Commun. math. Phys. 46, 253—262 (1976)

Communications in Mathematical Physics
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# Correlation Inequalities in Quantum Statistical Mechanics and Their Application in the Kondo Problem

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**Abstract.** We consider a large class of models which share the essential features of the Kondo model. Bounds on the susceptibility of the impurity spin are derived as consequences of general inequalities for quantum correlation functions. We also obtain bounds for the spin polarization in the presence of an external field.

## 1. Introduction

The Kondo model for the interaction of the conduction electrons with localized magnetic moments, in its most idealized version, concerns an isolated spin immersed in an electron gas. The purpose of the present work is to investigate the behavior of a single spin coupled to a heat bath and, in particular, to place lower and upper bounds on the susceptibility $\chi$ as a function of the temperature $T$ and the coupling constant $J$. From these bounds it is seen that, as $J \to 0$, the deviation of $\chi^{-1}$ from the Curie law tends to zero *uniformly* in $T$. This result refutes the singular $T$-dependence of $\chi^{-1}$ obtained from the Kondo model in perturbation theory [1, 2], but it does not contradict $\chi(T=0)$ being finite.

First, we clarify terminology and notation. Let $\langle \cdot \rangle_{\beta H}$ denote the thermal average with respect to the hamiltonian $H$ and the inverse temperature $\beta = 1/kT$. For any two operators $A$ and $B$, Bogoliubov [3] introduced the inner product

$$(A, B) = \int_0^\beta d\lambda \langle e^{\lambda H} A^* e^{-\lambda H} B \rangle_{\beta H}$$

with the remarkable property

$$(A, B) = (B^*, A^*) .$$

The physical significance of this inner product becomes apparent if $A$ and $B$ are chosen to be selfadjoint and if by chance the hamiltonian contains a term $-xB$. Then

$$d/dx \langle A \rangle_{\beta H} = (A, B) - \beta \langle A \rangle_{\beta H} \langle B \rangle_{\beta H} .$$

A similar formula valid in classical statistical mechanics suggests to call $\beta^{-1}(A, B)$ the canonical correlation [4] between $A$ and $B$. In accordance with this notion, the observables $A$ and $B$ are said to be uncorrelated (for fixed $\beta$ and $H$) if

$$\beta^{-1}(A, B) = \langle A \rangle_{\beta H} \langle B \rangle_{\beta H}$$

meaning that the thermal average $\langle A \rangle_{\beta H}$ is invariant under an infinitesimal change $H \to H - xB$.

As a response to an external magnetic field $B=\{B_1, B_2, B_3\}$, a term $-B\cdot M$ is introduced into the hamiltonian, $M$ being the vector operator of the magnetic moment. The simplest, although by no means trivial, system is that of a magnetic moment generated by a single spin, in which case the Hilbert space naturally takes the form of a tensor product $\mathscr{H}\otimes\mathbb{C}^{2s+1}$ and

$$M=\mu\mathbb{1}\otimes S \tag{1}$$

where $S$ stands for the conventional spin operator pertaining to the spin $s$. Note that the Kondo model provides a specific example of this general structure. We are free to choose $\mu=1$ which we shall use in the sequel.

Macroscopic observations refer to the magnetization $\langle M\rangle_{\beta(H-B\cdot M)}$ or, if merely the first order response is considered, are concerned with the susceptibility $\chi$ given by

$$\chi\delta_{ik}=(M_i, M_k)=(\partial/\partial B_k)\langle M_i\rangle_{\beta(H-B\cdot M)}|_{B=0} \tag{2}$$

where rotational invariance and continuous differentiability with respect to $B$ is assumed. In the case of no coupling, we have $[H, M]=0$ and consequently, if we adopt (1), $\chi=1/3\,s(s+1)\beta$ which is the Curie law.

## 2. A Convexity Argument

Our main objective is to control the positive quantity $(A, A)$ as a function of $\beta$ with the example $\mathbb{1}\otimes S_3$ for the operator $A$ in the back of our mind. In order to fix our ideas and to simplify the discussion, we shall assume that, throughout this section, the hamiltonian $H$ acts on a finite dimensional Hilbert space. For any operator $A$ in this space we shall write

$$A(x)=(\mathrm{Tr}\,e^{-\beta H})^{-1/2}e^{(x-\beta)H/4}Ae^{-(x+\beta)H/4}\,.$$

Then, Bogoliubov's inner product may be rewritten as

$$(A, B)=\tfrac{1}{2}\int_{-\beta}^{\beta} dx\,\mathrm{Tr}\,A(x)^*B(x) \tag{3}$$

showing that $(A, B)$ is a positive hermitian nondegenerate form. In addition, it satisfies:

$$(A, B)=(B^*, A^*) \tag{4}$$

$$(\mathbb{1}, B)=\beta\langle B\rangle_{\beta H}=\beta\,\mathrm{Tr}\,e^{-\beta H}B/\mathrm{Tr}\,e^{-\beta H} \tag{5}$$

$$(A, [H, B])=\langle[A^*, B]\rangle_{\beta H}\,. \tag{6}$$

Indeed, (4) and (5) are immediate consequences of the definition, while (6) follows from the identity

$$\int_0^\beta d\lambda e^{(\lambda-\beta)H}[H, B]e^{-\lambda H}=\int_0^\beta d\lambda(d/d\lambda)(e^{(\lambda-\beta)H}Be^{-\lambda H})=[B, e^{-\beta H}]\,.$$

By virtue of the basic properties of the trace, we obtain two relations

$$\operatorname{Tr} A(x)^* A(y) = \operatorname{Tr} A((x+y)/2)^* A((x+y)/2) \geqq 0$$

$$|\operatorname{Tr} A(x)^* A(y)|^2 \leqq \operatorname{Tr} A(x)^* A(x) \operatorname{Tr} A(y)^* A(y)$$

which, if taken together, prove the inequality

$$f((x+y)/2) \leqq \tfrac{1}{2}(f(x)+f(y)) \tag{7}$$

for the real valued function $f$ given by

$$f(x) = \log \operatorname{Tr} A(x)^* A(x)\,.$$

Since the function $f$ is continuous, the inequality (7) states that $f$ is convex.

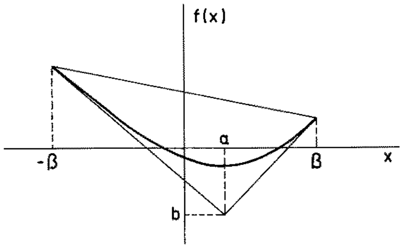


**Fig. 1**

In particular $f$ is convex for $-\beta \leqq x \leqq \beta$ and hence stays inside the triangle (Fig. 1) given by the vertices $(\beta, f(\beta))$, $(-\beta, f(-\beta))$, and $(a, b)$, where the coordinates $a$ and $b$ are to be calculated from

$$f(\beta) + (a-\beta) f'(\beta) = f(-\beta) + (a+\beta) f'(-\beta) = b\,.$$

We emphasize the fact that, given $\beta$, the triangle is completely determined by the following four expectation values

$$\langle A^* A \rangle_{\beta H} = e^{f(\beta)}, \qquad \langle A A^* \rangle_{\beta H} = e^{f(-\beta)}$$

$$\langle [A^*, H] A \rangle_{\beta H} = \langle A^* [H, A] \rangle_{\beta H} = 2 f'(\beta) e^{f(\beta)} \tag{8}$$

$$\langle [A, H] A^* \rangle_{\beta H} = \langle A [H, A^*] \rangle_{\beta H} = -2 f'(-\beta) e^{f(-\beta)} \tag{9}$$

and the geometrical assertion is adequately represented by the following bounds on $f(x)$:

$$(\beta + x)(2\beta)^{-1} f(\beta) + (\beta - x)(2\beta)^{-1} f(-\beta) \geqq f(x)$$

$$f(x) \geqq \begin{cases} f(\beta) + (x-\beta) f'(\beta) & a \leqq x \leqq \beta \\ f(-\beta) + (x=\beta) f'(-\beta) & -\beta \leqq x \leqq a\,. \end{cases}$$

Let us first concentrate on the upper bound. Taking the exponential and carrying out the integration we are lead to the inequality

$$\int_{-\beta}^{\beta} dx e^{f(x)} \leqq 2\beta (e^{f(\beta)} - e^{f(-\beta)}) / (f(\beta) - f(-\beta))\,,$$

thereby proving the first desired relation

$$(A, A) \leqq \beta/2 \langle \{A^*, A\} \rangle_{\beta H} r / \tanh^{-1} r \tag{10}$$

where

$$\tanh^{-1} r = \tfrac{1}{2} \log((1+r)/(1-r)), \qquad r = \langle [A^*, A] \rangle_{\beta H} / \langle \{A^*, A\} \rangle_{\beta H}$$

and $\{A, B\} = AB + BA$. Since $r^{-1} \tanh^{-1} r \geqq 1$ for real $r$, a weaker statement is also implied:

$$(A, A) \leqq \beta/2 \langle \{A^*, A\} \rangle_{\beta H}$$

which was previously derived and used to obtain Bogoliubov's inequality [5].

Next, we turn to the lower bound for $f(x)$. By a simple integration,

$$\int_{-\beta}^{\beta} dx e^{f(x)} \geqq (e^b - e^{f(-\beta)})/f'(-\beta) + (e^{f(\beta)} - e^b)/f'(\beta)$$

which, after a little algebra, can be brought into the form

$$(A, A) \geqq 1/c \{\alpha \langle AA^* \rangle_{\beta H} + (1-\alpha) \langle A^*A \rangle_{\beta H} - \langle AA^* \rangle_{\beta H}^{\alpha} \langle A^*A \rangle_{\beta H}^{1-\alpha} e^{-\beta c}\} \tag{11}$$

where $\alpha$ and $c$ may be obtained from the equations

$$\alpha \langle [A, H] A^* \rangle_{\beta H} = c \langle AA^* \rangle_{\beta H}$$

$$(1-\alpha) \langle [A^*, H] A \rangle_{\beta H} = c \langle A^*A \rangle_{\beta H} .$$

If $A = A^*$, the inequalities (10) and (11) specialize to

$$\langle A^2 \rangle_{\beta H} (1 - e^{-\beta c})/c \leqq (A, A) \leqq \beta \langle A^2 \rangle_{\beta H} \tag{12}$$

where $c$ now satisfies

$$4c \langle A^2 \rangle_{\beta H} = \langle [[A, H], A] \rangle_{\beta H} = ([A, H], [A, H]) \tag{13}$$

and therefore $c \geqq 0$ and $c = O(\beta)$ as $\beta \to 0$.

## 3. Infinite Systems

The next problem we encounter is to give meaning to various expressions like $(A, B)$ and $\langle [A, H] A^* \rangle_{\beta H}$ in the thermodynamic limit, i.e. if we pass from finite to infinite systems. Here, we must refrain from considering global observables and restrict ourselves to quasilocal operators accommodated within a $C^*$-algebra $\mathfrak{A}$ which we always assume to be simple (i.e. it has no nontrivial two-sided *-ideals). As a substitute for Gibbs' formula

$$\langle A \rangle_{\beta H} = \mathrm{Tr}\, e^{-\beta H} A / \mathrm{Tr}\, e^{-\beta H}$$

we characterize the equilibrium state by the KMS condition [6; Chapter 7.6]: For $A, B \in \mathfrak{A}$ there exists a function $F_{AB}(z)$, analytic in the strip $0 < \mathrm{Im}\, z < \beta$ and continuous for $0 \leqq \mathrm{Im}\, z \leqq \beta$ such that for real $t$

$$F_{AB}(t) = \langle BA_t \rangle_{\beta H} \quad \text{and} \quad F_{AB}(t + i\beta) = \langle A_t B \rangle_{\beta H}$$

where

$$A_t = e^{iHt} A e^{-iHt}.$$

Apparently, this function serves to define a scalar product on $\mathfrak{A}$:

$$(A, B) = \int_0^\beta dx F_{A^*B}(ix)$$

which, for finite systems, is easily shown to coincide with the previously defined product (3). Let us now assume that the infinite system under consideration emerges as a limit of suitably defined finite systems. Then the function $f(x) = \log F_{A^*A}(i(\beta + x)/2)$, being a limit of convex functions, is itself convex for $-\beta \leqq x \leqq \beta$. It may or may not be differentiable at the endpoints of that interval. If it is, then $\langle [A^*, H]A \rangle_{\beta H}$ and $\langle [A, H]A^* \rangle_{\beta H}$ exist and are given by (8) and (9) respectively. All inequalities derived for finite systems then also hold for the infinite system. We now turn to the susceptibility of a single spin in a heat bath. Abstractly speaking, by a "heat bath" we mean a tripel $(\mathscr{H}_0, \mathfrak{A}_0, H_0)$ consisting of a Hilbert space $\mathscr{H}_0$, a concrete $C^*$-Algebra $\mathfrak{A}_0$ of operators on $\mathscr{H}_0$ and a hamiltonian $H_0$, such that time translations act continuously on $\mathfrak{A}_0$ and that there exists a KMS state $\langle \cdot \rangle_{\beta H_0}$ on $\mathfrak{A}_0$. The total system, spin + heat bath, may then be represented by a tripel $(\mathscr{H}, \mathfrak{A}, H)$ where

$$\mathscr{H} = \mathscr{H}_0 \otimes \mathbb{C}^{2s+1}$$

$$\mathfrak{A} = \mathfrak{A}_0 \otimes M_{2s+1}(\mathbb{C})$$

$$H = H_0 \otimes I + H^k \otimes S_k. \tag{14}$$

Here, $M_n(\mathbb{C})$ stands for the algebra of all complex $n \times n$-matrices and, as for the hamiltonian, summation over $k = 1, 2, 3$ is tacitly assumed. The interaction is linear in $S$ and therefore, except for $s = 1/2$, it is not the most general Ansatz. However, it underlies the Kondo model [7]. Intuitively, if the operators $H^k$ are sufficiently "gentle", the total system will admit a KMS state as well.

From now on the crucial, although by no means compelling, assumption will be made that the operators $H^k$ belong to $\mathfrak{A}_0$. This assumption, phrased in a more physical language, means that the perturbation is local which is the key assumption of the Kondo model.

To establish the existence of an equilibrium state for the locally perturbed system we first observe that the uncoupled system $(\mathscr{H}, \mathfrak{A}, H_0 \otimes \mathbb{1})$ admits a unique KMS state such that

$$\langle A_0 \otimes a \rangle_{\beta H_0 \otimes \mathbb{1}} = \langle A_0 \rangle_{\beta H_0} (2s+1)^{-1} \operatorname{Tr} a$$

for $A_0 \in \mathfrak{A}_0$ and $a \in M_{2s+1}(\mathbb{C})$. By assumption, the interaction part of the hamiltonian,

$$V = H^k \otimes S_k$$

is an element of the algebra $\mathfrak{A}$. Thus, appealing to a general result of Araki [8], we conclude that $(\mathscr{H}, \mathfrak{A}, H)$ admits a KMS state

$$\langle A \rangle_{\beta H} = F(A)/F(\mathbb{1}) \qquad A \in \mathfrak{A} \tag{15}$$

where the positive functional $F$ on $\mathfrak{A}$ is defined by the perturbation expansion

$$F(A)=\langle A\rangle_{\beta H_0\otimes\mathbb{1}}+\sum_{n=1}^{\infty}(-1)^n\int_0^{\beta}dx_n\int_0^{x_n}dx_{n-1}\dots\int_0^{x_2}dx_1 f_n^A(x_1,\dots,x_n)$$

where $f_n^A$ is the unique analytic function in $n$ variables satisfying

$$\begin{aligned}&f_n^A(-it_1,\dots,-it_m,\beta-it_{m+1},\dots,\beta-it_n)=\langle V_{t_{m+1}}\dots V_{t_n}AV_{t_1}\dots V_{t_m}\rangle_{\beta H_0\otimes\mathbb{1}}\\&V_t=e^{itH_0}H^ke^{-itH_0}\otimes S_k\end{aligned}\tag{16}$$

for $m=0,\dots,n$ and any real $t_1,\dots,t_n$. The domain of analyticity is known to contain the tube $T_S=\{z\in\mathbb{C}^n;\,\mathrm{Re}\,z\in S\}$ with basis $S\subset\mathbb{R}^n$ given by the inequalities $0<x_1<x_2<\dots<x_n<\beta$ [9]. It should perhaps be stressed that the perturbation series converges absolutely for any fixed temperature $\beta^{-1}$. This conclusion can be drawn from the estimate

$$|f_n^A(z)|\leqq\|A\|\,\|V\|^n\tag{17}$$

valid for $z\in T_S$, implying that $F(A)$ is entire analytic with respect to the coupling constant

$$J=\|V\|$$

and that it is of at most exponential growth: $|F(A)|\leqq\|A\|\exp\beta J$. We shall now give the details of the proof of (17) for finite systems. On writing $K=H_0\otimes\mathbb{1}+\|H_0\|\mathbb{1}$ we have

$$f_n^A(z)=\mathrm{Tr}\,Ae^{-z_1K}Ve^{(z_1-z_2)K}V\dots e^{(z_{n-1}-z_n)K}Ve^{(z_n-\beta)K}/\mathrm{Tr}\,e^{-\beta K}$$

which is entire analytic. Since $K\geqq0$, $|f_n^A(z)|$ is bounded in the tube $T_S$ and by an extension of the "three lines theorem" to several complex variables [10; Chapter VI, Theorem 2] the function

$$F_n^A(x)=\sup_{t\in\mathbb{R}^n}|f_n^A(x-it)|$$

is logarithmically convex on the convex set $\bar{S}=\{x\in\mathbb{R}^n;\,0\leqq x_1\leqq\dots\leqq x_n\leqq\beta\}$ assuming its supremum in one of the extreme points of $\bar{S}$. Since $\bar{S}$ is a $n$-dimensional simplex, its extreme points are the vertices $x^0,x^1,\dots,x^n$ with coordinates $x_i^m=0$ if $i<m$ and $x_i^m=\beta$ if $i\geqq m$. It is quickly realized that $f_n^A(x-it)$ assumes the value (16) for $x=x^m$. Therefore, $|f_n^A(x^m-it)|\leqq\|A\|\,\|V\|^n$ which proves (17). It seems hopeless to apply the perturbation expansion in the limit $\beta=\infty$; i.e. at zero temperature. The worst models in this respect are those satisfying $[H_0,H^k]=0$, where the $n$th order corrections to $\langle A\rangle$ and $(A,A)$ in general grow like $\beta^n$ resp. $\beta^{n+1}$. There are better behaved models, e.g. of the Kondo type, where the second order correction to the susceptibility grows like $\beta\log\beta$ instead of $\beta^3$. However, this does in no way reveal the true behavior of the quantity under study.

A second remark concerns the denominator in (15). We have

$$F(\mathbb{1})\geqq1\tag{18}$$

and so it never becomes small. To prove this result, we start from Klein's inequality [6; Chapter 2.5]

$$\operatorname{Tr}\{e^{-A}-e^{-B}+(A-B)e^{-B}\}\geqq 0$$

valid for arbitrary hermitian $n\times n$-matrices $A$ and $B$.

On putting $A=\beta H$ and $B=\beta H_0\otimes\mathbb{1}$ in a finite system we obtain

$$\operatorname{Tr}e^{-\beta H}-\operatorname{Tr}e^{-\beta H_0\otimes\mathbb{1}}\geqq -\beta/(2s+1)\operatorname{Tr}e^{-\beta H_0}H^k\operatorname{Tr}S_k=0$$

as a consequence of $\operatorname{Tr}S_k=0$.

Therefore,

$$F(\mathbb{1})=\langle e^{-\beta H}e^{\beta H_0\otimes\mathbb{1}}\rangle_{\beta H_0\otimes\mathbb{1}}=\operatorname{Tr}e^{-\beta H}/\operatorname{Tr}e^{-\beta H_0\otimes\mathbb{1}}\geqq 1$$

and (18) is still valid for infinite systems appearing as limits of finite systems.

## 4. Bounds on the Susceptibility

We are now in the position to apply the correlation inequality (12) to the operator $A=\mathbb{1}\otimes S_3$, thereby obtaining bounds for the susceptibility

$$\chi=(A,A)$$

The crucial property of $A$ is $[A,H]\in\mathfrak{A}$ though $H\notin\mathfrak{A}$ in all cases of interest. Note that, in any rotational invariant theory, $\langle A^2\rangle_{\beta H}=1/3\,s(s+1)$ and

$$0\leqq\langle[[A,H],A]\rangle_{\beta H}=-2/3\langle V\rangle_{\beta H}$$

which simplifies the result:

$$1/3\,s(s+1)(1-e^{-\beta c})/c\leqq\chi\leqq 1/3\,s(s+1)\beta$$
$$c=-[2s(s+1)]^{-1}\langle V\rangle_{\beta H}\geqq 0\,.$$

We see that in general the susceptibility is smaller than the Curie law predicts but exceeds some positive quantity involving the thermal average of the interaction energy which is negative. If this energy is small as compared to $kT$, the susceptibility is close to its Curie value.

Note that $c^{-1}(1-e^{-\beta c})$ is a monotone decreasing function of $c$. This suggests to look for upper bounds on $-\langle V\rangle_{\beta H}$. The obvious bound $-\langle V\rangle_{\beta H}\leqq\|V\|=J$ is not the best possible for all temperatures. A more refined analysis yields

$$-\langle V\rangle_{\beta H}\leqq J\tanh\beta J\,. \tag{19}$$

This way we get a result which no longer involves the details of the dynamics:

$$\begin{aligned}&1/3\,s(s+1)(1-e^{-\varepsilon\beta})/\varepsilon\leqq\chi\leqq 1/3\,s(s+1)\beta\\&\varepsilon=J\tanh\beta J/2s(s+1)\,.\end{aligned}\tag{20}$$

In order to prove (19) we consider the thermal average $\langle V\rangle$ with respect to the hamiltonian $H_0\otimes\mathbb{1}+\lambda V$ and obtain

$$\beta\langle V\rangle^2-d\langle V\rangle/d\lambda=(V,V)\leqq\beta\langle V^2\rangle\leqq\beta J^2\,.$$

Upon setting $f(\lambda)=\tanh^{-1}(-J^{-1}\langle V\rangle)$ we have $f'(\lambda)\leqq\beta J$ and $f(0)=0$ implying $f(\lambda)\leqq\beta J\lambda$ which, for $\lambda=1$, is the assertion (19). It has become common practice to plot $\chi^{-1}$ against $T$. The allowed area for such a plot is shown in Fig. 2. As a measure for the deviation from the Curie law, we introduce the quantity

$$\delta=\sup_T(\chi^{-1}-3kT/s(s+1))$$

which not only proves to be finite but also tends to zero for small $J$ because

$$\delta\leqq\Delta\sup_{x>0}(1/(1-e^{-x})-1/x)=\Delta=3J/2s^2(s+1)^2\,. \tag{21}$$

It should be stressed that this behavior of $\delta$ cannot be inferred from perturbation theory.

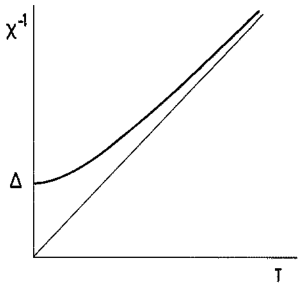


Fig. 2

## 5. Nonzero External Field

Our next problem concerns the mean polarization caused by a homogeneous magnetic field in the direction of the 3-axis. We shall restrict the discussion to the simplest case which is $s=1/2$ and write

$$\mathbb{1}\otimes S_k=\tfrac{1}{2}\sigma_k\,.$$

The total hamiltonian now reads

$$H'=H-x\sigma_3 \qquad x\geqq 0$$

where we introduced a variable $x$ proportional to the magnetic field. Thermal averages are taken with respect to $H'$. However, we shall shorten the notation and omit the subscript $\beta H'$, writing for instance

$$d\langle\sigma_3\rangle/dx=(\sigma_3,\sigma_3)-\beta\langle\sigma_3\rangle^2\,.$$

Since $|\langle\sigma_3\rangle|\leqq 1$ for all $x$, we may set $\langle\sigma_3\rangle=\tanh y(x)$ and thus obtain

$$y'(x)=(1-\langle\sigma_3\rangle^2)^{-1}d\langle\sigma_3\rangle/dx=\langle A^2\rangle^{-1}(A,A)$$

where $A=\sigma_3-\langle\sigma_3\rangle\mathbb{1}$. In particular, $4\chi=y'(0)$. From the conclusion reached in Section 2 we know that

$$0\leqq y'(x)\leqq\beta\,.$$

Since $\langle\sigma_3\rangle=0$ for $x=0$ assuming rotational invariance, we may write

$$\langle\sigma_3\rangle=\tanh\int_0^x d\xi y'(\xi)$$

thereby establishing the following results:

$\langle\sigma_3\rangle$ is a monotone function of the magnetic field variable $x$ and is majorized by the Brillouin function for a free spin, i.e.

$$0\leqq\langle\sigma_3\rangle\leqq\tanh\beta x\,.$$

In order to improve upon the lower bound, we obviously need, with regard to (12), and upper bound for

$$c=\tfrac{1}{2}\langle[A,H']A\rangle\langle A^2\rangle^{-1}$$

the problem being that there can be no estimate uniformly in $x$, since $\langle A^2\rangle$ tends to zero as $x$ increases. In this situation the best general result is obtained by applying Cauchy's inequality:

$$c\leqq\tfrac{1}{2}\langle A^2\rangle^{-\frac{1}{2}}\langle(i[A,H'])^2\rangle^{\frac{1}{2}}\leqq\tfrac{1}{2}\|[\sigma_3,V]\|(1-\langle\sigma_3\rangle^2)^{-\frac{1}{2}}$$
$$\leqq J\cosh y\,.$$

Then the essential content of (12) is the differential inequality

$$(1-e^{-\beta J\cosh y})/J\cosh y\leqq y'\leqq\beta \tag{22}$$

to be supplemented by $y(0)=0$. Because $y(x)$ is monotone, we may pass to the inverse function $x(y)$, thus obtaining the inequality

$$x'(y)\leqq J\cosh y(1-e^{-\beta J\cosh y})^{-1}\,.$$

Integrating both sides and introducing the function

$$\phi_\alpha(y)=\int_0^y dt\cosh t(1-e^{-\alpha\cosh t})^{-1}\qquad\alpha>0$$

we get

$$x(y)=\int_0^y dt x'(t)\leqq J\phi_{\beta J}(y)\,.$$

We emphasize that both $x$ and $\phi_\alpha$ are monotone functions of $y$. Therefore, $\phi_\alpha^{-1}$ exists and $\phi_{\beta J}^{-1}(J^{-1}x)\leqq y(x)$. Summarizing:

$$\tanh\phi_{\beta J}^{-1}(J^{-1}x)\leqq\langle\sigma_3\rangle\leqq\tanh\beta x\,. \tag{23}$$

For small $\beta$ these bounds are very tight, they fall apart if $\beta$ becomes large. Still, at zero temperature we get an interesting answer. Since $\phi_\infty(y)=\sinh y$, we conclude that

$$x(J^2+x^2)^{-1/2}\leqq\lim_{\beta\to\infty}\langle\sigma_3\rangle\leqq 1 \tag{24}$$

assuming that the limit exists. Although for any finite $\beta$

$$\lim_{x \to 0} \langle \sigma_3 \rangle = 0$$

it is feasible that

$$\lim_{x \to 0} \lim_{\beta \to \infty} \langle \sigma_3 \rangle \neq 0$$

and consistent with (24).

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Communicated by J. L. Lebowitz

Received June 10, 1975