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Ground-State Energy of a Heisenberg-Ising Lattice

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The Heisenberg-Ising Hamiltonian $H=-\frac{1}{2}\{\alpha(\sigma_x\sigma_x'+\sigma_y\sigma_y')+\epsilon(\sigma_z\sigma_z')\}$ for rectangular one-, two-, or three-dimensional lattices are considered. The sum is over nearest neighbors and $\Delta=\epsilon/\alpha$ measures the anisotropy of the coupling. Upper and lower bounds for the ground-state energy are established and these bounds apply equally well to lattices of one, two, or three dimensions. Furthermore, it is shown that the ground-state energy per nearest-neighbor pair is nondecreasing as the dimension of the lattice (one, two or three) increases.

INTRODUCTION AND DEFINITIONS

THIS paper discusses some properties of the eigenvalues of the following Hamiltonian:

$$H(\alpha,\epsilon)=-\tfrac{1}{2}\sum\{\alpha(\sigma_x\sigma_x'+\sigma_y\sigma_y')+\epsilon\sigma_z\sigma_z'\}\,, \tag{1}$$

where the sum extends over all nearest-neighboring pairs of spins $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$ on a lattice. σ_x, σ_y, σ_z are the Pauli spin matrices at a particular site.

$$(\sigma_x^2=\sigma_y^2=\sigma_z^2=1)\,,$$

α and ϵ are numerical constants. We consider one-dimensional (linear), two-dimensional (square), and three-dimensional (simple-cubic) lattices. For definiteness we consider only periodic lattices with the number of sites along each side even.

The Hamiltonian (1) has been a subject of study of many papers.[1] Our interest in it originated in the recent discussions[2] of the quantum lattice gas[3] as a model of the critical phenomena in liquid-gas transitions.[4]

We shall study the lowest eigenvalue $\mathfrak{N}zF(\alpha,\epsilon,y)$ and the highest eigenvalue $\mathfrak{N}zG(\alpha,\epsilon,y)$ of (1) for a fixed eigenvalue y of

$$Y=(1/\mathfrak{N})(\textstyle\sum\sigma_z)\,, \tag{2}$$

where z is the number of nearest neighbors per site and $\mathfrak{N}$ is the total number of spins. (Obviously H commutes with Y.)

Theorem 1: $H(\alpha,\epsilon)$ and $H(-\alpha,\epsilon)$ have the same spectrum for the same eigenvalue y of Y.

Proof: Consider the operator

$$A=\textstyle\prod'\sigma_z\,, \tag{3}$$

where the product runs thru every other side. (In the two-dimensional case, for example, the sites whose σ_z are included in the product form a checkerboard pattern.) It is clear that A commutes with Y, and

$$AH(\alpha,\epsilon)A^{-1}=H(-\alpha,\,\epsilon)\,. \tag{4}$$

The theorem follows.

This theorem tells us that the sign of α is irrelevant if one is interested only in the spectrum. We can, therefore, take α to be positive and will simplify our discussion by considering the Hamiltonian $H(1,\Delta)=(1/\alpha)H(\alpha,\epsilon)$. Furthermore, from (4) it follows that

Theorem 2: $F(\alpha,\epsilon,y)=-G(\alpha,\,-\epsilon,y)$.

Thus we need only study $F(1,\Delta,y)$ to obtain all information about the maximum and minimum eigenvalues of $H(\alpha,\epsilon)$.

PROPERTIES OF $F(1,\Delta,y)$

Theorem 3: $F(1,\Delta,y)=F(1,\Delta,\,-y)$.

Proof: The operator

$$B=\textstyle\prod\sigma_x\,, \tag{5}$$

where the product extends thru the whole lattice anticommutes with Y and commutes with H. Hence the theorem.

Theorem 4: $F(1,\Delta,1)=-\frac{1}{4}\Delta$.

Proof: The state with $y=1$ has all spins lined up in the $+z$ direction. For such a state, only the term $\sum\sigma_z\sigma_z'$ contributes to H and one easily obtains this theorem.

Theorem 5:

$$F(1,\Delta,y)\leqq-\tfrac{1}{4}-\tfrac{1}{4}(\Delta-1)(\mathfrak{N}y^2-1)/(\mathfrak{N}-1)\,. \tag{6}$$

Proof: Consider a state symmetrical with respect to all spins of the lattice

ψ_0 = normalized sum with equal weights of all states representing spin arrangements with a fixed number of up spins. (7)

[1] Some of the results of this paper are well known or implied in much of published literature. For references to some of these see J. C. Bonner and M. Fisher, Phys. Rev. **135**, A640 (1964).

[2] C. N. Yang and C. P. Yang, Phys. Rev. Letters **13**, 303 (1964).

[3] The lattice gas was first discussed by T. D. Lee and C. N. Yang, Phys. Rev. **87**, 410 (1952); the quantum lattice gas was first discussed by T. Matsubara and H. Matsuda, Progr. Theoret. Phys. (Kyoto) **16**, 569 (1956); **17**, 19 (1957). See also R. T. Whitlock and P. R. Zisel, Phys. Rev. **131**, 2409 (1963).

[4] M. R. Moldover and W. A. Little, Phys. Rev. Letters **15**, 54 (1965).

To evaluate the expectation value of H with respect to this state, we write

$$H(1,\Delta)=-\tfrac{1}{2}\sum[\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'+(\Delta-1)\sigma_z\sigma_z']. \quad (8)$$

ψ_0, being symmetrical with respect to any two spins, belongs to the triplet state for any two spins. Thus

$$\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'\psi_0=\psi_0. \quad (9)$$

Also

$$\langle\psi_0|(\sum\sigma_z)^2|\psi_0\rangle=\mathfrak{N}+(\mathfrak{N}^2-\mathfrak{N})\langle\psi_0|\sigma_z\sigma_z'|\psi_0\rangle. \quad (10)$$

Equation (6) follows immediately.

Theorem 6:

$$F(1,\Delta,y)\geqq -\tfrac{1}{4}+\tfrac{1}{4}(\Delta-1)(1-2|y|), \quad \text{if} \quad \Delta\leq 1; \quad (11)$$

$$F(1,\Delta,y)\geqq -\tfrac{1}{4}\Delta, \quad \text{if} \quad \Delta>1. \quad (12)$$

Proof: To prove (11), we have from (8)

$$\mathfrak{N}zF(1,\Delta,y)\geqq\sum[-\tfrac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}']_{\min}+\tfrac{1}{2}(1-\Delta)[\sum\sigma_z\sigma_z']_{\min}.$$

But $[-\frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}']_{\min}=-\frac{1}{2}$. To find the minimum of $\sum\sigma_z\sigma_z'$ for a given y we notice that it is attained when the number of antiparallel neighboring spin pairs is maximized. Equation (11) is then easily obtained.

To prove (12) we use the fact that each term in the sum in (8) has a maximum eigenvalue equal to Δ, if $\Delta>1$.

Theorem 7: $F(1,\Delta,y)$ is a convex function of Δ for fixed y.

Proof: $H(1,\Delta)$ is linear in Δ. Thus if

$$\Delta=a\Delta_1+(1-a)\Delta_2,\ 1>a>0,$$

then

$$H(1,\Delta)=aH(1,\Delta_1)+(1-a)H(1,\Delta_2).$$

The theorem follows immediately.

LIMIT AS LATTICE SIZE $\rightarrow\infty$

We introduce, for any finite lattice, an interpolated $\mathfrak{F}$ as a function of y:

$$\mathfrak{F}(1,\Delta,y)=F(1,\Delta,y'),$$

where y' is the largest eigenvalue of Y which is $\leqq y$. $\mathfrak{F}$ is thus defined for all y between $(-1, 1)$. The question of the existence of a limit for $\mathfrak{F}$ as the lattice size $\rightarrow\infty$ in all directions is similar to the problem in classical mechanics of the existence of a limit for thermodynamic functions.[5] The present problem can be simply treated with the following lemmas. We limit our considerations to three dimensions in the lemmas and theorems of this section. But they hold similarly for any dimension. A fundamental point in these considerations is that the interaction between two neighboring sites is a bounded operator. Surface effects are thus negligible for big volumes.

Lemma 1: Let box L be of size $mn\times mn\times mn$, and box S of size $n\times n\times n$, where m=integer. Let y_S be a possible y value for box S. Then

$$F_L(1,\Delta,y_S)\leqq F_S(1,\Delta,y_S)+K_1/n, \quad (13)$$

where K_1 is a numerical constant independent of m, n and y_S.

Proof: Divide L into m^3 small boxes S. Take as a trial wave function for L, the product of the wave functions of the ground states of the small boxes S. The interactions between the different boxes S is bounded from above. One thus obtains Lemma 1.

Lemma 2: If a series of numbers a_n satisfies

$$a<a_n, \quad a_{n+1}<a_n+b_{n+1},$$

and $\sum^\infty b_n$ is convergent, then $\lim_{n\rightarrow\infty} a_n$ exists.

Proof: Define

$$a_n'=a_n-\sum_2^n b_n.$$

Then

$$a_{n+1}'<a_n'$$

and a_n' is bounded below. Thus $a_n'\rightarrow$ a limit as $n\rightarrow\infty$. The lemma follows immediately.

Lemma 3: For any given box,

$$|F(1,\Delta,y_1)-F(1,\Delta,y_2)|\leqq K_2|y_1-y_2| \quad (14)$$

for all y_1, y_2 in any closed interval (a,b), $0<a<b<1$. K_2 is independent of y_1 and y_2, independent of the size of the box; but dependent on Δ, a and b.

Proof: Consider the normalized ground state ψ for the eigenvalue y_1 of Y. Let $\sigma_\pm=\frac{1}{2}(\sigma_x\pm i\sigma_y)$ at a specific site s. We have

$$H(1,\Delta)\sigma_+=\sigma_+H(1,\Delta)+D,$$

where D is a sum of six terms each relating to a neighboring pair of spins containing s. Thus

$$\langle\sigma_+\psi|H(1,\Delta)|\sigma_+\psi\rangle =\mathfrak{N}zF(1,\Delta,y_1)\langle\sigma_+\psi|\sigma_+\psi\rangle+\langle\sigma_+\psi|D\psi\rangle. \quad (15)$$

But

$$\langle\sigma_+\psi|\sigma_+\psi\rangle=\langle\psi|\sigma_+{}^+\sigma_+\psi\rangle =\tfrac{1}{2}\langle\psi|1-\sigma_z|\psi\rangle=\tfrac{1}{2}(1-y_1). \quad (16)$$

Also

$$|\langle\sigma_+\psi|D\psi\rangle|^2\leqq\langle\sigma_+\psi|\sigma_+\psi\rangle\langle D\psi|D\psi\rangle =\tfrac{1}{2}(1-y_1)\langle\psi|D^+D|\psi\rangle\leqq K_3. \quad (17)$$

Now use $\sigma_+\psi$ as a trial wave function. It describes a state with one more up spin than ψ. Thus it belongs to the eigenvalue $y_1+2/\mathfrak{N}$ of Y. Equations (15)–(17) show that

$$F(1,\Delta,y_1+2/\mathfrak{N})\leqq F(1,\Delta,y_1)+K_4/\mathfrak{N}. \quad (18)$$

[5] L. Von Hove, Physica **15**, 951 (1949). The problem for a grand canonical ensemble was discussed by C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952). Recent discussions are found in D. Ruelle, Helv. Phys. Acta **36**, 183, 789 (1963); Michael E. Fisher, Archives Rational Mechanics Analysis **17**, 377 (1964).

By using $\sigma_-\psi_1$ as a trial wave function where ψ_1 is the ground state for the eigenvalue $y_1+2/\mathfrak{N}$ of Y, one obtains an identity similar to (18). Combining the two results one obtains

$$|F(1,\Delta,y_1+2/\mathfrak{N})-F(1,\Delta,y_1)|<2K_2/\mathfrak{N}. \quad (19)$$

(14) then follows by repeated application of (19).

Lemma 4: Consider the series of boxes: $2\times2\times2$, $4\times4\times4$, $8\times8\times8$, etc. For these boxes (of size $2^l\times2^l\times2^l$),

$$f(\Delta,y)=\lim \mathfrak{F}(1,\Delta,y)$$

exists as $l\rightarrow\infty$.

Proof: Consider two boxes $S=2^l\times2^l\times2^l$ and $L=2^{l+1}\times2^{l+1}\times2^{l+1}$. Let y' be the largest eigenvalue of Y (for box S) that is $\leqq y$. Apply Lemma 1 to the two boxes S and L at y'. Use Lemma 3 to limit the difference of $\mathfrak{F}$ between y' and y. Lemma 2 then yields the present lemma. (Lemma 3 does not apply when $y=\pm1$. But then Theorems 3 and 4 give Lemma 4 immediately).

Theorem 8: Consider the periodic cubic boxes $n\times n\times n$.

$$f(\Delta,y)=\lim \mathfrak{F}(1,\Delta,y) \quad (20)$$

exists as $n\rightarrow\infty$.

Proof: Lemma 4 defines an f function. For any $\epsilon>0$ to prove that

$$\mathfrak{F}(1,\Delta,y)\leqq f(\Delta,y)+\epsilon \quad (21)$$

for sufficiently big n we take $n\geq M2^l$ where M and l are both big. We then compare the $n\times n\times n$ box with its subboxes $2^l\times2^l\times2^l$, obtaining (21). To prove that

$$\mathfrak{F}(1,\Delta,y)\geqq f(\Delta,y)-\epsilon \quad (22)$$

for sufficiently large n we choose a very large box $2^L\times2^L\times2^L$ and consider it a collection of M_1^3 boxes $n\times n\times n$ with some left over surface effects. $(M_1+1)n>2^L\geqq M_1n$. Equation (22) then follows for sufficiently large n (and M_1).

PROPERTIES OF $f(\Delta,y)$

Theorem 9: $f(\Delta,y)$ is a continuous function of y for $-1\leqq y\leqq1$. It concaves upwards. [i.e., if

$$y=ay_1+(1-a)y_2 \quad 1>a>0,$$
$$f(y)\leqq af(y_1)+(1-a)f(y_2)]. \quad (23)$$

Proof: The basic idea of the proof rests on the fact that if a big box V is divided into two subboxes V_1 and V_2 one can use as a trial wave function for V the product of the ground-state wave functions for boxes V_1 and V_2 with y values y_1 and y_2. Surface effects do not contribute to f. Thus one proves (23). The continuity of f in the open interval $-1<y<1$ follows from (23). To prove continuity at $y=\pm1$, use Theorems 3–6.

The following are immediate consequences of the theorems on F and the above theorem:

$$f(\Delta,y)=f(\Delta,-y), \quad (24)$$

$$f(\Delta,1)=-\tfrac{1}{4}\Delta, \quad (25)$$

$$f(\Delta,y)\leqq-\tfrac{1}{4}-\tfrac{1}{4}(\Delta-1)y^2 \quad (26)$$

$$f(\Delta,y)\geqq-\tfrac{1}{4}+\tfrac{1}{4}(\Delta-1)(1-2|y|) \quad \text{if} \quad \Delta\leqq1 \quad (27)$$

$$f(\Delta,y)\geqq-\tfrac{1}{4}\Delta \quad \text{if} \quad \Delta\geqq1. \quad (28)$$

$f(\Delta,y)$ is a convex function of Δ for fixed y. (29)

Theorem 10: $f(\Delta,y)=-\tfrac{1}{4}\Delta$ for $\Delta\geqq1$.

Proof: Relations (23), (24), (25), and (28) lead to this theorem directly.

Theorem 11: Let $f^{\mathrm{III}}(\Delta,y)$, $f^{\mathrm{II}}(\Delta,y)$ and $f^{\mathrm{I}}(\Delta,y)$ be the f functions for three, two and one dimensions. Then

$$f^{\mathrm{III}}(\Delta,y)\geqq f^{\mathrm{II}}(\Delta,y)\geqq f^{\mathrm{I}}(\Delta,y). \quad (30)$$

Proof: Consider a two-dimensional *periodic* lattice of size $m\times m$. We write

$$H^{\mathrm{II}}(1,\Delta)=[H^{\mathrm{I}}(1,\Delta)]_h+[H^{\mathrm{I}}(1,\Delta)]_v+D_1, \quad (31)$$

where $[H^{\mathrm{I}}(1,\Delta)]_h$ consists of all the horizontal links in H^{II} in the *open* $m\times m$ lattice plus m links to connect the *end of the* ith *row* with the *beginning of the* $(i+1)$th *row*. $[H^{\mathrm{I}}(1,\Delta)]_h$ describes thus the Hamiltonian of a one dimensional chain of m^2 spins forming one *cyclic* lattice. Similarly $[H^{\mathrm{I}}(1,\Delta)]_v$ is defined. $(-D_1)$ consists of all the $2m$ added connecting links minus the $2m$ links which make the original lattice periodic. Let ψ be the minimum eigenfunction of H^{II} for a given y. Taking the expectation value of (31) for ψ, we obtain

$$4m^2F^{\mathrm{II}}(1,\Delta,y)\geqq2\{[H^{\mathrm{I}}(1,\Delta)]_h\}_{\min\text{ at }y}+\{D_1\}_{\min}$$
$$=4m^2F^{\mathrm{I}}(1,\Delta,y)+\{D_1\}_{\min}.$$

The last term is $\leqq0(m)$ in absolute value. Thus

$$f^{\mathrm{II}}(\Delta,y)\geqq f^{\mathrm{I}}(\Delta,y),$$

for $y=$ rational. For irrational values of y use Theorem 9. The other inequality in (30) can be similarly proved.

Theorem 12:

$$f^{\mathrm{II}}(\Delta,y)\leqq\tfrac{1}{2}f^{\mathrm{I}}(\Delta,y)-\tfrac{1}{8}\Delta y^2, \quad (32)$$

$$f^{\mathrm{III}}(\Delta,y)\leqq\tfrac{2}{3}f^{\mathrm{II}}(\Delta,y)-\tfrac{1}{12}\Delta y^2. \quad (33)$$

Proof: Consider an $m\times m$ periodic lattice. Consider the normalized ground state wave function ψ_i for its ith row at a given y value for that row. Keeping the same y for all rows, let

$$\psi=\prod_{i=1}^{m}\psi_i.$$

Use ψ as a trial wave function of the whole $m\times m$ lattice:

$$4m^2F^{\mathrm{II}}(1,\Delta,y)\leqq2m^2F^{\mathrm{I}}(I,\Delta,y)$$
$$+\langle\psi|\sum(\text{vertical links})|\psi\rangle.$$

But for each vertical link the two spins are *independently* described in ψ. Thus

$$\begin{aligned}\langle\psi|\text{ one vertical link }|\psi\rangle &= -\tfrac{1}{2}\langle\psi|\sigma_x|\psi\rangle\langle\psi|\sigma_x'|\psi\rangle \\ &\quad -\tfrac{1}{2}\langle\psi|\sigma_y|\psi\rangle\langle\psi|\sigma_y'|\psi\rangle \\ &\quad -\tfrac{1}{2}\Delta\langle\psi|\sigma_z|\psi\rangle\langle\psi|\sigma_z'|\psi\rangle \\ &= -\tfrac{1}{2}\Delta[\langle\psi|\sigma_z|\psi\rangle]^2 \\ &= -\tfrac{1}{2}\Delta y^2.\end{aligned}$$

(32) follows. (33) can be similarly proved.

For suitable y and Δ (for example, $y=0$, $\Delta=$large negative) Theorem (12) gives more stringent upper bounds for f^{II} and f^{III} than (26).

Theorem 13:

$$\begin{aligned}\frac{\partial f}{\partial y}\Big|_{y=1} &= 0 && \text{for } \Delta\geqq 1, \\ &= -\tfrac{1}{2}(\Delta-1) && \text{for } \Delta\leqq 1.\end{aligned}$$

Proof: Use (26), (27) and Theorem 10.

This theorem yields the $T=0$ magnetic field $\mathcal{H}$ necessary to produce 100% magnetization.

$$\begin{aligned}\mathcal{H} = z\frac{\partial f}{\partial y} &= 0, && \text{for } \Delta\geqq 1; \\ &= z\tfrac{1}{2}(1-\Delta), && \text{for } \Delta\leq 1.\end{aligned}$$

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Temperature-Dependent Lifetimes of Nonequilibrium Fe^{3+} Ions in CoO from the Mössbauer Effect*

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The lifetime of the nonequilibrium Fe^{3+} state in a CoO:Co^{57} source has been determined in the temperature range 78 to 1000°K. The intensity of the ferrous state is highly temperature-dependent and was hardly detectable above 800°K. The width of the nuclear excited level of the nonequilibrium state is determined by the nuclear decay time τ and the atomic decay time $\theta(3)$. The expected changes in the linewidth of the nonequilibrium Fe^{3+} state in the Mössbauer spectra have been observed. The observed deviation of the temperature variation of the hf magnetic field at the nuclei of both Fe^{2+} and Fe^{3+} ions from that expected by the molecular-field theory may be due to a possible biquadratic exchange interaction in CoO, with $j/J_2 \simeq 0.022$.

1. INTRODUCTION

IN the electron-capture decays of nuclei various highly ionized atomic states are produced as a consequence of Auger electron emission.[1] It has been shown earlier[2] that the Mössbauer effect offers a possibility of detecting some of these nonequilibrium charge states whose lifetimes are comparable with that of the excited state of the nucleus producing the Mössbauer emission. In metallic lattices these highly charged nonequilibrium states relax to the stable state in a time very much smaller as compared to the nuclear lifetime and hence only the stable state is observed in the Mössbauer spectrum. However, employing dielectric source lattices in which the relaxation times can be of the order of the nuclear lifetime, some of the nonequilibrium charge states can be detected. Indeed, nonequilibrium Fe^{3+} state has been observed in cobalt oxide[3] and nickel oxide[4] using the Fe^{57} Mössbauer effect.

In nickel oxide we have reported[4] a strong temperature dependence of the intensity of the ferrous state which indeed vanished above about 466°K. The present paper deals with the temperature dependence of the lifetime and the linewidth of the nonequlibrium Fe^{3+} state in CoO over the temperature range, 78 to 1000°K. Wertheim[3] has reported earlier Fe^{57} Mössbauer measurements in CoO used as a source over the range 78°K to room temperature. Our observations, in this range of temperature, pertaining to the hf magnetic fields at the Fe^{2+} and Fe^{3+} nuclei are in agreement with those reported by Wertheim.[3] Above the room temperature, and indeed even below this, we observed a decrease in the intensity of the ferrous peak with increasing temperature to almost negligible value above about 800°K. This behavior is seen to be closely connected with the semiconducting properties of this oxide

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[1] I. Bergström, in *Beta- and Gamma-Ray Spectroscopy*, edited by K. Siegbahn (North-Holland Publishing Company, Amsterdam, 1955), p. 624.

[2] H. Frauenfelder and R. Steffen, in *Alpha, Beta and Gamma Ray Spectroscopy*, edited by K. Siegbahn (North-Holland Publishing Company, Amsterdam, 1964), Vol. 2, p. 1182. G. K. Wertheim, *Mössbauer Effect: Principles and Applications* (Academic Press Inc., New York, 1964), p. 100.

[3] G. K. Wertheim, Phys. Rev. **124**, 764 (1961).

[4] V. G. Bhide and G. K. Shenoy, Phys. Rev. **143**, 309 (1966).