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Critical Temperature Bounds of Quantum Lattice Gases

W. Greenberg
Department of Mathematics, Indiana University
Bloomington, Indiana

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Abstract. We prove rigorous critical temperature upper bounds of quantum lattices in the infinite volume limit and with many-body potentials which conserve the number of particles. The results are obtained from the analyticity properties of the reduced correlation functionals. As an example the isotropic Heisenberg model is considered. The method also extends previous results on the analyticity and the critical temperature of a classical lattice.

I. Introduction

In recent papers [1, 3], it has been proved that the reduced correlation functionals of a quantum lattice gas in the infinite volume limit are analytic in fugacity z in a region of the $\beta - z$ plane corresponding to high temperatures. The method depends upon estimates on the kernels of a set of integral equations for the finite volume correlation functionals. Here we consider potentials which conserve particle number, and we extend the region of analyticity sufficiently to obtain an upper bound on the critical temperature of the lattice. In addition, for particular potentials we provide a means of selecting contributions to the kernels which are significant, and of estimating the remainder. In the last sections, the results are applied to the isotropic Heisenberg model and to classical lattices. Enlarged regions of analyticity and improved critical temperature bounds are obtained for both the classical [2, 4] and the quantum [1, 5] potentials.

II. Notation

The states of a ν-dimensional lattice $\mathbb{Z}^\nu$ are given by subsets $X \subset \mathbb{Z}^\nu$. If we associate with each lattice point x a two-dimensional vector space $\mathscr{H}_x$ generated by the creation and annihilation operators a_x^+, a_x, and with each finite subset the tensor product $\mathscr{H} = \bigotimes_{x \in \Lambda} \mathscr{H}_x$, then the vector $|X\rangle = a^+(X)|\emptyset\rangle$ in $\mathscr{H}$, $X \subset \Lambda$, corresponds to a state of the lattice with sites $y \in X$ occupied and $y \in \Lambda - X$ unoccupied. Let $\mathfrak{A}(\Lambda)$ denote the bounded operators on $\mathscr{H}_\Lambda$.

Interactions of the lattice are given by a sequence $\{\varphi^n\}$ of potentials, where $\varphi^n(x_1, \ldots, x_n)$ is an n-body potential which is a Hermitian, translation-covariant, bounded operator on $\mathscr{H}_{x_1 \cup \ldots \cup x_n}$. We shall assume that $\{\varphi^n\}$ commutes with the number of particles operator: $[\varphi^n(x_1, \ldots, x_n), N] = 0$ for all n, where $N = \sum_{x \in \mathbf{Z}^\nu} a_x^+ a_x$. In addition, we impose the norm requirement: $\|\varphi\| = \sum_{k=1}^{\infty} \|\varphi\|_k < \infty$. Here $\|\varphi\|_k = \sum_{\substack{0 \notin X \subset \mathbf{Z}^\nu \\ N(X) = k-1}} \|\varphi^k(0 \cup X)\|$ and $\|\varphi^k(Y)\|$ is the operator norm of $\varphi^k(Y)$. With this norm the potentials form a Banach space B. Translation covariance and commutation with N implies $\beta\varphi^1(x) = -\ln z a_x^+ a_x$ (plus a multiple of the identity, which corresponds to an irrelevant rescaling of the energy), and this serves to define the fugacity z. The energy operator is $U_\varphi(\Lambda) = \sum_{X \subset \Lambda} \varphi(X)$.

The correlation functional for a lattice of finite volume Λ is defined by $\varrho_\Lambda^\varphi(X, Y) = Z_\Lambda^{-1} \operatorname{Tr}\{e^{-\beta U_\varphi(\Lambda)} a^+(X)\, a(Y)\}$. Then $\varrho_\Lambda \in \mathscr{L}^\infty$, the Banach space of bounded sequences, and satisfies a generalized Kirkwood-Salzburg integral equation [3]:

Theorem 2.1. *$\varrho_\Lambda = (I - K_\Lambda)^{-1}\alpha$, where $\alpha \in \mathscr{L}^\infty$ and $K_\Lambda \in$ Hom$(\mathscr{L}^\infty)$, the algebra of bounded operators on $\mathscr{L}^\infty$. The matrix elements of K_Λ are given by*

$$K_\Lambda(X, Y; P, Y' \cup R) = \begin{cases} \displaystyle\sum_{\substack{V \subset R \cap P \\ R \cap (y_1 \cup X) \subset V}} (-1)^{N(V)} \langle P - V|\, e^{\beta U(\Lambda)} a_{y_1} e^{-\beta U(\Lambda)} \cdot |X \cup (R - V)\rangle \\ \qquad \text{if } Y \neq \emptyset,\ (X \cup y_1) \cap R \subset P \\ \displaystyle\sum_{\substack{V \subset R \cap (P - X') \\ x_1 \cap P \subset V}} (-1)^{N(\Lambda)} \langle P - X' - V|\, e^{-\beta U(\Lambda)} a_{x_1}^+ \cdot e^{\beta U(\Lambda)} |R - V\rangle \\ \qquad \text{if } Y = \emptyset,\ x_1 \cap P \subset R,\ X' \subset P \end{cases}$$

and zero otherwise, for $y_1 \in Y$, $Y' = Y - y_1$, $x_1 \in X$, $X' = X - x_1$, and

$$\alpha(X, Y) = \begin{cases} 1 & \text{if } X \cup Y = \emptyset \\ 0 & \text{otherwiese}. \end{cases}$$

III. General Quantum Potentials

A subset B_c, $c \in \mathbb{R}$, of the Banach space B is given by those potentials in B which satisfy:

$$\Gamma(\varphi) = (2/\pi)^{1/4} \cdot \sum_{n=1}^{\infty} \sum_{k_1=2}^{\infty} \cdots \sum_{k_n=2}^{\infty} \|\varphi\|_{k_1} \cdots \|\varphi\|_{k_n} \sum_{r=0}^{Q(n)} \cdot \sum_{j=0}^{r} \binom{Q(n)}{r} \binom{r}{j} \frac{2^{n + \frac{1}{2}(Q(n) - j)}}{(Q(n) - j + \frac{2}{\pi}\delta(Q(n) = j))^{1/4}} \frac{1}{n!} \cdot \prod_{s=1}^{n-1} Q(s) < c$$

for $Q(s) = \sum_{i=1}^{s} (k_i - 1) + 1$ and $\delta(A = B) = \begin{cases} 1, & A = B \\ 0, & \text{otherwise}. \end{cases}$

Theorem 3.1. *If* $\beta\varphi \in B_c$, $c < z^{-1}$, *then in the limit* $\Lambda \to \infty$, $K_\Lambda \to K \in \mathrm{Hom}(\mathscr{L}^\infty)$ *in the sense that the adjoints converge weakly in* $\mathscr{L}^1$. *Thus* $\varrho_\Lambda(X, Y) \to \varrho(X, Y)$ *pointwise, and the functions* $\varrho(X, Y)$, *the infinite volume correlation functionals, are analytic in fugacity* z.

The proof of 3.1, as well as much of what is to follow, depends upon an estimate of the kernels K which is proved in [3]. Expand K_Λ in multicommutators to obtain K^n_Λ, $K_\Lambda = \sum\limits_{n=0}^{\infty} \frac{1}{n!} K^n_\Lambda$.

Theorem 3.2.

$$\sum_{\substack{P,R\subset\Lambda\\ R\cap Y'=\emptyset}} \|K^n_\Lambda(X, Y; P, Y' \cup R)\| \leqq \sum_{y_2\in S_1} \cdots \sum_{y_n\in S_{n-1}} \sum_{\substack{Y_1\subset\Lambda\\ Y_1\cap y=\emptyset}} \cdots \sum_{\substack{Y_n\subset\Lambda\\ Y_n\cap y_n=\emptyset}}$$

$$\cdot \sum_{P,R\subset S_n} \sum_{V\subset R\cap P} \beta^n |\langle P - V| \, [\varphi(y_n \cup Y_n), \ldots, [\varphi(Y_1 \cup y), a_y] \ldots]$$

$$\cdot \, |(Y \cap S_n) \cup (R - V)\rangle| \text{ where } S_p = Y_p \cup Y_{p-1} \cup \cdots \cup Y_1 \cup y.$$

Proof of 3.1. In [3], the Schwarz inequality is employed to sum over P. However, as φ conserves particle number, $\langle P - V| \, [\varphi, a_y]^{(n)} |(X \cap S_n) \cup (R - V)\rangle = 0$ unless $N(P - V) = N((X \cap S_n) \cup (R - V)) - 1$, since $[\varphi, a_y]^{(n)} \equiv H$ annihilates one particle. Therefore, there are not $2^{N(S_n) - N(V)}$ terms in the sum over P, but at most $\sup\limits_{0 \leqq j \leqq N(S_n) - N(V)} \binom{N(S_n) - N(V)}{j}$. Use the inequality $\sup\limits_j \binom{N(S_n) - N(V)}{j} \leqq (2/\pi)^{1/2} \dfrac{2^{N(S_n)-N(V)}}{\left(N(S_n) - N(V) + \frac{2}{\pi}\delta\right)^{1/2}}$, where the δ indicates that the denominator is to be taken equal to $\sqrt{2/\pi}$ if $N(S_n) - N(V) = 0$. Then $\sum\limits_{R\subset S_n} \sum\limits_{V\subset R} \sum\limits_{T\subset S_n - V} |\langle T|H|(X\cap S_n)\cup(R - V)\rangle|$

$$\leqq \sum_{R\subset S_n} \sum_{V\subset R} \|H\| \left\{\sqrt{\frac{2}{\pi}} \frac{2^{N(S_n)-N(V)}}{\left(N(S_n) - N(V) + \frac{2}{\pi}\delta\right)^{1/2}}\right\}^{1/2}$$

$$\leqq \sum_{r=0}^{N(S_n)} \binom{N(S_n)}{r} \sum_{j=0}^{r} \binom{r}{j} (2/\pi)^{1/4} \frac{2^{\frac{1}{2}(N(S_n)-j)}}{\left((N(S_n) - j + \frac{2}{\pi}\delta\right)^{1/4}} \|H\|.$$

From 3.2 and the inequalities $\|[\varphi, a_y]^{(n)}\| \leqq 2^n \|\varphi\|^n$, $N(S_p) \leqq Q(p)$, obtain $\|K^n_\Lambda\| \leqq (2/\pi)^{1/4} \, 2^n \beta^n \sum\limits_{k_1=2} \cdots \sum\limits_{k_n=2} \|\varphi\|_{k_1} \cdots \|\varphi\|_{k_n} \sum\limits_{r=0}^{Q(n)} \sum\limits_{j=0}^{r} \binom{Q(n)}{r}$

$$\cdot \binom{r}{j} \frac{2^{\frac{1}{2}(Q(n)-j)}}{\left(Q(n) - j + \frac{2}{\pi}\delta\right)^{1/4}} \prod_{s=1}^{n-1} Q(s).$$

To prove $\sup\limits_j \binom{N}{j} \leqq \sqrt{2/\pi} \; 2^N \left(N + \frac{2}{\pi}\delta\right)^{-1/2}$, assume N odd and use the Stirling expansion: $n! = \sqrt{2\pi/n} \, n^n e^{-n} e^{r(n)}$, where $r(n)$ is an error term which satisfies $1/12n - 1/360n^3 < r(n) < 1/12n$ [6]. Then $\sup_j \binom{N}{j} = N!/((N+1)/2)!((N-1)/2)! \leqq \sqrt{2/\pi}\, 2^N N^{-1/2} N^{N+1}(N-1)^{-N/2} \cdot (N+1)^{-1-N/2} \exp(1/12N - 1/6(N+1) + 1/45(N+1)^3 - 1/6(N-1) + 1/45(N-1)^3$. However, $\frac{1}{12N} - \frac{1}{6(N+1)} + \frac{1}{45(N+1)^3} - \frac{1}{6(N-1)} + \frac{1}{45(N-1)^3} < 0$ for $N > 2$, and $N^{N+1}(N-1)^{-\frac{1}{2}N}(N+1)^{-1-\frac{1}{2}N} = \left(\left(1-\frac{1}{N^2}\right)\left(1+\frac{1}{N}\right)^{2/N}\right)^{-1} < 1$ for $N > 2$, since:

$$\begin{aligned}\left(1-\frac{1}{N^2}\right)\left(1+\frac{1}{N}\right)^{2/N} &= \left(1-\frac{1}{N^2}\right)\left(1+\frac{2}{N}\cdot\frac{1}{N}+\frac{1}{2!\,N^2}\left(\frac{2}{N}\right)\left(\frac{2}{N}-1\right)\right.\\ &\quad \left.+\frac{1}{3!\,N^3}\left(\frac{2}{N}\right)\left(\frac{2}{N}-1\right)\left(\frac{2}{N}-2\right)+\cdots\right)\\ &\geqq \left(1-\frac{1}{N^2}\right)\left(1+\frac{2}{N^2}-\frac{2}{N}\left(\frac{1}{2!}\cdot\frac{1}{N^2}+\frac{3!}{4!}\cdot\frac{1}{N^4}+\frac{5!}{6!}\cdot\frac{1}{N^6}+\cdots\right)\right)\\ &= 1+\frac{1}{N^2}-\frac{1}{N^3}-\frac{2}{N^4}+\frac{2}{N}\left(\left(\frac{1}{2}-\frac{1}{4}\right)\frac{1}{N^4}+\left(\frac{1}{4}-\frac{1}{6}\right)\frac{1}{N^6}+\cdots\right)\\ &\geqq 1+\frac{1}{N^2}-\frac{1}{N^3}-\frac{2}{N^4}\geqq 1\,.\end{aligned}$$

If $K(X, Y; P, R)$ is chosen to be the limit $\lim_{\Lambda\to\infty} K_\Lambda(X, Y; P, R)$, then $\lim \sum_{P,R} \|K_\Lambda(X, Y; P, R \cup Y') - K(X, Y; P, R \cup Y')\| = 0$ uniformly in fugacity. From this and the bound $\|K_\Lambda\| <$ constant < 1, it follows that for any $\chi \in \mathscr{L}^1$ and $\xi \in \mathscr{L}^\infty$, $\chi(K_\Lambda \xi) \to \chi(K\xi)$. Then, for $\chi(X, Y) = \delta(X, Y)$ and $\xi = \alpha$, the convergence of $\chi\left(\frac{1}{1-K_\Lambda}\xi\right) \to \chi\left(\frac{1}{1-K}\xi\right)$ uniformly in z completes the proof of the theorem.

It is possible to extend the region of analyticity in the $\beta - z$ plane by employing hole-particle symmetry. Toward this end, define the hole-particle inversion $\mathscr{L}: (\mathscr{L}^{-1}B_c) \to B_c$ by

$$(\mathscr{L}\varphi)(X) = (-1)^{N(X)} \sum_{Y \supset X} \mathrm{Tr}_{\mathscr{H}_{Y-X}} \varphi(Y)$$

which may be interpreted as giving physical significance to unoccupied lattice sites (holes) rather than particles, and define the symmetry operator $s: \mathfrak{A}(\Lambda) \to \mathfrak{A}(\Lambda)$ by

$$s(A) = \sum_{T \subset \Lambda} (-1)^{N(T)} \mathrm{Tr}_{\mathscr{H}_{\Lambda-T}} A\,.$$

Note $\mathscr{L}^2 = I$, $s^2 = I$. These generalize to quantum lattices the hole-particle symmetry of a classical lattice dissussed in [2].

Lemma 3.3. $A \in \mathfrak{A}(\Lambda) \Rightarrow \mathrm{Tr}_{\mathscr{H}_\Lambda} A = \mathrm{Tr}_{\mathscr{H}_\Lambda} s(A)$.

Proof. $\mathrm{Tr}\, s(A) = \sum_{T\subset\Lambda} \sum_{V\subset\Lambda} (-1)^{N(V)} \sum_{W\subset\Lambda-V} \langle (T\cap V)\cup W| A |(T\cap V)\cup W\rangle$

$$= \sum_{T\subset\Lambda} \sum_{\substack{W_1\subset\Lambda\\ W_1\cap T=\emptyset}} \sum_{W_2\subset T} \sum_{\substack{V_2\subset T\\ V_2\cap W_2=\emptyset}} \sum_{\substack{V_1\subset\Lambda-T\\ V_1\cap W_1=\emptyset}} (-1)^{N(V_1)-N(V_2)} \langle V_2\cup W_1\cup W_2|\, A\,|V_2 \cup W_1\cup W_2\rangle,$$

where we have written $V_2 = V \cap T$, $V_1 = V - V_2$, $W_2 = W \cap T$, and $W_1 = W - W_2$. But $\sum_{\substack{V_1 \subset \Lambda - T \\ V_1 \cap W_1 = \emptyset}} (-1)^{N(V_1)} = 0$ unless $\Lambda - (T \cup W_1) = \emptyset$.

Therefore $T = \Lambda - W_1$, $V_1 = \emptyset$, and

$$\begin{aligned}
&\operatorname{Tr} s(A) \\
&= \sum_{W_1 \subset \Lambda} \sum_{\substack{W_2 \subset \Lambda \\ W_1 \cap W_2 = \emptyset}} \sum_{\substack{V_2 \subset \Lambda \\ V_2 \cap (W_1 \cup W_2) = \emptyset}} (-1)^{N(V_2)} \langle V_2 \cup W_1 \cup W_2 | A | V_2 \cup W_1 \cup W_2 \rangle \\
&= \sum_{R \subset \Lambda} \langle R | A | R \rangle D(R),
\end{aligned}$$

where $D(R)$ is the number of ways of disjointly choosing V_2, W_1, W_2, so that $V_2 \cup W_1 \cup W_2 = R$, weighted by $(-1)^{N(V_2)}$. Thus, $D(R) = \sum_{n=0}^{N(R)} \cdot \binom{N(R)}{n} \sum_{j=0}^{N(R)-n} \binom{N(R)-n}{j} (-1)^n = \sum_{n=0}^{N(R)} \binom{N(R)}{n} (-1)^n (1+1)^{N(R)-n}$ $= (1+1-1)^{N(R)} = 1$ and $\operatorname{Tr} s(A) = \sum_{R \subset \Lambda} \langle R | A | R \rangle = \operatorname{Tr} A$.

Lemma 3.4. $A, B \in \mathfrak{A}(\Lambda) \Rightarrow s(AB) = s(B)\, s(A)$.

Proof. The case $N(\Lambda) = 1$ is trivial. Assume $A, B \in \mathfrak{A}(\Lambda)$ and observe s is linear on $\mathfrak{A}(x)$. Then $s(AB) = \sum_{T \subset \Lambda} (-1)^{N(T)} \operatorname{Tr}_{\mathscr{H}_{\Lambda - T}} \left(\bigotimes_{x \in \Lambda} A_x B_x \right)$

$$= \bigotimes_{x \in \Lambda} \left(\sum_{y \subset x} (-1)^{N(y)} \operatorname{Tr}_{\mathscr{H}_{x-y}} A_x B_x \right) = \bigotimes_{x \in \Lambda} s(A_x B_x) = \bigotimes_{x \in \Lambda} s(B_x)\, s(A_x)$$
$$= s\left(\bigotimes_{x \in \Lambda} B_x \right) s\left(\bigotimes_{x \in \Lambda} A_x \right) = s(B)\, s(A).$$

Lemma 3.5. $s(U_\varphi(\Lambda)) = U_{\mathscr{L}\varphi}(\Lambda) + N(\Lambda) E_0 + S(\Lambda)$, *where* $E_0 = \sum_{0 \in X} \operatorname{Tr}_{\mathscr{H}_X} \varphi(X)/N(X)$ *and* $S(\Lambda)$ *is a boundary term with the property:* $\lim_{\Lambda \to \infty} \|S(\Lambda)\|/N(\Lambda) = 0$.

Proof. From the definition of s and $\mathscr{L}$:

$$\begin{aligned}
&s(U_\varphi(\Lambda)) \\
&= \sum_{X \subset \Lambda} \sum_{T \subset X} (-1)^{N(T)} \operatorname{Tr}_{\mathscr{H}_{X-T}} \varphi(X) = \sum_{T \subset \Lambda} \left\{ (-1)^{N(T)} \sum_{\substack{X \subset \Lambda \\ X \supset T}} \operatorname{Tr}_{\mathscr{H}_{X-T}} \varphi(X) \right\} \\
&= \sum_{\substack{T \subset \Lambda \\ T \neq \emptyset}} (\mathscr{L}\varphi)(T) + (\mathscr{L}\varphi)(\emptyset) + S_1(\Lambda)
\end{aligned}$$

where

$$S_1(\Lambda) = \sum_{T \subset \Lambda} (-1)^{N(T)} \sum_{\substack{X \supset T \\ X \cap \Lambda \neq X}} \operatorname{Tr}_{\mathscr{H}_{X-T}} \varphi(X)$$

is a boundary term. Then compute:

$$\begin{aligned}
(\mathscr{L}\varphi)(\emptyset) &= \sum_{Y} \operatorname{Tr}_{\mathscr{H}_Y} \varphi(Y) = \sum_{n=1}^{\infty} \sum_{y \in \mathbf{Z}^\nu} \sum_{\substack{y \notin Y \subset \mathbf{Z}^\nu \\ N(Y) = n-1}} \operatorname{Tr}_{\mathscr{H}_{y \cup Y}} \varphi(y \cup Y)/n \\
&= \sum_{n=1}^{\infty} N(\Lambda) \sum_{\substack{Y \not\ni 0 \\ N(Y) = n-1}} \operatorname{Tr}_{\mathscr{H}_{0 \cup Y}} \varphi(0 \cup Y)/n + S_2(\Lambda).
\end{aligned}$$

Corollary 3.6. *The pressure* $P_\Lambda(\varphi) = (1/N(\Lambda)) \log \mathrm{Tr}_{\mathscr{H}_\Lambda} e^{-\beta U_\varphi(\Lambda)}$ *satisfies* $P_\Lambda(\varphi) = P_\Lambda(\mathscr{L}\varphi) - \beta E_0 + S_0(\Lambda)$ with $\lim_{\Lambda\to\infty} S_0(\Lambda) = 0$.

Proof. Use the bounds due to van Kampen [7]:

$$P_\Lambda(\varphi) - \beta\sigma/N(\Lambda) \leqq (1/N(\Lambda)) \log \mathrm{Tr}_{\mathscr{H}_\Lambda} e^{-\beta(U_\varphi(\Lambda)+S)} \leqq P_\Lambda(\varphi) - \beta\tau/N(\Lambda),$$

where σ and τ are the maximum and minimum eigenvalues, respectively, of S.

Theorem 3.7. *If* $\beta\mathscr{L}\varphi$ and $\beta\varphi$ *both satisfy the hypothesis of Theorem 3.1, then* $\varrho^\varphi(X, Y) = (-1)^{N(X)+N(Y)} \sum_{T\subset X\cap Y} (-1)^{N(T)} \varrho^{\mathscr{L}\varphi}$

$$\cdot (X - X\cap Y + T, Y - X \cap Y + T).$$

Proof. For a lattice of finite volume:

$$\begin{aligned}\varrho_\Lambda(X, Y) &= Z_\Lambda^{\varphi-1} \mathrm{Tr}\{s(a(Y)\, e^{-\beta U_\varphi}\, a^+(X))\} = Z_\Lambda^{\varphi-1}(-1)^{N(X)+N(Y)} \\ &\quad\cdot \mathrm{Tr}\{a^+(X)\, e^{-\beta s(U_\varphi)}\, a(Y)\} \\ &= (-1)^{N(X)+N(Y)} Z_\Lambda^{\varphi-1} \sum_{S\supset X\cup Y} \langle S - X|\, e^{-\beta s(U_\varphi)} |S - Y\rangle\end{aligned}$$

since all partial traces of $a(X)$ on $\mathscr{H}_T$ vanish for $T\subset X$ except $\mathrm{Tr}_{\mathscr{H}_\emptyset} a(X) = (-1)^{N(X)} a(X)$. Let $X = \hat{X} + X\cap Y$, $Y = \hat{Y} + X\cap Y$, and compute from Lemma 3.5:

$$\varrho_\Lambda^\varphi(X,Y) = (-1)^{N(X)+N(Y)} Z_\Lambda^{\mathscr{L}\varphi-1} \sum_{\substack{T\subset\Lambda \\ T\cap(X\cup Y)=\emptyset}} \langle T\cup\hat{Y}|\, e^{-\beta\mathscr{L}\varphi}\, |T\cup\hat{X}\rangle + S(\Lambda)$$

with $\lim_{\Lambda\to\infty} S(\Lambda) = 0$. Then from the identity

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

letting

$$T\cup V = W,\ W - (X\cap Y)\cap W = V',$$

$$\varrho_\Lambda^\varphi(X, Y) = (-1)^{N(X)+N(Y)} \sum_{\substack{W\subset\Lambda \\ V'\subset W-(X\cap Y)\cap W \\ W\cap(\hat{X}\cup\hat{Y})=\emptyset}} (-1)^{N(X\cap Y\cap W)}$$

$$\cdot (-1)^{N(V')} \varrho_\Lambda^{\mathscr{L}\varphi}(\hat{X}\cup W, \hat{Y}\cup W) + S(\Lambda).$$

However, the sum $\sum_{V'\subset W-(X\cap Y)\cap W} (-1)^{N(V')}$ vanishes unless $W - (X\cap Y)\cap W = \emptyset$, thus $W\subset X\cap Y$, and the theorem follows from the finiteness of the sum over $T\subset X\cap Y$ for finite X, Y as $\Lambda\to\infty$.

Define the transformed fugacity $\mathscr{L}z$ by $(\mathscr{L}\varphi)^1(x) = \mu I - \beta^{-1} \cdot \log(\mathscr{L}z)\, a_x^+ a_x$, μ, $\mathscr{L}z \in \mathbb{R}$.

Corollary 3.8. *If* $\beta\mathscr{L}\varphi \in B_c$, $c < (\mathscr{L}z)^{-1}$, *but* $\beta\varphi \notin B_c$, *then 3.6 provides an analytic continuation of the components* $\varrho^\varphi(X, Y)$ *of* ϱ^φ.

Theorem. 3.9. *Suppose* $\varphi \in B_c, c < \infty$, *and define* $\Gamma(\varphi)$ *as before Theorem 3.1. Then the critical temperature* T_0 *of an infinite volume lattice with potential* φ *is bounded by* $T_0 \leqq (k\beta_1)^{-1}$ *for* β_1 *the solution of the simultaneous equations*: $z\Gamma(\beta\varphi) = 1$, $\mathscr{L}z\Gamma(\beta\mathscr{L}\varphi) = 1$.

Theorem 3.9 follows directly from the observation that $\Gamma(\beta\varphi)$ is a monotonically decreasing function of β.

A case of special interest is the general two-body potential, $\varphi^i = 0$, $i > 2$.

Corollary 3.10. *If* $\varphi \in B_c, c < \infty$, *and* $\varphi^i = 0, i > 2$, *then the critical temperature* T_0 *of the infinite volume lattice satisfies* $T_0 \leqq 31\,\|\varphi\|/k$.

Proof. Compute $\mathscr{L}\varphi$. $(\mathscr{L}\varphi)^i = 0, i > 2$, and $(\mathscr{L}\varphi)^2 = \varphi^2$. $(\mathscr{L}\varphi)^1(0) = z^{-1}\exp\left\{-\beta\sum_{x \neq 0} \mathrm{Tr}_{\mathscr{H}_x}\varphi(0 \cup x)\right\}$, and since $\left\|\sum_{x \neq 0} \mathrm{Tr}_{\mathscr{H}_x}\varphi(0 \cup x)\right\| \leqq 2\|\varphi\|$, $z^{-1}e^{-4\beta\|\varphi\|} \leqq \mathscr{L}z \leqq z^{-1}e^{4\beta\|\varphi\|}$. As $\varrho^{\mathscr{L}\varphi}$ is analytic for $\mathscr{L}z < 1/\Gamma(\beta\varphi)$, ϱ^φ is analytic for $z^{-1}e^{4\beta\|\varphi\|} < 1/\Gamma(\beta\varphi)$, and the critical temperature is determined by the solution β_1 of $z = 1/\Gamma(\beta\varphi)$, $z^{-1} = e^{-4\beta\|\varphi\|}/\Gamma(\beta\varphi)$.

For a two-body potential, $k_i = 2$, $Q(s) = s + 1$, and $\Gamma(\beta\varphi) = (2/\pi)^{1/4} \cdot \sum_{n=1}^{\infty} (2\beta\|\varphi\|)^n \sum_{r=0}^{n+1} \sum_{j=0}^{r} \binom{n+1}{r}\binom{r}{j} \dfrac{2^{\frac{1}{2}(n+1-j)}}{\left(n+1-j+\frac{2}{\pi}\delta\right)^{1/4}}$. The critical temperature bound is the solution of $\sum_{n=1}^{\infty} c_n x^n = \exp(-x/2\sqrt{2})$ with $x = 2\sqrt{2}\,\beta_1\|\varphi\|$ and $c_n = 4\sqrt{\frac{8}{\pi}} \sum_{r=0}^{n+1} \sum_{j=0}^{r} \binom{n+1}{r}\binom{r}{j} 2^{-\frac{1}{2}j}\left(n+1-j+\frac{2}{\pi}\delta\right)^{-1/4}$. Calculating the first several c_n and estimating the remainder by $c_n \leqq \left(\frac{4}{\pi}\right)^{1/4} \sum_{r=0}^{n+1} \sum_{j=0}^{r} \cdot \binom{n+1}{r}\binom{r}{j} 2^{-\frac{1}{2}j} = \left(\frac{4}{\pi}\right)^{1/4}\left(2+\sqrt{\frac{1}{2}}\right)^{n+1}$ gives $x = 0.09$.

IV. The Heisenberg Model

The estimates of $\|K_\Lambda^n\|$ in Theorem 3.2, along with the proof of 3.1, provide a method of obtaining an improved upper bound on the critical temperature for some potentials. Namely, the multiple-commutators and their matrix elements occurring in 3.2 can be explicitly evaluated for the first few partial kernels K_Λ^n, thereby obtaining better bounds on $\|K_\Lambda^n\|$, $n = 1, 2, \ldots, N$, and then the remaining partial kernels can be estimated as in 3.1.

As an example, consider the isotropic Heisenberg model: $\varphi^2(x, y) = V(x, y)\, a_x^+ a_x a_y^+ a_y - \frac{1}{2} V(x - y)(a_x^+ - a_y^+)(a_x - a_y)$. The first three multicommutators have been calculated explicitly, and then from 3.2 the contributions to $\|K_\Lambda^n\|$, $n = 1, 2, 3$, counted, enumerating the non-zero matrix elements and taking a supremum over $X \subset S$. The result is

$$\|K_\Lambda^1\| \leqq \frac{7}{\sqrt{2}}\beta\|\varphi\|z, \quad \frac{1}{2}\|K_\Lambda^2\| \leqq \frac{25}{2\sqrt{2}}\beta^2\|\varphi\|^2 z, \quad \frac{1}{6}\|K_\Lambda^3\| \leqq \frac{78}{2\sqrt{2}}\beta^3\|\varphi\|^3 z.$$

The remainder $\sum_{n=4}^{\infty} \frac{1}{n!} \|K_\Lambda^n\|$ can be estimated as in 3.10, using $\| [\varphi(x_n, y_n), [\ldots[\varphi(x_1, y), a_y] \ldots]]\| \leqq 2^{n-4.5}\, 3 \|\varphi(x_n, y_n)\| \ldots \|\varphi(x_1, y)\|$ for $n \geqq 3$ since $\|[\varphi(x_3, y_3), [\ldots [\varphi(x_1, y)]]]\| \leqq \frac{3}{2\sqrt{2}} \|\varphi(x_3, y_3)\| \ldots \|\varphi(x_1, y)\|$. Finally, compute: $(\mathscr{L}\varphi)(x) = \left(\beta^{-1} \log z + \frac{1}{2} \sum_{y \neq x} V(y-x)\right) a_x^+ a_x$ and so $z^{-1} e^{-\frac{1}{2}\beta\|\varphi\|} \leqq \mathscr{L} z \leqq e^{\frac{1}{2}\beta\|\varphi\|} z^{-1}$.

Theorem 4.1. *Let $f(t) = 4.95t + 17.7t^2 + 165t^3 + 1325t^4(1 - 7.66t)^{-1}$. The correlation functionals of the isotropic Heisenberg model are analytic in the regions $zf(\beta\|\varphi\|) < 1$ and $z^{-1}e^{\frac{1}{2}\beta\|\varphi\|} f(\beta\|\varphi\|) < 1$. The critical temperature T_0 satisfies $T_0 \leqq 10\|\varphi\|/k$.*

V. The Classical Lattice

A similar calculation can be carried out for the classical lattice: $\varphi^n(X) = V(X)\, a^+(X)\, a(X)$. Here $\varrho(X, Y) = 0$ unless $X = Y$, and the commutators can all be explicitly evaluated. $[\varphi(X_n), \ldots, [\varphi(X_1), y] \ldots] = a^+(X_n \cup \ldots \cup X_1 - y)\, a(X_n \cup \ldots \cup X_1 - y)\, a_y$ if $y \in X_n \cap \ldots \cap X_1$, zero otherwise. There obviously is precisely one non-zero contribution to $\|K_\Lambda^n\|$ in the sum over P, R, and V (Theorem 3.2), and so $\|K_\Lambda^n\| \leqq \prod_{i=1}^{n} \cdot \sum_{\substack{Y_i \subset \Lambda \\ y \notin Y_i}} |V(Y_i \cup y)|$. Finally, $\mathscr{L} z \leqq z^{-1} e^{\beta\|\varphi\|}$.

Theorem 5.1. *The correlation functionals of the classical lattice are analytic in fugacity z in the regions $z(e^{\beta\|\varphi\|} - 1) < 1$ and $z^{-1}e^{\beta\|\varphi\|}(e^{\beta\|\varphi\|} - 1) < 1$. A bound on the critical temperature is given by $T_0 \leqq 1.8\|\varphi\|/k$,* or for *nearest neighbor interaction in ν-dimensions, $T_0 \leqq 3.6\nu E/k$.*

VI. Summary

The region of analyticity of the correlation functionals for a two-body quantum potential is graphed in Fig. 1, along with the larger region of analyticity for the isotropic Heisenberg model. By a different method [1], Gallavotti, Miracle-Sole, and Robinson have predicted $T_0 < 10{,}000\|\varphi\|/k$ for the Heisenberg model, while our result is $T_0 < 10\|\varphi\|/k$. This compares to the non-rigorous critical temperature estimate of $T_0 \approx 0.7\|\varphi\|/k$ calculated by Dombs, see [8].

For the classical lattice, the region of analyticity is also an enlargement of the region found by the same authors [1, 2] (Fig. 2). Their result was $2ze^{\beta\|\varphi\|}\{\exp(e^{\beta\|\varphi\|} - 1\} < 1$ (plus the extended region hole-particle symmetry), obtained in a manifestly classical manner by estimating the kernels of the classical Kirwood-Salzburg equation. Actually, the estimates in [1, 2] can be improved by noticing that (for,e.g.,

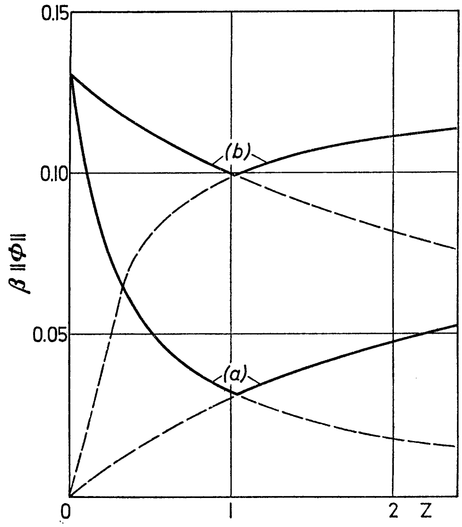

Fig. 1. The region of analyticity for the correlation functionals with: *(a)* a two-body quantum potential; *(b)* the Heisenberg model

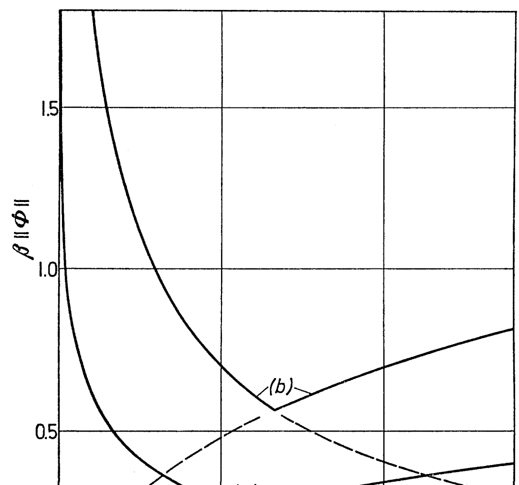

Fig. 2. The region of analyticity for the correlation functionals of a classical lattice: *(a)* as obtained by GALLAVOTTI, MIRACLE-SOLE, and ROBINSON [3]; *(b)* according to Theorem 5.1

a two body potential) the bound on the kernels is

$$\sum_{R \neq \emptyset} \sum_{r \in R} (e^{-\varphi(r,y)} - 1) \leqq \sum_{R \neq \emptyset} \prod_{r \in R} \sum_{n=1}^{\infty} |\varphi(r,y)|^n / n! = \sum_{N=1}^{\infty} \sum_{\substack{r_1,\ldots,r_N \in Z^\nu \\ r_1 < \ldots < r_N}} \sum_{n_1,\ldots n_N = 1}^{\infty}$$

$$\cdot |\varphi(r_1, y)|^{n_1} \ldots |\varphi(r_N, y)|^{n_N} / n_1! \ldots n_N!$$

which is the sum of all monomials of all degrees in all $\varphi(r, y)$ (weighted by $n_r!$). Summing up by order, this is just

$$\sum_{N=1}^{\infty} \sum_{\substack{r_1,\ldots,r_N \leqq Z^\nu \\ r_1 < \ldots < r_N}} \sum_{\substack{n_1,\ldots,n_N = 0 \\ n_1 + \ldots + n_N = N}} |\varphi(r, y)|^{n_1} \ldots |\varphi(r_N, y)|^{n_N} / n_1! \ldots n_N! = \sum_{N=1}^{\infty} \prod_{i=1}^{N}$$

$$\cdot \left(\sum_{r \neq y} |\varphi(r, y)| \right) \Big/ N! = e^{\|\varphi\|} - 1 .$$

Our method predicts a critical temperature bound for classical lattices of $T_0 < 1.8 \, \|\varphi\| / k$. The critical temperature of the Ising lattice (nearest neighbor interaction) has been calculated rigorously in two dimensions: $T_0 = 0.14 \, \|\varphi\| / k$. Mean field theory predicts for the Ising lattice in arbitrary dimension [9]. $T_0 < 0.25 \, \|\varphi\| / k$.

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W. GREENBERG
Department of Mathematics
Indiana University
Bloomington, Indiana, USA