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Correlation Functionals of Infinite Volume Quantum Spin Systems*

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Abstract. The existence and analyticity of the correlation functionals of a quantum lattice in the infinite volume limit is proved. The result is valid at sufficiently high temperatures and for a large class of interactions. Our method estimates the kernel K^φ for a set of Kirkwood-Salzburg equations. While a naive estimate would indicate that $\|K^\varphi\| = \infty$, we take into account cancellations between different contributions to K^φ in order to show that for sufficiently high temperatures $\|K^\varphi\| < 1$, and this estimate is independent of the volume of the system.

I. Introduction

The algebraic theory of statistical mechanics applied to quantum spin systems has recently been studied by D. Robinson [1, 2, 3]. In this note, it is proved that the correlation functional of an infinite volume quantum lattice satisfies a Kirkwood-Salzburg equation and is analytic in the fugacities, for sufficiently high temperatures and a large class of multiparticle potentials. This generalizes results of Dobrushin [4] and Gallavotti [5] for classical lattices.

In order to describe a ν-dimensional quantum lattice, assign to every point x of $\mathbb{Z}^\nu$ a Hilbert space $\mathfrak{H}_x$ of dimension N, and to every finite set $\Lambda \subset \mathbb{Z}^\nu$ the tensor product $\mathfrak{H}_\Lambda = \bigoplus_{x \in \Lambda} \mathfrak{H}_x$. The algebra of bounded operators on $\mathfrak{H}_\Lambda$, denoted $\mathfrak{A}(\Lambda)$, is called the algebra of strictly local observables, and the closure of the union $\bigcup_{\Lambda \subset \mathbb{Z}^\nu} \mathfrak{A}(\Lambda)$ is called the algebra of quasi-local observables $\mathfrak{A}$.

We will assume $N = 2$ to simplify notation, although the results are true for arbitrary N. Let the vectors $|X\rangle$, $X \subset \Lambda$, be an orthonormal basis for $\mathfrak{H}_\Lambda$. Then the algebra $\mathfrak{A}(\Lambda)$ is generated by creation and annihilation operators $a^+(X)$, $a(X)$, $X \subset \Lambda$, defined with Fermi-Dirac commutation relations at each lattice site and commutation between different lattice sites.

$$a^+(X) \equiv a^+(x_1)\, a^+(x_2) \ldots a^+(x_n)\,, \qquad X = x_1 \cup x_2 \cup \cdots \cup x_n$$
$$a^+(x_i)\, |\emptyset\rangle = |x_i\rangle$$
$$[a(x_1), a^+(x_2)]_+ = \delta_{x_1, x_2}.$$

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We will assume that the interaction of particles on the lattice is given by a Hermitian, translation-invariant, many-body potential $\{\varphi^k\}$ such that $\varphi^k(x_1, \ldots, x_k) \in \mathfrak{A}(x_1 \cup \cdots \cup x_k)$. With the norm $\|\varphi\| = \sum_{k=1}^{\infty} \|\varphi\|_k$, where $\|\varphi\|_k = \sum_{\substack{0 \notin X \subset \mathbb{Z}^\nu \\ N(X) = k-1}} \|\varphi^k(0 \cup X)\|$, $\|\varphi^k(X)\|$ is the operator norm of $\varphi^k(X)$, and $N(X)$ is the number of elements in X, the potentials $\{\varphi^k\}$ of finite norm form a Banach space B. Since the potential is translation-invariant, φ^1 can be uniquely specified by $\beta\varphi^1(x) = -\sum_{i=0}^{3} \ln z_i \sigma_i$, where the σ_i are generators of the algebra $\mathfrak{A}(x)$. This serves to define the fugacities z_i. For the choice $\sigma_0 = a^+(x)\,a(x)$, z_0 agrees with the usual notion of fugacity in the classical limit. The energy operator $U_\varphi(\Lambda) = \sum_{X \subset \Lambda} \varphi(X)$ satisfies $|U_\varphi(\Lambda)| \leqq N(\Lambda)\,\|\varphi\|$.

The space B is too large to carry out the intended proofs. It is necessary rather to consider the subsets B_α, $\alpha \in \mathbb{R}$, of those multiparticle potentials $\{\varphi^k\}$ which satisfy

$$\sum_{q_1=1}^{\infty} \cdots \sum_{q_n=1}^{\infty} \|\varphi\|_{q_1} \|\varphi\|_{q_2} \cdots \|\varphi\|_{q_n} (\alpha)^{q_1 + \cdots + q_n} \prod_{j=1}^{n-1} \cdot \left(\sum_{i=1}^{j} (q_i - 1) + 1 \right) < r^n\, n!$$

for some number r depending on φ.

II. Kirkwood-Salzburg Equation

The partition function Z_Λ and the correlation functional ϱ_Λ of a finite lattice are defined by:

$$Z_\Lambda = \mathrm{Tr}_{\mathfrak{H}_\Lambda}\left(e^{-\beta U_\varphi(\Lambda)}\right)$$

$$\varrho_\Lambda(X, Y) = Z_\Lambda^{-1}\, \mathrm{Tr}_{\mathfrak{H}_\Lambda}\left(e^{-\beta U_\varphi(\Lambda)}\, a^+(X)\, a(Y)\right).$$

Theorem. *The correlation functional $\varrho_\Lambda(X, Y)$ satisfies the following generalization of the Kirkwood Salzburg equation:*

$$\varrho_\Lambda(X, Y) = \sum_{\substack{R, P \subset \Lambda \\ R \cap Y' = \emptyset}} \varrho(P, Y' \cup R)\, K_\Lambda(X, Y; P, Y' \cup R) + \alpha(X, Y).$$

where

$$y_1 \in Y,\ Y' = Y - y_1,\ x_1 \in X,\ X' = X - x_1,\ \alpha(X, Y) = \begin{cases} 1 & \text{if } X \cup Y = \emptyset \\ 0 & \text{otherwise} \end{cases}$$

and the kernel is given by

$$K_\Lambda(X,Y;\, P, Y'\cup R) = \begin{cases} \sum\limits_{\substack{V\subset R\cap P \\ R\cap(y_1\cup X)\subset V}} (-1)^{N(V)} \langle P-V|\, e^{\beta U(\Lambda)} a_{y_1} e^{-\beta U(\Lambda)} |X\cup(R-V)\rangle & \text{if } Y \neq \emptyset,\ (X\cup y_1)\cap R\subset P \\ \sum\limits_{\substack{V\subset R\cap(P-X') \\ x_1\cap P\subset V}} (-1)^{N(V)} \langle P-X'-V|\, e^{-\beta U(\Lambda)} a^+_{x_1} e^{\beta U(\Lambda)} |R-V\rangle & \text{if } Y=\emptyset,\ x_1\cap P\subset R,\ X'\subset P \\ \text{zero otherwise} \end{cases}$$

If $\varphi \in B_\alpha$, $\alpha = 2\sqrt{2}+1$, and if β is sufficiently small, then in the limit $\Lambda\to\infty$ this equation is well defined, has a unique solution, and the solution is an analytic function of the fugacities in a region of $z_i - \beta$ space.

Proof. Viewed as an operator equation on $\mathcal{L}^\infty$, the Kirkwood-Salzburg equation can be written $(I - K_\Lambda^\varphi)\,\varrho_\Lambda = \alpha$. We will prove that if $\varphi\in B_\alpha$ and β is sufficiently small, then the operator K_Λ^φ approaches a limit K^φ of norm $\|K^\varphi\| < 1$ as $\Lambda\to\infty$, uniformly in (complex) fugacities z_i. Therefore, the equation is well defined in the infinite volume limit, $K_\Lambda^\varphi \to K^\varphi$, and $(I - K^\varphi)$ is invertible.

The solutions of the equation $(I-K^\varphi)\,\varrho = \alpha$ are the infinite volume correlation functionals ϱ. Since $\|K^\varphi\| < 1$, $(I-K_\Lambda^\varphi)^{-1} \to (I-K^\varphi)^{-1}$ as $\Lambda\to\infty$, and thus $\varrho_\Lambda = (I-K_\Lambda^\varphi)^{-1}\alpha \to \varrho$. Moreover, the functions $z_i \to K_\Lambda^{(z_i,\varphi)} \to (I - K_\Lambda^{(z_i,\varphi)})^{-1} \to \varrho_\Lambda(X, Y)$ of $\mathbb{C}\to \mathrm{Hom}(\mathcal{L}^\infty) \to \mathrm{Hom}(\mathcal{L}^\infty) \to \mathbb{C}$ are analytic, and so the composite functions $z_i \to \varrho_\Lambda$ are analytic. By the uniform convergence of K_Λ^φ, the functions $z_i \to \varrho(X, Y)$ restricted to the real lines are analytic functions.

To derive the equation for the case $Y\neq\emptyset$, use cyclicity of the trace and a sum over intermediate states:

$$\begin{aligned}
\varrho_\Lambda(X, Y) &= Z_\Lambda^{-1}\,\mathrm{Tr}_{\mathfrak{H}_\Lambda}\big(a(Y)\, e^{-\beta U_\varphi(\Lambda)}\, a^+(X)\big) \\
&= Z_\Lambda^{-1} \sum_{\substack{S\subset\Lambda \\ S\cap(Y\cup X)=\emptyset}} \langle S\cup Y|\, e^{-\beta U_\varphi(\Lambda)}\, |S\cup X\rangle \\
&= Z_\Lambda^{-1} \sum_{\substack{S\subset\Lambda \\ S\cap(Y\cup X)=\emptyset}} \langle S\cup Y'|\, e^{-\beta U_\varphi(\Lambda)}\, e^{\beta U_\varphi(\Lambda)}\, a_{y_1}\, e^{-\beta U_\varphi(\Lambda)} |S\cup X\rangle \\
&= Z_\Lambda^{-1} \sum_{\substack{S,T\subset\Lambda \\ S\cap(Y\cup X)=\emptyset}} \langle S\cup Y'|\, e^{-\beta U_\varphi(\Lambda)}\, |T\rangle \\
&\quad\cdot \langle T|\, e^{\beta U_\varphi(\Lambda)}\, a_{y_1}\, e^{-\beta U_\varphi(\Lambda)}\, |S\cup X\rangle\,.
\end{aligned}$$

From the identity,

$$\langle A|\, e^{-\beta U_\varphi(\Lambda)}\, |B\rangle = Z_\Lambda \sum_{\substack{V\subset\Lambda \\ V\cap(A\cup B)=\emptyset}} (-1)^{N(V)}\, \varrho_\Lambda(B\cup V, A\cup V)$$

obtain

$$\varrho_A(X, Y) = \sum_{\substack{V, S, T \subset A \\ S \cap (Y \cup X) = \emptyset \\ V \cap (Y' \cup S \cup T) = \emptyset}} \varrho_A(T \cup V, Y' \cup S \cup V) (-1)^{N(V)} \cdot \langle T | e^{\beta U_\varphi(A)} a_{y_1} e^{-\beta U_\varphi(A)} | S \cup X \rangle .$$

Making the change of summation indices, $P = T \cup V$ and $R = S \cup V$, completes the derivation. The case $Y = \emptyset$ is similar [6].

We shall calculate $\|K_A^\varphi\| = \sup_{X, Y \subset A} \sum_{\substack{R, P \subset A \\ R \cap Y' = \emptyset}} \|K_A(X, Y; P, Y' \cup R)\|$ by expanding $e^{\beta U(A)} a_{y_1} e^{-\beta U(A)}$ in multicommutators:

$$e^{\beta U(A)} a_{y_1} e^{-\beta U(A)} = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \operatorname{ad}^n (U(A), a_{y_1}) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} [U(A), a_{y_1}]^{(n)} .$$

Then

$$K_A(X, Y; P, Y' \cup R) = \sum_{n=0}^{\infty} \frac{1}{n!} K_A^n(X, Y; P, Y' \cup R) ,$$

where

$$K_A^n(X, Y; P, Y' \cup R) = \sum_{\substack{V \subset R \cap P \\ R \cap (y_1 \cup X) \subset V}} (-1)^{N(V)} \langle P - V | \beta^n [U(A), a_{y_1}]^{(n)} | X \cup (R - V) \rangle .$$

If in estimating $\|K_A^\varphi\|$ the factor $(-1)^{N(V)}$ is omitted, then we obtain $\|K_A^\varphi\| = \infty$. Hence this factor must be used to take into account cancellations between different contributions to the sum for K_A^φ.

A bound on $\|K_A^\varphi\|$ is given by the Lemma.

Lemma.

$$\sum_{\substack{R, P \subset A \\ R \cap Y' = \emptyset}} \|K_A^n(X, Y; P, Y' \cup R)\| \leqq \alpha \left(2 \frac{\beta}{\alpha}\right)^n \sum_{k_1=1}^{\infty} \cdots \sum_{k_n=1}^{\infty} \|\varphi\|_{k_1} \cdots \|\varphi\|_{k_n} \cdot (\alpha)^{k_1 + \cdots + k_n} \prod_{p=1}^{n-1} \left(\sum_{i=1}^{p} (k_i - 1) + 1 \right)$$

for $\alpha = 2\sqrt{2} + 1$.

Proof. The proof is based on the commutativity $[\varphi(Y_1), \varphi(Y_2)] = 0$ whenever $Y_1 \cap Y_2 = \emptyset$, and the identity $\sum_{Y \subset X} (-1)^{N(Y)} \equiv 0$ for any set $X \neq \emptyset$. From the first we have

$$[U(A), a_y]^{(n)} = \sum_{\substack{Y_1 \subset A \\ Y_1 \cap y = \emptyset}} \sum_{y_2 \in S_1} \sum_{\substack{Y_2 \subset A \\ Y_2 \cap y_2 = \emptyset}} \cdots \sum_{y_n \in S_{n-1}} \sum_{\substack{Y_n \subset A \\ Y_n \cap y_n = \emptyset}} \cdot [\varphi(y_n \cup Y_n), [\varphi(y_{n-1} \cup Y_{n-1}), \ldots, [\varphi(y \cup Y_1), a_y] \ldots]]$$

where $\mathrm{Sp} = Y_P \cup Y_{P-1} \cup \cdots \cup Y_1 \cup y$. By setting $W = R \cap P - V$, write K_Λ^n in the form

$$K_\Lambda^n(X, Y; P, Y' \cup R) = (-1)^{N(R \cap P)} \sum_{W \subset R \cap P - (X \cup y) \cap R} (-1)^{N(W)}$$
$$\cdot \langle P - (R \cap P) + W \,|[\beta U(\Lambda), a_y]^{(n)}\,| X \cup (R - R \cap P + W) \rangle .$$

In evaluating $\sum_{\substack{R, P \subset \Lambda \\ R \cap Y' = \emptyset}} \|K_\Lambda^n(X, Y; P, Y' \cup R)\|$, we may interchange the order of summation at finite Λ and sum last over the arguments of the potentials $Y_1, y_2, Y_2, \ldots, y_n, Y_n$, as it will become clear from the proof of the Lemma and the definition of B_α that the resulting series is absolutely convergent uniformly in Λ. Therefore, let $\tau = R \cap P$, $\hat{R} = R - \tau$, $\hat{P} = P - \tau$, and consider the sum

$$\sum_{\substack{\hat{P}, \hat{R} \subset \Lambda \\ \hat{R} \cap (Y' \cup \hat{P} \cup X \cup y) = \emptyset}} \sum_{\tau \subset \Lambda - (\hat{P} \cup \hat{R} \cup Y')} (-1)^{N(\tau)} \sum_{W \subset \tau - (X \cup y) \cap \tau} (-1)^{N(W)} \beta^n \langle \hat{P} \cup W|$$
$$\cdot \left[\varphi(y_n \cup Y_n), [\ldots[\varphi(y \cup Y_1), a_y] \ldots]\right] |X \cup \hat{R} \cup W\rangle .$$

The sum $\sum_{W \subset \tau - (X \cup y) \cap \tau} (-1)^{N(W)}$ can be written

$$\sum_{W_1 \subset (\tau - (X \cup y) \cap \tau) \cap S_n} (-1)^{N(W_1)} \sum_{W_2 \subset (\tau - (X \cup y) \cap \tau) \cap (\Lambda - S_n)} (-1)^{N(W_2)}$$

which vanishes unless $(\tau - (X \cup y) \cap \tau) \cap (\Lambda - S_n) = \emptyset$, since, from the observation $[U(\Lambda), a_y]^{(n)} \in \mathfrak{A}(S_n)$, the matrix element is clearly independent of W_2. Note that this implies $\tau \subset S_n \cup X$. With these restrictions, the matrix element becomes

$$\langle \hat{P} \cup W_1| \left[\varphi, [\ldots [\varphi, a_y] \ldots]\right] |X \cup \hat{R} \cup W_1\rangle$$
$$= \langle (\hat{P} \cap S_n) \cup W_1| \left[\varphi, [\ldots [\varphi, a_y] \ldots]\right] |(X \cup \hat{R} \cup W_1) \cap S_n\rangle$$
$$\cdot \langle \hat{P} \cap (\Lambda - S_n) \,|\, (X \cup \hat{R}) \cap (\Lambda - S_n)\rangle$$

which vanishes unless $\hat{P} \cap (\Lambda - S_n) = X \cap (\Lambda - S_n)$, $\hat{R} \cap (\Lambda - S_n) = \emptyset$.

Now suppose $\tau \cap (\Lambda - S_n) \neq \emptyset$, i.e., $\tau \cap (X \cap (\Lambda - S_n)) \neq \emptyset$. Then $\tau \cap (\hat{P} \cap (\Lambda - S_n)) \neq \emptyset$, which is impossible, since $\tau \subset \Lambda - \hat{P}$. Hence $\tau \subset S_n$. Combining these results, we may write

$$\sum_{\substack{P, R \subset \Lambda \\ R \cap Y' = \emptyset}} \|K_\Lambda^n(X, Y; P, Y' \cup R)\|$$
$$\leqq \sum_{y_2 \in S_1} \cdots \sum_{y_n \in S_{n-1}} \sum_{\substack{Y_1 \subset \Lambda \\ Y_1 \cap y = \emptyset}} \cdots \sum_{\substack{Y_n \subset \Lambda \\ Y_n \cap y_n = \emptyset}} \sum_{P, R \subset S_n} \sum_{W \subset R \cap P}$$
$$\cdot \beta^n \left|\langle P - (R \cap P) + W| \left[\varphi, [\cdots [\varphi, a_y] \cdots]\right] | (X \cap S_n) \cup (R - R \cap P + W)\rangle\right| .$$

Let $[\varphi, [\cdots [\varphi, a_y] \cdots]] = B$, $V = R \cap P - W$, and $T = P - V$, and employ the Schwarz inequality in summing over T.

$$\sum_{P, R \subset S_n} \sum_{W \subset R \cap P} |\langle P - (R \cap P) + W | B | (X \cap S_n) \cup (R - (R \cap P) + W)\rangle|$$

$$= \sum_{R \subset S_n} \sum_{V \subset R} \sum_{T \subset S_n - V} |\langle T | B | (X \cap S_n) \cup (R - V)\rangle|$$

$$\leqq \sum_{R \subset S_n} \sum_{V \subset R} (\sqrt{2})^{N(S_n) - N(V)} \|B\| = \|B\| \sum_{R \subset S_n} (\sqrt{2})^{N(S_n)} (1 + \sqrt{1/2})^{N(R)}$$

$$= \|B\| (\sqrt{2}(2 + \sqrt{1/2}))^{N(S_n)}$$

where we have used the fact that for any set S and number z,

$$\sum_{A \subset S} (z)^{N(A)} = \sum_{r=0}^{N(S)} \binom{N(S)}{r} (z)^r = (z+1)^{N(S)} .$$

Finally, since $\|[\varphi, a_y]^{(n)}\| \leqq 2 \|\varphi\| \, \|[\varphi, a_y]^{(n-1)}\|$, and

$$N(S_p) \leqq \sum_{i=1}^{p} (k_i - 1) + 1$$

for $k_i = N(Y_i) + 1$,

$$\sum_{\substack{P, R \subset \Lambda \\ R \cap Y' = \emptyset}} \|K^n(X, Y; P, Y' \cup R)\|$$

$$\leqq 2^n \beta^n \sum_{k_1 = 1}^{\infty} \cdots \sum_{k_n = 1}^{\infty} \|\varphi\|_{k_1} \cdots \|\varphi\|_{k_n}$$

$$\cdot (2\sqrt{2} + 1)^{N(S_n)} \prod_{p=1}^{n-1} N(S_p)$$

which proves the Lemma.

The case $n = 0$ can be explicitly evaluated, writing $\delta(A = B)$

$$= \begin{cases} 1 & \text{if } A = B \\ 0 & \text{otherwise} . \end{cases}$$

$$\sum_{\substack{P, R \subset \Lambda \\ R \cap Y' = \emptyset}} K_\Lambda^0(X, Y; P, Y' \cup R) \, \varrho_\Lambda(P, Y' \cup R)$$

$$= \delta(y \cap X \neq \emptyset) \, [\varrho_\Lambda(X - y, Y') - \varrho_\Lambda(X, Y)] .$$

Thus the Kirkwood-Salzburg equation takes the form

$$\varrho_\Lambda(X, Y) = \frac{1}{1 + \delta(y \cap X \neq \phi)} \Bigg[\delta(y \cap X \neq \emptyset) \, \varrho_\Lambda(X - y, Y')$$

$$+ \sum_{n=1}^{\infty} \sum_{\substack{P, R \subset \Lambda \\ R \cap Y' = \emptyset}} \frac{1}{n!} K_\Lambda^n(X, Y; P, Y' \cup R) \, \varrho_\Lambda(P, Y' \cup R) + \alpha(X, Y) \Bigg]$$

and it is evident that if $\varphi \in B_\alpha$, then β can be made sufficiently small so that $|K_\Lambda^\varphi| < 1$. The convergence of K_Λ^φ as $\Lambda \to \infty$ and the uniformity in fugacities can easily be checked, completing the proof of the Theorem.

Corollary 1. *If $U_\varphi(\Lambda)$ conserves particle number, there exists a strictly positive monotonically decreasing function of fugacity $\beta_c(z)$ such that the infinite volume correlation functional is analytic in fugacity for $\beta < \beta_c(z)$.*

Proof. If $U_\varphi(\Lambda)$ conserves particle number, z can be factored from K^φ_Λ.

Corollary 2. *Suppose $\varphi \in B$, $\varphi_i = 0$ if $i > 2$, and suppose $U_\varphi(\Lambda)$ conserves particle number. Then $\varrho(X, Y)$ is analytic in fugacity z if $\beta(1 + z\alpha) < (2\alpha \|\varphi\|_2)^{-1}$, where $\alpha = 2\sqrt{2} + 1$.*

We are investigating if the Theorem provides, in the case that $U(\Lambda)$ commutes with particle number, a better value for an upper bound of the critical temperature than that found by G. GALLAVOTTI [7].

Applications of the integral equation and other properties of the correlation functionals for classical systems have been described by D. RUELLE [8] and G. GALLAVOTTI [9].

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