we apply the Schwarz inequality to the integral with respect to $dP(q)$ in (19):

$$|b_n(X_n)| \le \beta^{n-1} \sum_\eta \int_0^1 (ds)_{n-1} f_\eta(s)_{n-2} \left(\int dP \prod_{2\le j\le n} V_{\eta(j),j}^2(q) \right)^{1/2} \times (\textstyle\int dP \exp[-2\beta V_0(X_n; (s)_{n-1}) - 2\beta V(X_n; (s)_{n-1})])^{1/2} .$$

The following two lemmas yield the final estimation.

Lemma 1.

$$\left(\int dP(q) \prod_{2\le j\le n} V^2_{\eta(j),j}(q)\right)^{1/2} \le (16\cdot z_0)^n \prod_{1\le k\le n-1} d_\eta(k)! \prod_{2\le j\le n} \tilde{V}_{Y_{\eta(j)},Y_j}\,, \quad (21)$$

where $\tilde{V}_{Y_1,Y_2}$ is defined in (20), *and $d_\eta(k)$ is the number of vertices j in the "tree" η for which $\eta(j) = k$ (see* [13] *for details), and* $z_0 = \max(\tilde{z}, 1)$.

Proof. First of all, in (4) we set

$$f(x) = \sum_{1\le j\le N} \alpha_j f_j(x)\,, \qquad \operatorname{supp} f_j \subset Y\,, \qquad j = 1, \ldots, N$$

and define

$$q(f_j) = \int_Y q(x) f_j(x)\, dx$$

and

$$\hat{f}_{i_1,\ldots,i_m} = \int_Y dx\, f_{i_1}(x)\ldots f_{i_m}(x)\,. \quad (22)$$

Differentiating now (4) with respect to $\alpha_1, \ldots, \alpha_N$ and putting $\alpha_1 = \ldots = \alpha_N = 0$, we obtain the following formula for moments of the measure

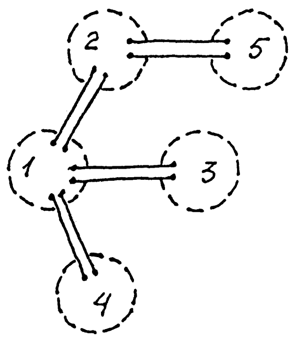
$$\begin{aligned}
&\int dP(q) q(f_1)\ldots q(f_N)\\
&\quad = \sum_{1\le l\le N_*} \sum_{\substack{m_1\nu_1+\ldots+m_l\nu_l=N\\ m_1<\ldots<m_l}} \tilde{z}^{\nu_1+\ldots+\nu_l} \sum_{\text{perm.}}\\
&\quad \times \hat{f}_{i_1^{(1)},\ldots,i_{m_1}^{(1)}} \cdots \hat{f}_{i_1^{(\nu_1)},\ldots,i_{m_1}^{(\nu_1)}} \cdots \hat{f}_{j_1^{(1)},\ldots,j_{m_l}^{(1)}} \cdots \hat{f}_{j_1^{(\nu_l)},\ldots,j_{m_l}^{(\nu_l)}}\,;\\
&\quad N_* = [1/2((8N+1)^{1/2}-1)]\,, \qquad i_1^{(1)}, \ldots, j_{m_l}^{(\nu_l)} \in (1, \ldots, N)\,, \qquad (23)
\end{aligned}$$

where $[x]$ is the integral part of x.

The number of terms on the right-hand side of (23) is

$$K_N = \frac{d^N}{dx^N}\left(e^{e^x-1}\right)\big|_{x=0} = \frac{1}{e}\sum_{k\ge 1}\frac{k^N}{k!} \le N!\,. \quad (24)$$

To use (23), let us integrate the product on the left-hand side of (21). We explain this more explicitly. The product on the left-hand side of (21) is the contribution of the tree-graph η (see the figure) in which each double line corresponds to the expression $V^2_{\eta(j),j}(q)$, where $V_{\eta(j),j}(q)$ is defined by (17)–(18) and (8)–(9). For example, the graph $\eta : \eta(2) = \eta(3) = \eta(4) = 1$; $\eta(5) = 2$ can be drawn as follows



Note here that for this graph we have

$$d_\eta(1) = 3\,, \qquad d_\eta(2) = 1\,, \qquad d_\eta(3) = d_\eta(4) = d_\eta(5) = 0\,.$$

In every k^{th} circle $2d_\eta(k) + 2$ fields (for $k = 1, 2d_\eta(1)$), are located which are integrated with the potential $V(x - \cdot)$ over the cube Y_k. According to the condition (13), the integral on the left-hand side of (21) factorizes into a product of n integrals. If we now introduce "sewing" m points $x_{i_1}, \ldots, x_{i_m}$, which are in the same circle by the formula (22) [analytically, this means that we insert the product of δ-functions $\delta(x_{i_1} - x_{i_2})\delta(x_{i_2} - x_{i_3} \ldots \delta(x_{i_{m-1}} - x_{i_m})$ into $(2d_\eta(k)+2)$-multiple integral], then we obtain, according to (23), after integration with respect to $dP(q)$ the sum of graphs with all kinds of "sewing" in every circle. The number of such graphs, according to (24), is less than

$$\prod_{1\le k\le n-1} [2d_\eta(k) + 2]!\,.$$

We should note here that for $k = 1$ in the points which correspond to the variables $x_1, \ldots, x_m$ of the function $\tilde{\varrho}_m$, there are no variables q as well as the integration with respect to them; therefore, theses points cannot be "sewed."

Now we bound the contributions of all these graphs by the right-hand side of (21) if we take into account the definition (20) of $\tilde{V}_{Y,Y'}$ and the following expression:

$$([2d_\eta(k) + 2]!)^{1/2} \le 4^{d_\eta(k)+1} d_\eta(k)!$$

and

$$\sum_{1\le k\le n-1} d_\eta(k) = n - 1\,.$$

Lemma 2.

$$\begin{gathered} I_V = (\textstyle\int dP(q) \exp[-2\beta V_0(X_n; (s)_{n-1}) - 2\beta V(X_n; (s)_{n-1})]^{1/2} \le C_m\,, \\ C_m = \exp\left[\tfrac{1}{2}\, m\tilde{z}c(2\beta)\, e^{mv_0}\right], \qquad c(\beta) = \int\limits_{\mathbb{R}^3} |e^{-\beta V(x)} - 1|\, dx\,, \end{gathered} \tag{25}$$

where m is the number of variables of $\varrho^\Lambda(x)_m$.

Proof. Recall that $V_0(X_n;(s)_{n-1})$ and $V(X_n;(s)_{n-1})$ are convex combinations of "diagonalized" terms (see the proof of Lemma 9.8 in [5])

$$V_0(X_n;(s)_{n-1}) = \sum_j \lambda_j V_0(Z_j)\,,$$
$$V(X_n;(s)_{n-1}) = \sum_j \lambda_j V(Z_j';Z_j')\,, \tag{26}$$
$$\sum_j \lambda_j = 1\,,$$

where λ_j is a product of parameters s_k and $(1-s_l)$, and $\bigcup_j Z_j = X_n$, $\bigcup_j Z_j' = X_n$. Now, we apply Hölder's inequality to obtain the upper bound

$$I_V \le \prod_j \left(\int dP(q)\exp[-2\beta V_0(Z_j) - 2\beta V(Z_j', Z_j')]\right)^{\lambda_j/2}.$$

The positive definiteness of $V(x-y)$ implies

$$\exp[-2\beta V(Z_j', Z_j')] \le 1\,.$$

Using (4) with

$$f(x) = i\cdot 2\beta \sum_{1\le j\le m} V(x_j - x)\,,$$

we obtain

$$\int dP(q)\, e^{-2\beta V_0(Z_j)} = \exp\left[z \int_{Z_j} \left(e^{-2\beta \sum\limits_{1\le i\le m} V(x_i - x)} - 1\right) dx \right]. \tag{27}$$

The estimation of (27) gives (25) if we take into account (26). This proves Lemma 2.

Now, to prove the convergence of (14) as $\Lambda \nearrow \mathbb{R}^3$ we use the Battle-Federbush estimate [13]

$$\sum_\eta \int_0^1 (ds)_{n-1} f_\eta (s)_{n-2} \prod_{1\le k\le n-1} d_\eta(k)! \le 4^n$$

and the well-known method of Kirkwood-Salsburg type equation for the function $f_\Lambda(X_n)$ on the sets of Λ. This gives the existence of the limit for the sequence (16) (see [5, 6, 10]):

$$\lim_{\Lambda\nearrow\mathbb{R}^3} f_\Lambda(X_n) = f(X_n)$$

and the following estimate

$$|f_\Lambda(X_n)| \le e^{c\cdot n}\,,$$

with some c independent of Λ. Now the proof of the theorem follows from these lemmas with $C(m,z,\beta) = C_m z_m e^c$.

5. Concluding Remarks

We want to stress that the representation (5)–(7) turns out to be very useful for the construction of cluster expansions in spite of the fact that the considered systems can be investigated by traditional methods [14, 15]. But we expect that this representation can be useful for studying more complicated models and various phenomena.

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