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On lattice oscillator equilibrium equation with positive infinite-range many-body potentials

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The symmetrized lattice Kirkwood-Salsburg (KS) equation for the Gibbs grand canonical correlation functions of the lattice oscillators, interacting via positive infinite-range manybody potentials, is solved. The symmetrization is based on the superstability condition for the potentials.

Key words: *lattice oscillators, Gibbs grand canonical ensemble, superstability, Kirkwood-Salsburg equation*

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We consider Gibbsian (equilibrium) systems of oscillators, whose one-dimensional coordinates $q_x \in \mathbb{R}$ are indexed by sites x of the hyper-cubic lattice $\mathbb{Z}^d$ with the potential energy (see also [1])

$$U_{\rm c}(q_\Lambda) = \sum_{x\in\Lambda} u(q_x) + U(q_\Lambda), \qquad U(q_\Lambda) = \sum_{|X|>1, X\subseteq\Lambda} \phi_X(q_X),$$

where the summation is performed over the one-point sets and sets with greater then 1 number of sites in the first and second sums, respectively, $q_X = (q_x, x \in X \subseteq \Lambda)$, u is an external potential, ϕ_X is a $|X|$-body positive interaction potential, $\Lambda \subset \mathbb{Z}^d$ and the number of sites in Λ is finite, that is $|\Lambda| < \infty$. States of these systems are described in the thermodynamic limit by the sequence ρ of grand canonical correlation functions $\rho = \{\rho(q_X), X \subset \mathbb{Z}^d, 1 \leqslant |X| < \infty\}$ satisfying the lattice oscillator Kirkwood-Salsburg (KS) equation (we derive it in the Appendix)

$$\rho = zK\rho + z\alpha,$$

where z is the activity(a thermodynamic parameter), $\alpha(q_X) = \delta_{|X|,1} = 0, |X| \neq 1, \delta_{|X|,1} = 1, |X| = 1$. The linear KS operator K is defined on sequences of measurable functions $F = \{F(q_X), X \subset \mathbb{Z}^d, 1 \leqslant |X| < \infty\}$as follows

$$(KF)(q_X) = \sum_{Y\subseteq X^{\rm c}} \int K(q_x|q_{X\backslash x}; q_Y)\left[F(q_{X\backslash x\cup Y}) - \int \nu({\rm d}q_x) F(q_{X\cup Y})\right]\nu({\rm d}q_Y), \quad 1 < |X| < \infty,$$

where the integrations are performed over $\mathbb{R}$ and $\mathbb{R}^{|Y|}$ in the integral within the square brackets and the other, respectively,

$$\nu({\rm d}q_Y) = \prod_{y\in Y} \nu({\rm d}q_y), \qquad \nu({\rm d}q) = {\rm e}^{-\beta u(q)}\left(\int {\rm e}^{-\beta u(q)}{\rm d}q\right)^{-1}{\rm d}q, \qquad X^{\rm c} = \mathbb{Z}^d\backslash X,$$

and $\beta > 0$ is the inverse temperature. If $X = x$, then the first term in the square bracket is missing. The KS kernels are defined as follows

$$K(q_x|q_{X\backslash x}; q_Y) = {\rm e}^{-\beta W(q_x|q_{X\backslash x})} \sum_{n=1}^{|Y|} \sum_{\cup Y_j = Y, Y_j\neq\emptyset} \prod_{j=1}^{n}\left({\rm e}^{-\beta W(q_X; q_{Y_j}|x)} - 1\right) = {\rm e}^{-\beta W(q_x|q_{X\backslash x})} K_x(q_X; q_Y),$$

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$$W(q_x|q_Y) = U(q_x, q_Y) - U(q_Y) \geqslant 0, \qquad W(q_X; q_Y|x) = \sum_{x\in Z\subseteq X} u_{Z\cup Y}(q_{Z\cup Y}).$$

Where the summation in the expression for the KS kernel is performed over n subsets whose union is Y. We will also demand that the superstability condition [2] for positive potentials should hold

$$u_Y(q_Y) \leqslant J_Y \sum_{y\in Y} v(q_y), \qquad N_0 = \int \mathrm{e}^{\beta\gamma v(q)}\nu(\mathrm{d}q) < \infty, \qquad \gamma > 0,$$

$||J||_1 = \max_x \sum_{Y, x\in Y} J_Y < \infty$ and the summation is performed over subsets of $\mathbb{Z}^d$ containing a site x.

Usually the considered systems are described by canonical correlation functions [3, 4] which are determined in the high-temperature regime by convergent cluster expansions. One hopes to show that they satisfy the KS equation by analogy with correlation functions of particle systems [5]. It is well known that the canonical ensemble correlation functions generate vacuum averages in the lattice boson Euclidean quantum field theory for the case of the nearest neighbor bilinear pair potential [6, 7].

The KS equation for an integer valued spin Ising model with a pair potential, whose solutions describe vacuum field averages in the two-dimensional lattice Higgs-Villain model, appeared earlier in [8]. The case of unbounded spins (oscillator variables sometimes are treated as unbounded continuous spins) is more complicated than the case of bounded spins or lattice gas and the results concerning solutions of the KS operator for the latter, exposed in [9], cannot be easily generalized to unbounded spins either for infinite-range manybody or non-positive potentials (this conclusion follows from [8]).

In [1] we considered the case of finite-range positive manybody potentials and super-stable pair potentials with a different representation of the KS kernels and showed that for positive pair potentials the KS equation is easily solved. For a non-positive pair potential we proposed to symmetrize the KS operator (with respect to the super-stability condition) and established that the symmetrized KS equation (the KS equation with the symmetrized KS operator) can be solved proving that the symmetrized KS operator is bounded in a natural Banach space $\mathbb{E}_{f,\xi}$ which will be used by us in this paper. But our method failed for infinite-range manybody potentials. Starting with the above representation for the KS kernels we are able to derive in this paper the basic bound

$$\bar{K}_x(q_X) \leqslant \exp\left\{\xi\beta(c_1 + c_2 v(q_x) + W'(x|q_X))\right\}, \tag{1}$$

where c_1, c_2 do not depend on oscillator variables and lattice sites and

$$\begin{aligned}
\bar{K}_x(q_X) &= \sum_{Y\subseteq X^{\mathrm{c}}} \xi^{|Y|} \int |K(q_x|q_{X\backslash x}; q_Y)|\nu'(\mathrm{d}q_Y), \qquad \nu'(\mathrm{d}q_Y) = \exp\left\{\sum_{x\in Y} f(q_x)\right\}\nu(\mathrm{d}q_Y),\\
W'(x|q_X) &= \sum_{y\in X\backslash x} v(q_y) \sum_{Y\subseteq(x\cup y)^{\mathrm{c}}} J_{x\cup y\cup Y}(1+N_0)^{|Y|}.
\end{aligned}$$

Note that positivity of W permits to substitute $K_x(q_X; q_Y)$ into the expression for the kernel $\bar{K}_x(q_X)$ instead of $K_x(q_X; q_Y)$. W' satisfies the following remarkable inequality

$$\begin{aligned}
\sum_{x\in X} W'(x|q_X) &= \sum_{x\in X} v(q_x) \sum_{y\in X\backslash x} \sum_{Y\subseteq(x\cup y)^{\mathrm{c}}} J_{y\cup x\cup Y}(1+N_0)^{|Y|}\\
&\leqslant \sum_{x\in X} v(q_x) \sum_{y\in(x)^{\mathrm{c}}} \sum_{Y\subseteq(x\cup y)^{\mathrm{c}}} J_{y\cup x\cup Y}(1+N_0)^{|Y|} \leqslant |J|_1 \sum_{x\in X} v(q_x),
\end{aligned} \tag{2}$$

where

$$|J|_l = \max_x |J|_l(x), \qquad |J|_l(x) = \sum_{Z\subseteq(x)^{\mathrm{c}}} J_{x\cup Z}(1+N_0)^{|Z|}(|Z|+1)^{l-1}, \qquad l \geqslant 1.$$

The basic bound (1) permits to symmetrize the KS operator and prove that the symmetrized operator is bounded in the Banach space $\mathbb{E}_{f,\xi}$ which is the linear space of sequences $F = \{F_X(q_X), X \subset \mathbb{Z}^d, 1 \leqslant |X| < \infty\}$ of measurable functions with the norm

$$||F||_{f,\xi} = \max_X \xi^{-|X|} ess \sup_{q_X} \exp\left\{-\sum_{x\in X} f(q_x)\right\} |F_X(q_X)|, \qquad f(q) = \gamma\beta v(q).$$

Let $\chi_x(q_X)$ be the characteristic(indication) function of the set D_x where the inequality

$$W'(x|q_X) \leqslant |J|_1 v(q_x) \tag{2'}$$

holds. Then (2) implies that $\cup_{x\in X} D_x = \mathbb{R}^{|X|}$ or

$$\sum_{x\in X} \chi_x(q_X) \geqslant 1$$

since D_x may intersect for different x. It is more convenient to deal with χ_x^*

$$\chi_x^*(q_X) = \left(\sum_{y\in X} \chi_y(q_X)\right)^{-1} \chi_x(q_X), \qquad \sum_{x\in X} \chi_x^*(q_X) = 1. \tag{3}$$

The symmetrized KS operator $\tilde{K}$ is given by

$$(\tilde{K}F)(q_X) = \sum_{x\in X} \chi_x^*(q_X) \sum_{Z\subseteq X^c} \int K(q_x|_{X\backslash x}; q_Z) \left[F(q_{X\backslash x\cup Z}) - \int \nu(\mathrm{d}q_x) F(q_{X\cup Z})\right] \nu(\mathrm{d}q_Z),$$

where for $X = x$ the first term in the square bracket corresponding to $Z = \emptyset$ is equal to zero. The symmetrized KS equation

$$\rho = z\tilde{K}\rho + z\alpha \tag{4}$$

is derived after multiplying both sides of the KS equation by the characteristic function $\chi_x^*(q_X)$ and applying (3). Our main result is formulated in the following theorem.

Theorem. *Let $\gamma \geqslant 2\xi|J|_1$, $G(\xi) = \xi N_0'|J|_2$, where $N_0' = N_0^{-1} \int v(q)\nu'(\mathrm{d}q)$. Then the norm of the symmetrized KS operator in the Banach space $\mathbb{E}_{f,\xi}$ satisfies the following bound $||\tilde{K}||_{f,\xi} \leqslant (\xi^{-1} + N_0)\mathrm{e}^{\beta G(\xi)}$ and the vector ρ from the space $\mathbb{E}_{f,\xi}$*

$$\rho = \sum_{n\geqslant 0} z^{n+1} \tilde{K}^n \alpha$$

determines the unique solution of the symmetrized KS equations in $\mathbb{E}_{f,\xi}$ if $|z| < ||\tilde{K}||_{f,\xi}^{-1}$.

Proof. If the basic bound (1) holds then the proof is almost trivial since for the norm of the KS operator we have the following inequality

$$||\tilde{K}||_{\xi,f} \leqslant (\xi^{-1} + N_0) \max_X ess \sup_{q_X} \bar{K}(q_X|f), \qquad \bar{K}(q_X|f) = \sum_{x\in X} \chi_x^*(q_X) \mathrm{e}^{-f(q_x)} \bar{K}_x(q_X).$$

As a result of (2′) and (3) one obtains for $\gamma \geqslant \xi(c_2 + |J|_1)$

$$\bar{K}(q_X|f) \leqslant \mathrm{e}^{c_1\xi\beta} ess \sup_q \exp\{-\gamma\beta v(q) + \beta\xi(c_2 + |J|_1)v(q)\} = \mathrm{e}^{c_1\xi\beta}.$$

The most simple choice is $\xi = (\beta c_1)^{-1}$. The theorem will be proved if we prove the basic bound (1) and show that $c_1 = N_0'|J|_2$, $c_2 = |J|_1$.

Proof of the basic bound (1). We have the following inequalities which are analogues of the inequalities for the KS kernels for the lattice gas systems from [9]

$$
\begin{aligned}
\bar{K}_x(q_X) &\leqslant \sum_{Y\subseteq X^{\mathrm{c}}} \xi^{|Y|} \sum_{l=1}^{|Y|} \sum_{\cup Y_j = Y} \prod_{j=1}^{l} \int |\mathrm{e}^{-\beta W(q_X; q_{Y_j}|x)} - 1| \nu'(\mathrm{d}q_{Y_j}) \\
&= \sum_{n\geqslant 0} \xi^n \sum_{|Y|=n, Y\subseteq X^{\mathrm{c}}} \sum_{l=1}^{n} \sum_{\cup Y_j = Y} \prod_{j=1}^{l} \int |\mathrm{e}^{-\beta W(q_X; q_{Y_j}|x)} - 1| \nu'(\mathrm{d}q_{Y_j}) \\
&\leqslant \sum_{n\geqslant 0} \frac{\xi^n}{n!} \left[\sum_{Y\subseteq X^{\mathrm{c}}} \int |\mathrm{e}^{-\beta W(q_X; q_Y|x)} - 1| \nu'(\mathrm{d}q_Y) \right]^n \\
&= \exp\left\{ \xi \sum_{Y\subseteq X^{\mathrm{c}}} \int |\mathrm{e}^{-\beta W(q_X; q_Y|x)} - 1| \nu'(\mathrm{d}q_Y) \right\}.
\end{aligned}
$$

Hence, for positive potentials $u_Y \geqslant 0$ one derives the following estimate

$$
\bar{K}_x(q_X) \leqslant \exp\left\{ \xi\beta \sum_{Y\subseteq X^{\mathrm{c}}} \int |W(q_X; q_Y|x)| \nu'(\mathrm{d}q_Y) \right\}. \tag{5}
$$

Moreover,

$$
\begin{aligned}
|W(q_X; q_Y|x)| &\leqslant \sum_{x\in Z\subseteq X} |u_{Z\cup Y}(q_{Z\cup Y})| \leqslant \sum_{x\in Z\subseteq X} J_{Z\cup Y} \sum_{y\subseteq Z\cup Y} v(q_y) \\
&= \sum_{x\in Z\subseteq X} J_{Z\cup Y} \left[\sum_{y\in Y} v(q_y) + \sum_{y\in Z\backslash x} v(q_y) + v(q_x) \right].
\end{aligned}
$$

Then the last inequality yields

$$
\int |W(q_X; q_Y|x)| \nu'(\mathrm{d}q_Y) \leqslant N_0^{|Y|} \sum_{Z\subseteq X\backslash x} J_{x\cup Z\cup Y} \left[N_0'|Y| + \sum_{y\in Z\backslash x} v(q_y) + v(q_x) \right]
$$

$$
= N_0^{|Y|} \sum_{Z\subseteq X\backslash x} J_{x\cup Z\cup Y} \left[N_0'|Y| + v(q_x) \right] + N_0^{|Y|} \sum_{y\in X\backslash x} v(q_y) \sum_{Z\subseteq X\backslash(x\cup y)} J_{y\cup x\cup Z\cup Y}.
$$

Here we utilized the equality

$$
\sum_{Y\subseteq\Lambda} \sum_{y\in Y} F(Y; y) = \sum_{y\in\Lambda\backslash X} \sum_{Y\subseteq\Lambda\backslash y} F(Y\cup y; y).
$$

As a result

$$
\sum_{Y\subseteq X^{\mathrm{c}}} \int |W(q_X; q_Y|x)| \nu'(\mathrm{d}q_Y) \leqslant N_0'|J|_2 + |J|_1 v(q_x) + W'(x|q_X).
$$

The last inequality and (5) prove the basic bound. The theorem is proven.

The analogue of the theorem can be easily proven for the quantum lattice oscillator KS equation generalizing the result of [10] where only finite-range manybody potentials (special non-positive) were considered. The theorem can be also easily generalized to the classical case of special non-positive infinite-range manybody potentials from [10].

1. Appendix

To derive the KS equation one has to start from the following expression for the grand canonical correlation functions in a compact set Λ

$$\rho^{\Lambda}(q_X)=\chi_{\Lambda}(X)\Xi_{\Lambda}^{-1}\sum_{Y\subseteq\Lambda\backslash X} z^{|Y\cup X|}\int\nu(\mathrm{d}q_Y)\mathrm{e}^{-\beta U(q_{X\cup Y})},$$

where χ_{Λ} is the characteristic function of Λ, the grand partition function Ξ_{Λ} coincides with the numerator of the right-hand side of the empty set X. The usual Gibbs correlation functions are derived by multiplying the righthand side of the last equality by the $\exp\{-\beta\sum_{x\in\Lambda}u(q_x)\}(\int\mathrm{e}^{-\beta u(q)}\mathrm{d}q)^{-|X|}$ and renormalizing the activity by the multiplier $\int\mathrm{e}^{-\beta u(q)}\mathrm{d}q$. We have the equality

$$U(q_{X\cup Y})=U(q_{X\cup Y\backslash x})+W(q_x|q_{X\backslash x\cup Y}). \tag{6}$$

In order to derive the finite-volume KS equation one has to represent the exponent of $-\beta W(q_x|q_{X\backslash x\cup Y})$ in terms of the KS kernels. Let

$$\tilde{W}(q_X;q_Y|x)=\sum_{x\in Z\subseteq X}\sum_{\emptyset\neq S\subseteq Y}u_{Z\cup S}(q_{Z\cup S})=\sum_{\emptyset\neq S\subseteq Y}W(q_X;q_S|x).$$

Then

$$W(q_x|q_{X\backslash x},q_Y)=W(q_x|q_{X\backslash x})+\tilde{W}(q_X;q_Y|x),$$

and

$$\mathrm{e}^{-\beta\tilde{W}(q_X;q_Y|x)}=\prod_{\emptyset\neq S\subseteq Y}\Big(1+\Big(\mathrm{e}^{-\beta W(q_X;q_S|x)}-1\Big)\Big)=\sum_{S\subseteq Y}K_x(q_X;q_S),\qquad K_x(q_X;q_{\emptyset})=1.$$

Then, using (6) and substituting this equality into the expression of the finite volume grand canonical correlation functions one obtains

$$\begin{aligned}
\rho^{\Lambda}(q_X) &= \Xi_{\Lambda}^{-1}\chi_{\Lambda}(X)\sum_{Y\subseteq\Lambda\backslash X}z^{|Y\cup X|}\int\nu(\mathrm{d}q_Y)\mathrm{e}^{-\beta U(q_{X\cup Y\backslash x})}\sum_{S\subseteq Y}K(q_x|q_{X\backslash x};q_S)\\
&= \Xi_{\Lambda}^{-1}\chi_{\Lambda}(X)\sum_{Y\subseteq\Lambda\backslash X}z^{|Y\cup X|}\sum_{S\subseteq Y}\int\nu(\mathrm{d}q_Y)K(q_x|q_{X\backslash x};q_S)\mathrm{e}^{-\beta U(q_{X\cup Y\backslash x})}\\
&= z\sum_{Z\subseteq\Lambda\backslash X}\int\nu(\mathrm{d}q_Z)K(q_x|q_{X\backslash x};q_Z)\Xi_{\Lambda}^{-1}\chi_{\Lambda}(X\cup Z)\\
&\quad\times\sum_{Y\subseteq\Lambda\backslash(Z\cup X)}z^{|Y\cup X\cup Z|-1}\int\nu(\mathrm{d}q_Y)\mathrm{e}^{-\beta U(q_{X\backslash x},q_Y)}.
\end{aligned}$$

The equality

$$\rho^{\Lambda}(q_{X\backslash x})=\Xi_{\Lambda}^{-1}\chi_{\Lambda}(X\backslash x)\sum_{Y\subseteq(\Lambda\backslash X)\cup x}z^{|Y\cup X|-1}\int\nu(\mathrm{d}q_Y)\mathrm{e}^{-\beta U(q_{X\backslash x},q_Y)}$$

leads to

$$\begin{aligned}
\Xi_{\Lambda}^{-1}\chi_{\Lambda}(X\cup Z)\sum_{Y\subseteq\Lambda\backslash(Z\cup X)}z^{|Y\cup X\cup Z|-1}\int\nu(\mathrm{d}q_Y)\mathrm{e}^{-\beta U(q_{X\backslash x},q_Y)}\\
=\chi_{\Lambda}(x)(\rho^{\Lambda}(q_{X\backslash x\cup Z})-\int\nu(\mathrm{d}q_x)\rho^{\Lambda}(q_{X\cup Z})).
\end{aligned}$$

It is clear that the terms with $x \in Y$ in the sum, representing the first term in the round brackets, are canceled by the same terms in the sum representing the second term in the brackets. That is, the KS equation is given for $x \in X, |X| > 1$ by

$$\rho^{\Lambda}(q_X) = z\chi_{\Lambda}(x) \sum_{Z \subseteq \Lambda \setminus X} \int K(q_x|q_{X\setminus x}; q_Z) \left[\rho^{\Lambda}(q_{X\setminus x \cup Z}) - \int \nu(\mathrm{d}q_x)\rho^{\Lambda}(q_{X\cup Z})\right] \nu(\mathrm{d}q_Z)$$

and for $X = x$ by

$$\begin{aligned} \rho^{\Lambda}(q_x) \quad = \quad & z\chi_{\Lambda}(x)\Bigg\{1 - \int \rho^{\Lambda}(q_x)\nu(\mathrm{d}q_x) \\ & + \sum_{|Z|\geqslant 1, Z\subseteq \Lambda\setminus x} \int K(q_x|q_Z) \left[\rho^{\Lambda}(q_Z) - \int \nu(\mathrm{d}q_x)\rho^{\Lambda}(q_{Z\cup x})\right] \nu(\mathrm{d}q_Z)\Bigg\}. \end{aligned}$$

The infinite volume KS equation is derived if one puts $\Lambda = \mathbb{Z}^d$.

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До рівняння рівноваги ґраткового осцилятора з позитивними нескінченносяжними багаточастинковими потенціалами

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Розв'язано симетризоване ґраткове рівняння Кірквуда-Зальзбурга для гіббсівських великоканонічних кореляційних функцій ґраткових осциляторів, що взаємодіють через позитивні нескінченносяжні багаточастинкові потенціали. Симетризація ґрунтується на умові суперстійкості для потенціалів.

Ключові слова: *ґраткові осцилятори, великий канонічний ансамбль Гіббса, суперстійкість, рівняння Кірквуда-Зальзбурга*