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A Numerical Investigation of a Certain One-Dimensional Ising Model

Jimmy Green
Western Kentucky University

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Jimmy

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A NUMERICAL INVESTIGATION

OF A

CERTAIN ONE-DIMENSIONAL ISING MODEL

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A NUMERICAL INVESTIGATION

OF A

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Recommended 2-13-81
_____
(Date)

George P. Moon
Director of Thesis

Ed S. Dorman

D. L. Humphrey

Approved _February 20, 1981_
(Date)

Elmer Gray
Dean of the Graduate College

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF ILLUSTRATIONS

A NUMERICAL INVESTIGATION OF A CERTAIN ONE-DIMENSIONAL ISING MODEL

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Directed by: George C. Moore, Douglas L. Humphrey, and Ed S. Dorman

Department of Physics and Astronomy   Western Kentucky University

The model is a linear chain in which each spin interacts with its 2r nearest neighbors, the interaction energy being proportional to 1/r. Using a method similar to that of Montroll, the partition function of the model in the thermodynamic limit is shown to be related to the largest eigenvalue of a certain matrix. The largest eigenvalue of the matrix is determined numerically for $3 \leq r \leq 12$.

Also, a correct method is demonstrated for evaluating an improper limit of the model, in which the interaction range is set to the chain length before the limit of an infinite number of spins is taken. Previously published works have performed this calculation incorrectly.

Although the numerical results show some evidence of convergence to the improper limit, the results are inconclusive and furthermore raise doubts about the practicality of the numerical method in this context.

CHAPTER I

INTRODUCTION

A. Ising Models

In 1925 Ernst Ising[1] proposed a simplified model of ferro-
magnetism in order to study the temperature dependent transition to
a ferromagnetic state. Since then, the Ising model has been modified
and reinterpreted to encompass other types of order-disorder phenomena.
The chief value of these models is that they are frequently simple
enough to yield analytic information while being more or less physi-
cally realistic.

The model proposed by Ising describes a one-dimensional lattice
of particles, each particle capable of possessing either a plus, "spin
up" state, or a minus, "spin down" state. Each particle interacts via a
nonmagnetic force with its two adjacent neighbors. Ising showed that
this model does not possess a phase transition, which by definition
exists when the average energy per particle or one of its derivatives
becomes discontinuous at a certain temperature. It is now known that
any one-dimensional system with a finite interaction range can not
undergo a phase transition. Interest in Ising-type systems has
therefore turned to higher dimensional models and one-dimensional
models with infinite interaction ranges.

The three-dimensional Ising model, which is of the most interest

physically, has yet to be solved. The solution to the two-dimensional nearest neighbor problem was first given by Lars Onsager[2] in an important paper in 1944, and since then several other solutions have appeared. However, a solution for the two-dimensional model in a magnetic field has yet to be offered.

The one-dimensional Ising models, or "Ising chains," which have been studied are generally characterized by an interaction strength that depends inversely in some manner on the interaction distance. G. A. Baker[3] has made an approximate calculation which suggests that a model with an interaction strength that decreases as $\exp(-\gamma d)$, where γ is a parameter and d is the interaction distance, approaches a phase transition as γ approaches zero. Another approximate calculation of a model,[4] in which all interaction strengths are equal and which could be considered as a limiting case of Baker's model, also suggests the presence of a phase transition. Numerical treatments of a model[5] suggested to be more physically realistic, which has an interaction strength that depends inversely on a power of the interaction distance, indicate that a phase transition might occur for certain values of the exponent.

Although approximate calculations and numerical treatments can never prove the existence or nonexistence of critical points, it is hoped that such methods will at least provide insight into the behavior of a model. This paper examines a method of numerically evaluating the properties of an infinite length Ising chain with a finite interaction range. The properties of models with increasing interaction ranges are computed and tabulated.

B. Review of Basic Statistical Mechanics

According to currently accepted theories, the state of a system of particles is completely specified by giving either a denumerable set of quantum numbers of the system or a denumerable set of variables which are functions of the quantum numbers. Two states of a system are said to be distinct if at least one of the quantum numbers or variables assumes a different value in the two states. For a system with bound states only, such as an Ising chain, the quantum numbers are discrete, and the distinct states are therefore denumerable. It is convenient to label the distinct states of such a system by a single subscript.

Let $E_j(N)$ be the total energy of N particles in state j, k be the Boltzmann constant and $\beta \equiv 1/kT$, where T is the absolute temperature. Notice that the case $E_j = E_\ell$ with $j \neq \ell$ is possible. A postulate due to Boltzmann states that the relative probability of occurrence of state j is equal to the so-called Boltzmann factor, $\exp(-\beta E_j(N))$, which implies that the probability the system will be observed to be in state j is

$$P_j(N) = Q_N^{-1} \exp(-\beta E_j(N)) \, ,$$

where the canonical partition function Q_N is defined to be

$$Q_N \equiv \sum_{\{j\}} \exp(-\beta E_j(N)) \, , \tag{1}$$

the sum extending over all distinct states of the system.

The average observed total energy $\langle E(N) \rangle$ is then given by

$$\langle E(N) \rangle = \sum_{\{j\}} P_j(N) \ E_j(N)$$

$$= \frac{-\partial}{\partial \beta} \ \ln Q_N \ ,$$

and the average energy per particle ε_N is

$$\varepsilon_N = N^{-1} \langle E(N) \rangle \ .$$

The quantity of physical interest is the "thermodynamic limit" of the last expression, which by definition is obtained by letting the "volume" of the system and the number of particles in the system approach infinity while the average particle density remains finite. These limits should be taken before any other limiting operation, such as differentiation, is performed. Since such a procedure has proved to be impossible in general, one reverses the order of the limits. In the special cases in which the limits can be properly evaluated, the order is irrelevant.

Also, when one is interested in the bulk properties of matter, it is necessary to examine the role surface effects have on those properties. If the thermodynamic limit is taken in such a way that the ratio of "surface" particles to "interior" particles goes to zero, one is assured that the quantities obtained are representative of particle-particle, rather than particle-boundary, interactions. For a one-dimensional system, such as an Ising chain, the surface particles are merely the end particles in the chain.

The average energy per particle ε in the thermodynamic limit is given by

$$\varepsilon = \lim_{N \to \infty} \varepsilon_N$$

$$= \lim_{N \to \infty} \left(-\frac{\partial}{\partial \beta} \ln Q_N^{1/N} \right) , \tag{2}$$

where it is assumed that

$$\lim_{N \to \infty} \left(-\frac{\partial}{\partial \beta} \ln Q_N^{1/N} \right) = -\frac{\partial}{\partial \beta} \lim_{N \to \infty} \left(\ln Q_N^{1/N} \right) .$$

If one had an analytic expression for ε, then virtually all questions of thermodynamic interest could be answered. This paper is concerned in particular with the specific heat c_x at constant variable x,

$$c_x = \left. \frac{\partial \varepsilon}{\partial T} \right|_x ,$$

where the standard thermodynamic notation for differentiation has been used.

C. The Specific Model

Let $\sigma = (\sigma_j^k | 1 \leq j \leq N, 1 \leq k \leq r)$, where the superscript is an identifier, be a set of independent variables, each of which can assume the value +1 or -1 only. Such quantities are called "spin" variables. For this discussion, it is convenient to group σ into r subsets $\sigma^k = (\sigma_j^k | 1 \leq j \leq N)$; in a later section it will also be convenient to group σ into N subsets $\sigma_j = (\sigma_j^k | 1 \leq k \leq r)$. Furthermore, a cyclic subscript convention is adopted so that

$$\sigma_{j+nN}^k = \sigma_j^k$$

for any integer n. Notice that Eq. (3) implies that

$$\sigma_{j+nN} = \sigma_j .$$

Consider a model whose total energy $E_N(\sigma^1)$ is given by

$$\beta E_N(\sigma^1) = -r^{-1} \kappa \sum_{j=1}^{N} \sigma_j^1 \left(\sum_{i=1}^{r} \sigma_{j+i}^1 \right) , \qquad (4)$$

where $\kappa \equiv \beta J$ and J is a coupling constant. In figurative language, Eq. (4) gives the total energy of a one-dimensional Ising model of a ferromagnet with N spins in which cyclic (von Karman) boundary conditions have been imposed. Each spin interacts with its 2r nearest neighbors, the interaction energy between a pair of spins being $r^{-1} J \sigma_j^1 \sigma_k^1$, $j+1 \le k \le j+r$.

From the definition of the partition function, Eq.(1), the partition function of the model is

$$Q_N = \sum_{\sigma^1} \exp(-\beta E_N(\sigma^1)) ,$$

where the sum is over the 2^N distinct, ordered N-tuples of +1's and -1's in σ^1.

The value of Q_N is determined with the aid of a certain $2^r \times 2^r$ matrix $A(\beta)$, in which A is independent of N. It will be shown in Chapter II, Section B, that the partition function can be expressed as the trace of A^N. In terms of the eigenvalues of A, the partition function can be expressed as

$$Q_N = \sum_{\ell=1}^{2^r} (\lambda_\ell(\beta))^N .$$

The elements of A have a physical interpretation which precludes their possessing negative values. A theorem of Frobenius[6] states that the eigenvalue of largest magnitude of such a matrix is positive and nondegenerate. If the eigenvalue of largest magnitude is denoted by λ_1, then

$$\lim_{N \to \infty} (\lambda_\ell/\lambda_1)^N = 0 , \qquad 2 \le \ell \le 2^r ,$$

and

$$\lim_{N \to \infty} Q_N^{1/N} = \lim_{N \to \infty} \left(\lambda_1^N \left(1 + \sum_{\ell=2}^{2^r} (\lambda_\ell/\lambda_1)^N \right) \right)^{1/N}$$

$$= \lambda_1 \lim_{N \to \infty} \left(1 + \sum_{\ell=2}^{2^r} (\lambda_\ell/\lambda_1)^N \right)^{1/N}$$

$$= \lambda_1 .$$

Denoting λ_1 by λ, it follows from the definition of ε that

$$\varepsilon = \frac{-1}{\lambda} \frac{\partial \lambda}{\partial \beta}$$

It is convenient to express ε as the derivative with respect to the scaled inverse temperature κ. Since $\kappa = \beta J$,

$$\varepsilon = \frac{-1}{\lambda} \frac{\partial \kappa}{\partial \beta} \frac{\partial \lambda}{\partial \kappa}$$

$$= \frac{-J}{\lambda} \frac{\partial \lambda}{\partial \kappa} . \tag{6}$$

It is also convenient to differentiate ε with respect to κ^{-1}

to get the scaled specific heat. Let $t \equiv \kappa^{-1} = kT/J$. Then,

$$c_x = \frac{\partial t}{\partial T} \frac{\partial \varepsilon}{\partial t}\bigg|_x$$

$$= \frac{k}{J} \frac{\partial \varepsilon}{\partial t}\bigg|_x$$

$$= \frac{k}{J} \frac{\partial}{\partial t}\left(\frac{-J}{\lambda} \frac{\partial \lambda}{\partial \kappa} \right)\bigg|_x$$

$$= -k \frac{\partial}{\partial t}\left(\frac{1}{\lambda} \frac{\partial \lambda}{\partial \kappa} \right)\bigg|_x . \tag{7}$$

CHAPTER II

THEORETICAL METHODS

A. Evaluation of the Infinite Range Model

It was noted above (page 1) that a one-dimensional system with
a finite range of interaction can not possess a phase transition. At
this time, however, no one has succeeded in exactly evaluating the
proper thermodynamic limit

$$\lim_{r \to \infty} \left(\lim_{N \to \infty} \chi \right) ,$$

where χ is some variable of interest. In the hope of obtaining some
information about the model, various workers, notably Baker,[3] have
evaluated

$$\lim_{\substack{r = N \\ N \to \infty}} \chi .$$

The result is not merely questionable because of the improper limit;
it is obtained by using a result which is valid for positive definite
matrices only, which is not the case for the matrix involved. There-
fore, a proper derivation is given below of

$$\lim_{\substack{r = N \\ N \to \infty}} c_x .$$

9

By setting the interaction range equal to the chain length, the total energy of the model in Eq. (4) is given by

$$\beta\, E_N(\sigma^1) \;=\; -N^{-1}\, \kappa\, \sum_{j=1}^{N} \sigma_j^1 \sum_{i=1}^{N} \sigma_{i+j}^1$$

$$=\; -\kappa\, N^{-1} \left(\sum_{i=1}^{N} \sigma_i^1 \right)^2 \,,$$

and the partition function is then given by

$$Q_N \;=\; \sum_{\sigma^1} \exp\!\left(\kappa\, N^{-1} \left(\sum_{i=1}^{N} \sigma_i^1 \right)^2 \right) \,,$$

where the sum is over all possible distinct sequences of $+1$'s and -1's that σ^1 can assume.

The integration formula[7]

$$\exp(\alpha^2/2) \;=\; \int_{-\infty}^{\infty} \exp(-x^2/2 + \alpha x)\,(2\pi)^{-\frac{1}{2}}\,dx$$

may now be used. Define

$$\alpha \;\equiv\; (2\kappa/N)^{\frac{1}{2}} \sum_{i=1}^{N} \sigma_i^1 \,.$$

Then

$$Q_N \;=\; \int_{-\infty}^{\infty} F\, \exp(-x^2/2)\,(2\pi)^{-\frac{1}{2}}\,dx \tag{8}$$

where

$$F \equiv \sum_{\sigma^1} \exp(\alpha x)$$

$$= \sum_{\sigma^1} \exp\left(x \ (2\kappa/N)^{\frac{1}{2}} \sum_{i=1}^{N} \sigma_i^1 \right)$$

$$= \prod_{i=1}^{N} \sum_{\sigma^1} \exp\left(x \ (2\kappa/N)^{\frac{1}{2}} \sigma_i^1 \right)$$

$$= (2 \ \cosh\mu)^N \ ,$$

where

$$\mu \equiv x(2\kappa/N)^{\frac{1}{2}} \ .$$

Thus, Eq. (8) is now

$$Q_N = 2^N \ N^{\frac{1}{2}} \ (2\pi\kappa)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \left(h(\mu)\right)^N \ d\mu \ ,$$

where

$$h(\mu) \equiv \exp\left(\frac{-\mu^2}{4\kappa}\right) \cosh\mu \ .$$

To obtain the thermodynamic limit it is necessary to evaluate

$$\lim_{N \to \infty} Q_N^{1/N} = \lim_{N \to \infty} \left(2^N \ N^{\frac{1}{2}} \ (2\pi\kappa)^{-\frac{1}{2}} \right)^{1/N}$$

$$\times \lim_{N \to \infty} \left(\int_{-\infty}^{\infty} \left(h(\mu)\right)^N \ d\mu \right)^{1/N} \ .$$

The left-most limit on the RHS is easily shown to be 2. The right-most limit on the RHS can be evaluated by using the known result[8]

$$\lim_{N \to \infty} \left(\int_{-\infty}^{\infty} \left(f(t) \right)^N dt \right)^{1/N} = \max_{-\infty \leq \xi \leq \infty} f(\xi) .$$

The function $h(\mu)$ has local extrema at those points where

$$\frac{d}{d\mu} h(\mu) = 0 ,$$

which yields

$$\mu = 2 \kappa \tanh\mu .$$

For $\kappa < \frac{1}{2}$, the only solution is $\mu = 0$, and h attains its global maximum there. For $\kappa > \frac{1}{2}$, the solution $\mu = 0$ is a local minimum; the maximum occurs for $\mu = \pm\xi$, where ξ is the unique positive root of

$$\xi = 2 \kappa \tanh\xi .$$

Thus, the partition function is

$$\lim_{N \to \infty} Q_N^{1/N} = 2 \qquad\qquad \text{for } \kappa < \frac{1}{2} ,$$

$$= 2 \exp\left(\frac{-\xi^2}{4\kappa}\right) \cosh\xi \qquad \text{for } \kappa > \frac{1}{2} .$$

It follows that the average energy per particle is

$$\varepsilon = 0 \qquad\qquad \text{for } \kappa < \frac{1}{2} ,$$

$$= -J \left(\tanh\xi\right)^2 \qquad \text{for } \kappa > \frac{1}{2} ,$$

and the specific heat is

$$c_x = 0 \qquad\qquad \text{for } \kappa < \frac{1}{2} ,$$

$$= \frac{k \, \xi^2 \, \tanh\xi}{\sinh\xi \, \cosh\xi - \xi} \qquad \text{for } \kappa > \frac{1}{2} .$$

Since

$$\lim_{\kappa \uparrow \frac{1}{2}} c_x = 0 \; ,$$

and

$$\lim_{\kappa \downarrow \frac{1}{2}} c_x = \frac{3}{2} k \; ,$$

the specific heat is discontinuous and a phase transition exists at $\kappa = \frac{1}{2}$.

B. Formulation of the Matrix Representation

As noted earlier (page 5), the set of independent spin variables σ may be grouped into r ordered N-tuples σ^k and N ordered r-tuples σ_j. In the following discussion σ^k and σ_j will be used to indicate both the symbolic sets and the specific sets of +1's and -1's. If the sense is not clear from the context, it will be explicitly mentioned. Finally, notice that the sum over all 2^{Nr} distinct sequences of +1's and -1's in σ can be expressed as

$$\sum_\sigma = \sum_{\sigma^1} \sum_{\sigma^2} \cdots \sum_{\sigma^r} = \sum_{\sigma_1} \sum_{\sigma_2} \cdots \sum_{\sigma_N} \; . \tag{9}$$

It will now be shown that the RHS of Eq. (5) may be written as the trace of a certain matrix. Let the $2^r \times 2^r$ matrix A have elements

$$A(\sigma_j, \sigma_k) = \exp(r^{-1} \kappa f_{j,k}) \; C_{j,k} \; , \tag{10}$$

where

$$f_{j,k} \equiv \sigma_j^1 \sum_{i=1}^{r} \sigma_k^i \ ,$$

and

$$C_{j,k} \equiv \prod_{i=1}^{r-1} \delta(\sigma_j^{i+1} - \sigma_k^i) \ ,$$

where $\delta(0) = 1$, $\delta = 0$ otherwise. Both of the indices of A, σ_j and σ_k, run over all 2^r distinct sequences of +1's and -1's.

Then, directly from definitions,

$$Tr(A^N) = \sum_{\sigma_1} \left(A(\sigma_1, \sigma_1)\right)^N$$

$$= \sum_{\sigma_1} \sum_{\sigma_2} \cdots \sum_{\sigma_N} \prod_{j=1}^{N} A(\sigma_j, \sigma_{j+1}) \ ,$$

which, by Eq. (9), is strictly equivalent to

$$Tr(A^N) = \sum_{\sigma^1} G(\sigma^1) \ ,$$

where

$$G(\sigma^1) = \sum_{\sigma^2} \sum_{\sigma^3} \cdots \sum_{\sigma^r} \prod_{j=1}^{N} A(\sigma_j, \sigma_{j+1})$$

$$= \sum_{\sigma^2} \sum_{\sigma^3} \cdots \sum_{\sigma^r} \exp\left(r^{-1}\kappa \sum_{j=1}^{N} f_{j,j+1}\right) \prod_{j=1}^{N} C_{j,j+1} \ . \qquad (11)$$

Thus, the problem is reduced to showing that $G(\sigma^1)$ is just the Boltzmann factor, $\exp(-\beta E_N(\sigma^1))$.

The sum in Eq. (11) has 2^{Nr-N} terms, but for a specific N-tuple

of +1's and -1's in σ^1, only one term is nonzero. For a nonzero term to occur, the double product over the δ's requires that

$$\sigma^i_{j+1} = \sigma^{i+1}_j , \qquad 1 \le j \le N,\ 1 \le i \le r-1 ,$$

which implies

$$\sigma^1_j = \sigma^2_{j-1} = \cdots$$

$$= \sigma^i_{j+1-i} = \cdots$$

$$= \sigma^r_{j+1-r} , \qquad 1 \le j \le N . \tag{12}$$

Thus, for a nonzero term, a specific N-tuple of σ^1 determines specific N-tuples of σ^2, σ^3, ..., σ^r, and the sum in Eq. (11) contains only one term for which that is the case.

After rewriting Eq. (12) as

$$\sigma^1_{j+i} = \sigma^i_{j+1} , \qquad 1 \le j \le N,\ 2 \le i \le r , \tag{13}$$

it follows that, for the nonzero term in $G(\sigma^1)$,

$$f_{j,j+1} = \sigma^1_j \left(\sigma^1_{j+1} + \sum_{i=2}^{r} \sigma^i_{j+1} \right) , \qquad \text{by definition,}$$

$$= \sigma^1_j \left(\sigma^1_{j+1} + \sum_{i=2}^{r} \sigma^1_{j+i} \right) , \qquad \text{by Eq. (13),}$$

$$= \sigma^1_j \sum_{i=1}^{r} \sigma^1_{j+i} ,$$

and therefore

$$G(\sigma^1) = \exp\left(r^{-1} \kappa \sum_{j=1}^{N} \sigma_j^1 \sum_{i=1}^{r} \sigma_{j+i}^1 \right)$$

$$= \exp\left(-\beta \, E_N(\sigma^1) \right) \, .$$

Hence,

$$Q_N = \sum_{\sigma^1} G(\sigma^1) = Tr(A^N) \, .$$

CHAPTER III

NUMERICAL METHODS

A. Purpose and Comments

The calculation of Chapter II, Section A, which was acknowledged
to be possibly unjustifiable, indicates that a phase transition occurs
for an infinite length, infinite interaction range Ising chain at
$\kappa^{-1} = 2$. In contrast, the nearest neighbor case, which is equivalent
to Ising's original model, possesses only a maximum, which occurs at
a lower numeric value of both c_x and κ^{-1} than the infinite range
maximum. It is anticipated that models with increasingly long inter-
action ranges possess maxima which in the limit become the critical
point of the infinite range model. It is therefore of interest to
attempt to locate these maxima.

As noted on page 7, the largest eigenvalue of the matrix A yields
the partition function of a finite interaction range, infinite length
Ising chain. Unfortunately, the matrix is not analytically diagonal-
izable, but the largest eigenvalue can be found by using a numerical
technique. From the largest eigenvalue the average energy per particle
at a specific value of κ can be found. From a table of these values,
the specific heat can be numerically calculated.

It is convenient for computational purposes that the indices of
the matrix A be integers; as defined in Eq. (10) they are the 2^r

17

distinct sequences of +1's and -1's of the r-tuple σ_i. Any scheme that puts these sequences into one-to-one correspondence with the integers 1, 2, ..., 2^r is valid, so the following scheme is used. Let the index σ_i of A be represented by the integer

$$\sigma_i \;\leftrightarrow\; 1 + \sum_{j=1}^{r} 2^{j-1} \frac{1 + \sigma_i^j}{2} \;.$$

As a specific example, consider the case where $r = 3$. The matrix A is then 8×8, with indices as in Table 1. The matrix A is shown explicitly in Figure 1.

Index	σ_i^1	σ_i^2	σ_i^3
1	-1	-1	-1
2	-1	-1	+1
3	-1	+1	-1
4	-1	+1	+1
5	+1	-1	-1
6	+1	-1	+1
7	+1	+1	-1
8	+1	+1	+1

Table 1.--Indices of A for corresponding sequences of σ_i for

$r = 3$

$$\begin{matrix}
\alpha^3 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \alpha & \alpha^{-1} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \alpha & \alpha^{-1} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \alpha^{-1} & \alpha^{-3} \\
\alpha^{-3} & \alpha^{-1} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \alpha^{-1} & \alpha & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \alpha^{-1} & \alpha & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \alpha & \alpha^3
\end{matrix}$$

Figure 1.--Matrix A for r = 3. Here,

$\alpha = \exp(\kappa/3)$.

B. Method of Finding the Largest Eigenvalue

Since the power method of obtaining the eigenvalue of largest magnitude of a given matrix is developed in most texts on numerical analysis,[9] the details peculiar only to the present problem are outlined here.

Let λ be the eigenvalue of largest magnitude with an associated eigenvector ϕ. One starts with an almost arbitrary initial vector u_0 ("almost arbitrary" to be defined later) and forms the sequence of vectors

$$w_i = A u_{i-1} , \tag{14a}$$

$$u_i = ||w_i||^{-1} w_i , \qquad i = 1, 2, \ldots, \tag{14b}$$

where $||w_i||$ is any suitable norm[10] of w_i. Then, for some component ℓ

of w_{i+1} and u_i,

$$\lim_{i \to \infty} \frac{w_{i+1}(\ell)}{u_i(\ell)} = \lambda . \tag{15}$$

Furthermore, the sequence of vectors $\{u_i\}_{i=0}^{\infty}$ converges to the eigen-vector ϕ associated with λ.

The choice of the initial vector u_0 is not completely arbitrary because u_0 must have a nonzero projection on ϕ. However, the matrix considered here has nonnegative elements, and a theorem of Frobenius[6] states that the eigenvector associated with the largest eigenvalue of such a matrix is real and has all positive components. If u_0 is chosen such that all its components are positive, then the inner product of u_0 and ϕ is the sum of positive numbers, and therefore not zero.

If u_0 has all positive components, then with the matrix considered here, the components of the w_i's are also all positive. In this case a suitable choice for the norm in Eq. (14b) is the first component of the w_i's, which results in the first component of the u_i's being always equal to one. The first component is also chosen for the ratio in Eq. (15); consequently, the first component of the w_i's are the successive approximations to λ.

The criteria for termination of the iterative process are problematical. A practical solution is to terminate when two succes-sive estimates of λ are satifactorily close. An improvement on this criterion can be made by observing that the relative error in the estimate of the eigenvalue is approximately equal to the square of the maximum relative error in the components of the estimate of the

corresponding eigenvector. Thus, the iterative process is terminated when the maximum relative change in the components of two successive estimates of the eigenvector is small.

The power method is outlined in the "RIGHT-ITERATION" algorithm below. It is assumed that the zeroth iterate of U, the matrix A, and the maximum allowable error $ERROR_{max}$ are chosen prior to execution of the algorithm. After execution, L is the approximation of λ and the last iterate of U is the approximation of ϕ.

RIGHT-ITERATION algorithm:

Step 1;   Set L_{old} to zero.

Set DONE to "false."

Step 2;   Set W to the matrix product AU.

Set L to W(1).

Set $ERROR_L$ to $\left| (L - L_{old}) / (L + L_{old}) \right|$.

Set L_{old} to L.

If $ERROR_L$ is greater than $ERROR_{max}$, then go to step 4.

Step 3;   Set $ERROR_U$ to $\underset{i}{\text{maximum}} \left| \left(W(i) - L \cdot U(i) \right) / \left(W(i) + L \cdot U(i) \right) \right|$.

If $ERROR_U$ is less than $ERROR_{max}$, then set DONE to "true."

Step 4;   Set U to W/L.

If DONE is equal to "false," then go to step 2.

Step 5;   The algorithm is completed.

C. Method of Finding the Average
Energy per Particle

Given a table of values of λ as a function of κ, it is possible in principle to numerically differentiate first λ with respect to κ to obtain the average energy per particle ε, and then ε with respect to

κ^{-1} to obtain the specific heat c_x. Numerical differentiation is generally undesirable, however, and in the present case is not necessary for obtaining ε.

Consider the left eigenvalue problem,

$$A^T \theta = \Lambda \theta ,$$

where A^T denotes the transpose of A, which is distinct from the right eigenvalue problem,

$$A \phi = \lambda \phi ,$$

which was discussed in the previous section. The sets of left and right eigenvalues are identical, since

$$\det(\Lambda I - A^T) = \det(\Lambda I - A^T)^T = \det(\Lambda I - A) .$$

The sets of left and right eigenvectors in general are distinct.

Denote the right and left eigenvectors associated with the largest eigenvalue λ as ϕ and θ, respectively, and use the standard notations for differentiation,

$$\chi' = \frac{d\chi}{d\kappa} ,$$

and the inner product,

$$(x,y) = \sum_i x(i) \, y(i) .$$

Then one may differentiate the identity,

$$\lambda(\theta,\phi) = (\theta, A\phi) ,$$

and obtain, after some manipulation,

$$\lambda' = (\theta, A'\phi)/(\theta, \phi) .$$

From Eq. (6) it follows that

$$-\varepsilon/J = \lambda'/\lambda = \lambda^{-1} (\theta, \phi)^{-1} (\theta, A'\phi) .$$

The elements of A' are simple to compute from Eq. (10), being

$$\frac{d}{d\kappa} \left(A(\sigma_j, \sigma_k) \right) = \frac{d}{d\kappa} \left(\exp(r^{-1} \kappa f_{j,k}) C_{j,k} \right)$$

$$= r^{-1} f_{j,k} A(\sigma_j, \sigma_k) .$$

The "AVERAGE-ENERGY" algorithm which follows, outlines the
procedure for finding values of $-\varepsilon/J$ at a sequence of different values
of κ. Since the values of scaled average energy per particle are used
via numerical differentiation to obtain c_x, it is convenient to
evaluated $-\varepsilon/J$ at equally spaced intervals of κ^{-1}, and all calculations
are performed with effectively 15 decimal digits accuracy.

The AVERAGE-ENERGY algorithm refers to the RIGHT-ITERATION
algorithm discussed above (page 21) and a "LEFT-ITERATION" algorithm.
The latter is identical to the RIGHT-ITERATION algorithm except that
"A^T" is substituted for "A" and "V" is substituted for "U" wherever
U and A appear in the RIGHT-ITERATION algorithm. The RIGHT-ITERATION
algorithm produces an approximation U of the right eigenvector ϕ and
the LEFT-ITERATION algorithm produces an approximation V of the left
eigenvector θ. Both algorithms produce an approximation L of the
largest eigenvalue λ.

AVERAGE-ENERGY algorithm:

Step 1; Choose the interaction range of the model, R.

Choose the initial scaled temperature (κ^{-1}), X.

Choose the size of the increments of X, ΔX.

Choose the number of values of $-\varepsilon/J$ desired, COUNT.

Choose the maximum allowable error, ERROR$_{max}$.

Set vectors U and V to (1, 1, ..., 1).

Set LOOPCOUNTER to zero.

Step 2; Set X to X + ΔX.

Set K to X^{-1}.

Compute the elements of A for the values of K and R.

Perform the RIGHT-ITERATION algorithm (returns U and L).

Perform the LEFT-ITERATION algorithm (returns V and L).

Set Y to the inner product (V,U).

Compute the elements of A´.

Set W to the matrix product A´U.

Set Z to the inner product (V,W).

Set LPRIME to Z/Y.

Print LPRIME/L.

Step 3; Set LOOPCOUNTER to LOOPCOUNTER + 1.

If LOOPCOUNTER is less than COUNT, then go to step 2.

Step 4; The algorithm is completed.

D. Numerical Differentiation

The procedure used for approximating the derivatives of ε is based on differentiation of a polynomial that is constructed to pass through a set of data points provided by the AVERAGE-ENERGY algorithm.

Denoting κ^{-1} by t and λ'/λ by E, the data points are ordered pairs (t_0, E_0), (t_1, E_1), ..., which are separated by equally spaced increments h ("ΔX" in the AVERAGE-ENERGY algorithm) of t. Then, at some point $t = t_0 + uh$, the approximation of E(t) can be given by Newton's forward difference interpolation polynomial, which uses n+1 points to form an nth degree polynomial in u;

$$P_n(t) = P_n(t_0 + uh)$$

$$= E_0 + u \, \Delta E_0 + \frac{u \, (u-1)}{2!} \Delta^2 E_0 + \cdots$$

$$+ \frac{u \, (u-1) \, \cdots \, (u-n+1)}{n!} \Delta^n E_0 \, , \tag{16}$$

where the forward differences $\Delta^i E_0$ are defined recursively by

$$\Delta E_j = \Delta^1 E_j = E_{j+1} - E_j \, ,$$

$$\Delta^{i+1} E_j = \Delta^i (\Delta E_j)$$

$$= \Delta^i E_{j+1} - \Delta^i E_j \, , \qquad 1 \le i \le n, \; 0 \le j \le n \, .$$

It follows from Eq. (7) that the derivative of Eq. (16) with respect to t,

$$\frac{d}{dt} P_n = \frac{du}{dt} \frac{d}{du} P_n$$

$$= \frac{1}{h} \frac{d}{du} P_n \, ,$$

is the approximation of $-c_x/k$. Furthermore, if Eq. (16) is differentiated twice with respect to t,

$$\frac{d^2}{dt^2} P_n = \frac{1}{h^2} \frac{d^2}{du^2} P_n \; ,$$

the result being set equal to zero and solved for u, the location of the maximum of c_x is found.

More accurate results are to be expected if u lies within the interval 0 to n, since, after all, P_n is an interpolation polynomial. Also, if the values of the E's have an uncertainty δ, then the forward differences $\Delta^i E$ will have an uncertainty on the order of $2^i \delta$. Eventually this uncertainty reaches the magnitude of the forward differences, at which point it becomes fruitless to use that or higher order differences in the polynomial. This cumulative error effectively places a limit on the number of useful data points, and hence the degree of the polynomial.

CHAPTER IV

RESULTS AND CONCLUSIONS

A. Presentation of Results

A FORTRAN computer program, which is reproduced in the Appendix, was written to implement the AVERAGE-ENERGY algorithm (page 24). Due to limitations on computer time and memory, the models examined were restricted to interaction ranges of twelve and less. The numerical results obtained for $3 \leq r \leq 12$ are presented in this section; the following section contains the interpretation of the results.

The curves of average energy per particle and specific heat shown in Figures 2 and 3, respectively, give a general indication of the behavior of the properties of the models. The values of $-\varepsilon/J$ for interaction ranges of eight, nine and ten, which yield the values of c_x/k plotted in Figure 3, were obtained from the computer program. Included in both Figures for comparison are curves for the infinite range model, from the calculations of Chapter II, Section A.

Table 2 lists the values of average energy per particle calculated by the computer program for the various models in the near vicinity of the specific heat maxima. In obtaining these values, the error level ("ERROR$_{max}$" in the AVERAGE-ENERGY algorithm) was set to 1×10^{-15}, and the scaled temperature increments ("ΔX" in the AVERAGE-ENERGY algorithm and "h" is the discussion of Chapter III, Section D)

27
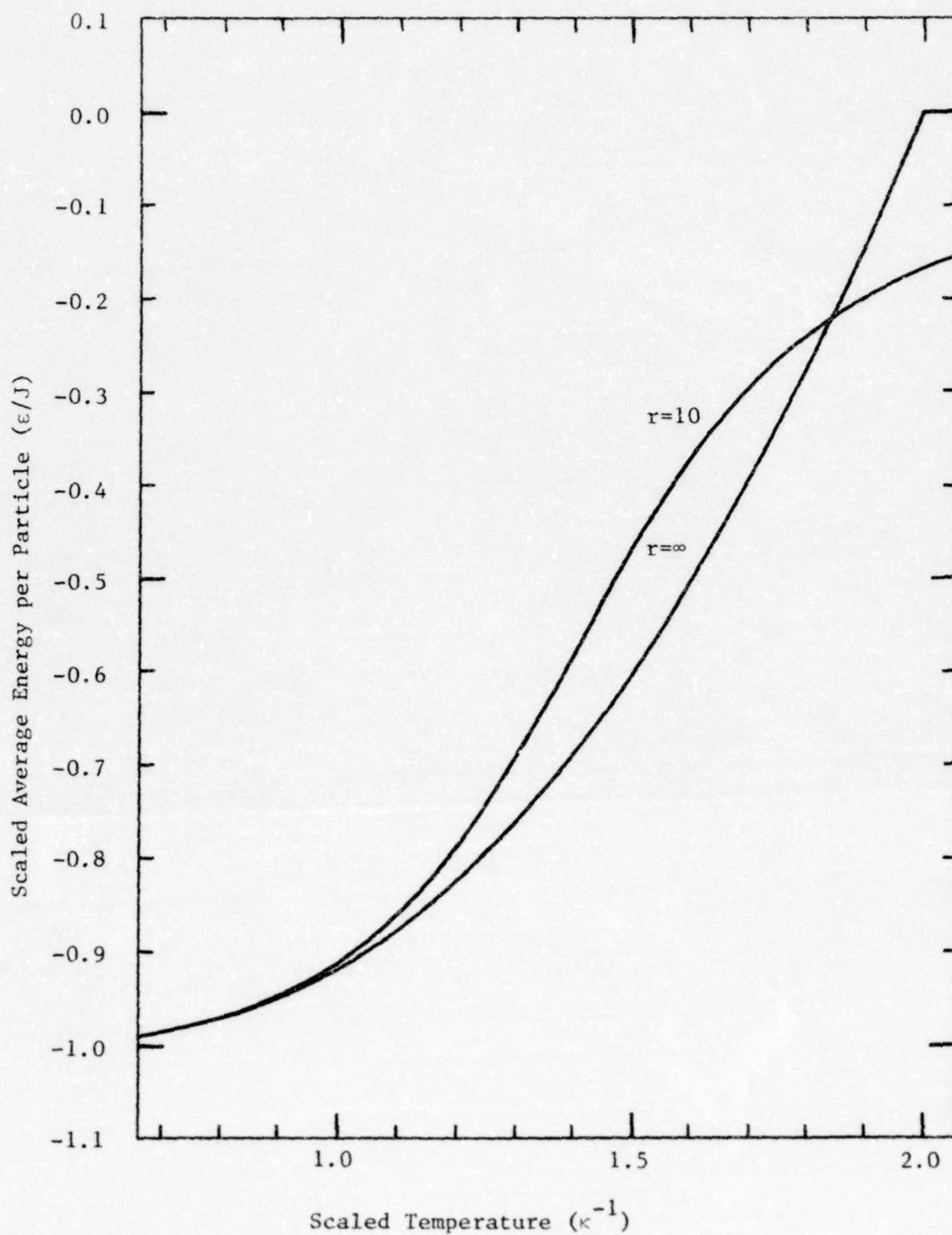
Figure 2. Average energy per particle as a function of temperature for r = 10 and r = ∞. The curves for r = 8 and r = 9 are not shown due to their closeness to the r = 10 curve.
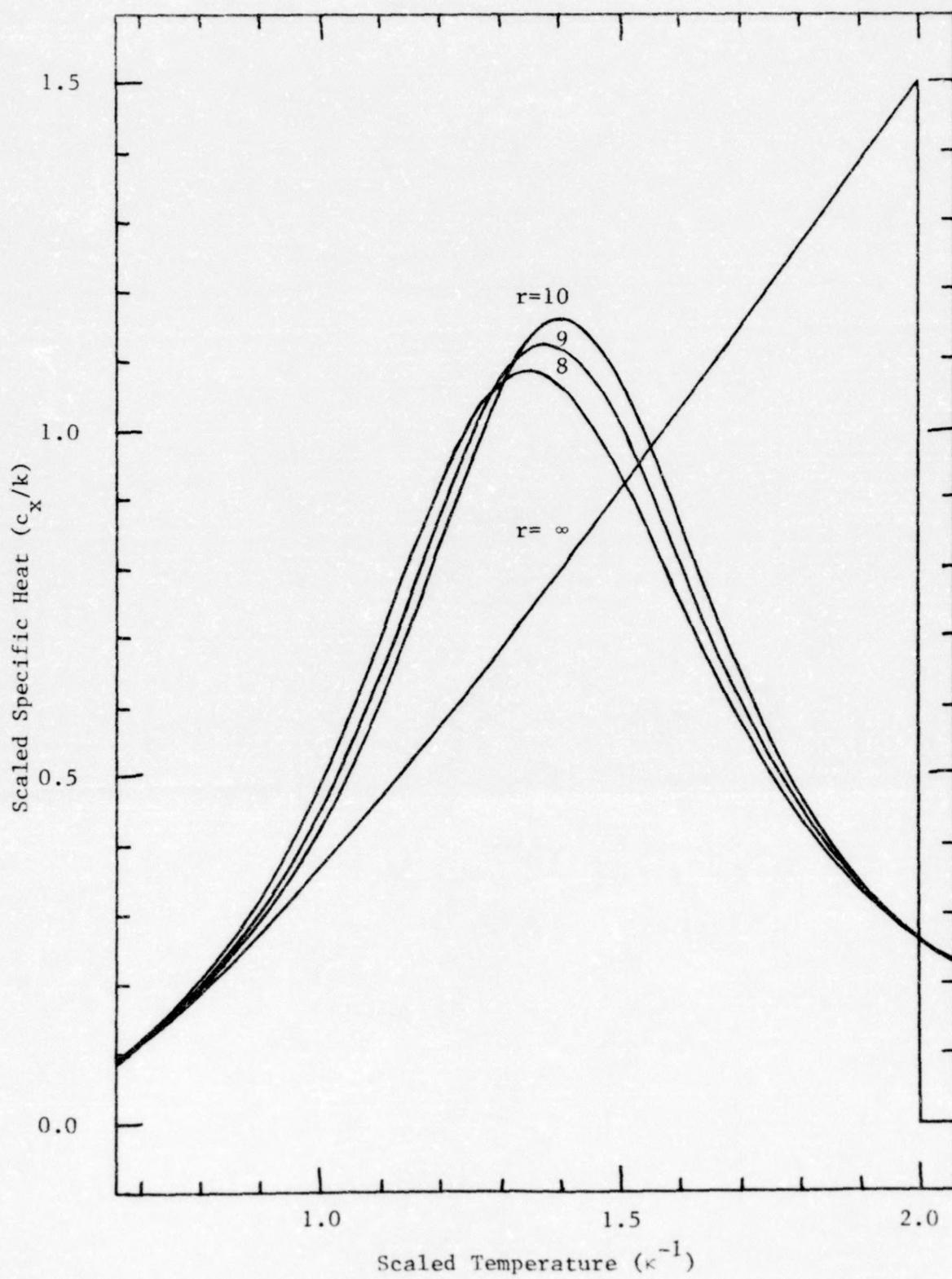
Figure 3. Specific heat as a function of temperature for r = 8, 9 and 10, and r = ∞.

r	κ^{-1}	$-\varepsilon/J$	r	κ^{-1}	$-\varepsilon/J$
3	1.1253	.7310634104614752	8	1.3498	.6134836060197968
	1.1254	.7309898581275500		1.3499	.6133756108104800
	1.1255	.7309163057887586		1.3500	.6132676155900362
	1.1256	.7308427534506940		1.3501	.6131596203747139
4	1.1892	.7022256325612256	9	1.3773	.5957747701254438
	1.1893	.7021422282103140		1.3774	.5956626636479821
	1.1894	.7020588238527287		1.3775	.5955505571566642
	1.1895	.7019754194961648		1.3776	.5954384506699093
5	1.2402	.6766523116218906	10	1.4017	.5794473400708567
	1.2403	.6765610250635233		1.4018	.5793316079137512
	1.2404	.6764697385051188		1.4019	.5792158757309540
	1.2405	.6763784519564878		1.4020	.5791001435430809
6	1.2825	.6536462430225259	11	1.4238	.5640370209995478
	1.2826	.6535484537190119		1.4239	.5639180598566488
	1.2827	.6534506644133556		1.4240	.5637990987243939
	1.2828	.6533528751174986		1.4241	.5636801376256132
7	1.3185	.6327329598260558	12	1.4435	.5500151909089815
	1.3186	.6326296813832862		1.4436	.5498933300995018
	1.3187	.6325264029287166		1.4437	.5497714692719470
	1.3188	.6324231244764320		1.4438	.5496496084513769

Table 2.--Values of average energy per particle vs. temperature in the near vicinity of the specific heat maxima for $3 \le r \le 12$

was set to 1×10^{-4}. This value of h resulted in the fourth forward differences being at the cumulative error level, with the assumption that the values of average energy per particle are accurate to one part in 10^{15}; therefore, the interpolating polynomial was truncated after the term including the third forward difference $\Delta^3 E_0$. Under this condition, the approximation of c_x'' evaluated at the maximum of c_x, which is a measure of the "sharpness" of the peak, is simply $\Delta^3 E_0 / h^3$.

Table 3 contains the interpolated locations of the maxima of c_x and the values of $-\epsilon/J$ at the maxima, along with the respective values of $\Delta^3 E_0 / h^3$. Figure 4 displays the maxima listed in Table 3 and the discontinuity of the infinite range model.

r	κ^{-1}	$-\epsilon/J$	c_x/k	$\Delta^3 E_0 / h^3$
3	1.125487	.7309258665141286	.735523394072	5.591
4	1.189387	.7020698978853619	.834043584245	7.693
5	1.240300	.6765607095248148	.912865600222	9.807
6	1.282618	.6535309427746348	.977893067684	11.937
7	1.318684	.6325431578413316	1.032784559599	14.085
8	1.349968	.6133016687060859	1.079952213976	16.242
9	1.377475	.5955783212286502	1.121064926722	18.425
10	1.401925	.5791873769686845	1.157321893956	20.613
11	1.423853	.5639735232274238	1.189611438633	22.830
12	1.443672	.5498054389533559	1.218608292121	25.056

Table 3.--Thermodynamic properties at the specific heat maxima for
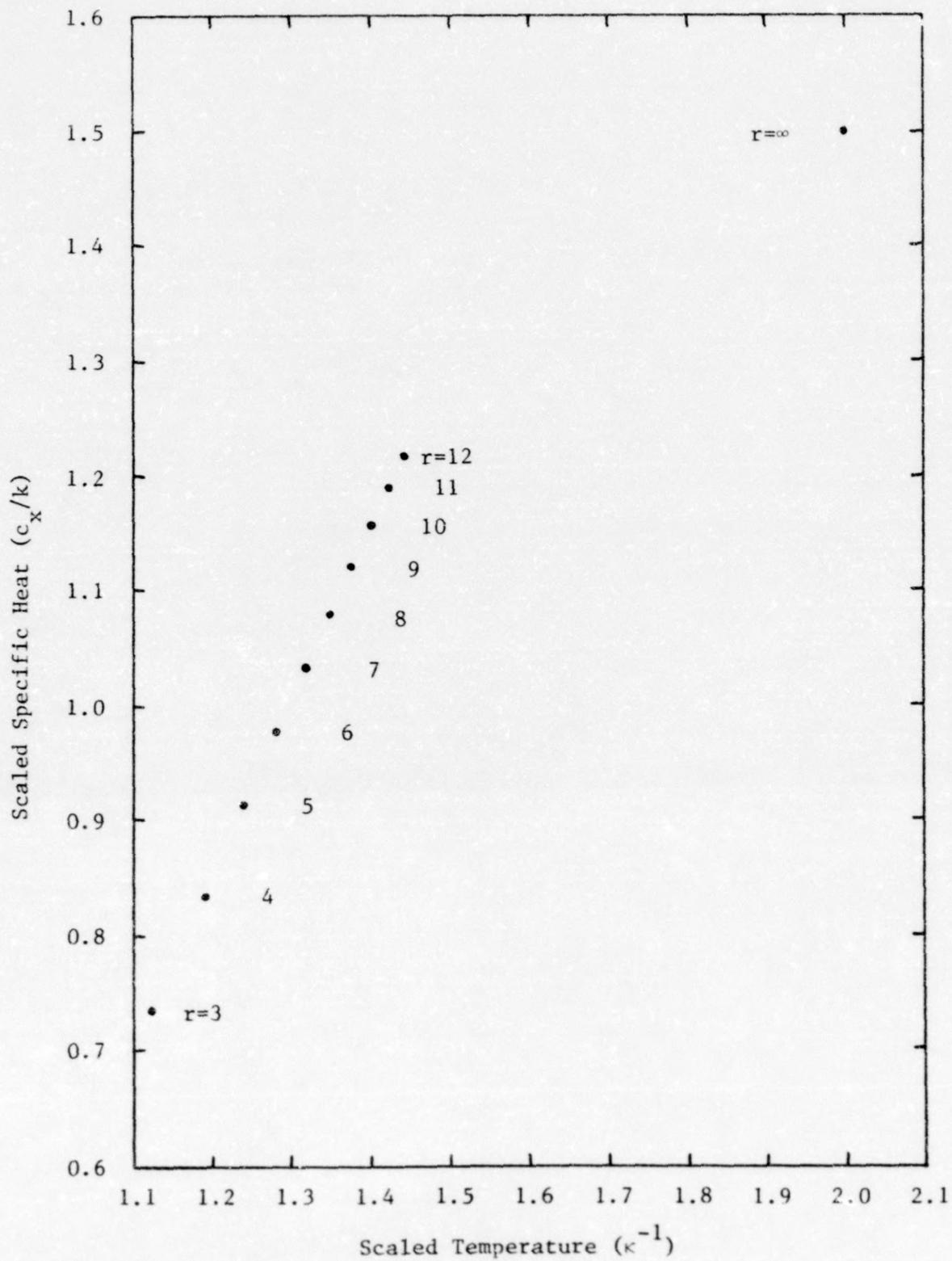
$$3 \leq r \leq 12$$

Figure 4. Locations of specific heat maxima for $3 \leq r \leq 12$ and $r = \infty$.

B. Interpretation of Results

From the results in the preceding section, a few qualitative observations can be made. From Figure 3 it is seen that the specific heat of each finite range model forms a bell-shaped curve that tends up and to the right with increasing r; since the models have specific heats that are close together at temperatures far enough from their maxima, Figure 3 gives the impression that the specific heat curves are skewing toward that of the infinite range model. Figure 4 indicates that the position of the maxima tend toward higher values of both c_x and temperature as r increases. Finally, from the values of $\Delta^3 E_0 / h^3$ in Table 4, the peaks are growing sharper with increasing r.

Unfortunately, these observations by themselves do not give sufficient reason to believe that the models converge to the infinite range model. The shape of the specific heat curves of the finite range models is too unlike that of the infinite range model, and the maxima lie on a line that appears quite linear and which shows no indication of turning toward the infinite range peak. However, an interaction range of twelve is very far indeed from an infinite interaction range; the tendency toward a phase transition may exist, with the evidence being obliterated by a slow convergence.

C. Suggestions for Future Work

It is apparent that the interaction ranges examined must be made longer, perhaps much longer, in order to show convincing evidence of a tendency toward a phase transition. Unfortunately, since the addition of each new spin to the interaction range requires doubling the array

size of the computer program, one soon reaches the limit of present
computers, probably without achieving the interaction ranges long
enough to provide additional insight. Therefore, an altogether
different approach is clearly in order.

For one so inclined, however, the methods used in this paper
could be adapted to other finite range Ising chains. For example, the
interaction energy between spins could be made to be a function of the
interaction distance. Also, a "magnetic field" could be introduced.
Again, the considerations of the preceding paragraph apply.

Appendix

The FORTRAN version of the AVERAGE-ENERGY algorithm (page 24)
is reproduced below. The subroutines RMUL and LMUL form the matrix
products AU and AV, respectively.

```
C       AVERAGE ENERGY MAIN ROUTINE
        IMPLICIT REAL*8(A-H,O-Z)
        REAL*8 L,LP
        COMMON A(8192),U(4096),V(4096),W(4096),E,ERR,L,N,M,MBY2
        READ(5,99) X,DX,NSTEP,N,ERR
99      FORMAT(2F6.0,2I3,D8.1)
        WRITE(6,100) X,DX,NSTEP,N,ERR
100     FORMAT('0',2F7.4,2I5,D8.1)
        M=2**N
        MBY2=M/2
        NSTEPM=NSTEP-1
                DO 1  I=1,M
                    U(I)=1.
                    V(I)=1.
1               CONTINUE
                DO 4  I=1,NSTEP
                    X=X+DX
                    E=1./X
                    CALL SETUP0
                    CALL RITER
                    CALL LITER
                    VU=0.
                        DO 2  J=1,M
2                       VU=VU+V(J)*U(J)
                    CALL SETUP1
                    CALL RMUL
                    VAU=0.
                        DO 3  J=1,M
3                       VAU=VAU+V(J)*W(J)
                    LP=VAU/VU
                    ENERGY=LP/L
                    WRITE(6,101) ENERGY
101                 FORMAT(/F20.16)
4               CONTINUE
        STOP
        END
C
```

```fortran
C
      SUBROUTINE SETUP0
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 L
      COMMON A(8192),U(4096),V(4096),W(4096),E,ERR,L,N,M,MBY2
      DIMENSION BITS(12)
          DO 4  I=1,M
                J1=2*I-2
                IF(J1.GE.M) J1=J1-M
                K=MBY2
                     DO 1  J=1,M
                           BITS(N-J+1)=-1.
                           IF(J1.LT.K) GOTO 1
                           BITS(N-J+1)=1.
                           J1=J1-K
1                    K=K/2
                X=0.
                     DO 2  J=1,N
2                    X=X+BITS(J)
                Y=X+2
                IF(I.GT.MBY2) GOTO 3
                X=-X
                Y=-Y
3               A(2*I-1)=DEXP(E*X/N)
                A(2*I)=DEXP(E*Y/N)
4         CONTINUE
      RETURN
      END
C
C
      SUBROUTINE RITER
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 L,LOLD
      COMMON A(8192),U(4096),V(4096),W(4096),E,ERR,L,N,M,MBY2
      LOLD=0.
      DONE=0.
1     CALL RMUL
      L=W(1)
      ERL=DABS((L-LOLD)/(L+LOLD))
      LOLD=L
      IF(ERL.GT.ERR) GOTO 3
      ERA=0.
          DO 2  I=2,M
                ERB=DABS((W(I)-L*U(I))/(W(I)+L*U(I)))
                IF(ERB.GT.ERA) ERA=ERB
2         CONTINUE
      IF(ERA.LT.ERR) DONE=1.
3         DO 4  I=2,M
4         U(I)=W(I)/L
      IF(DONE.EQ.0.) GOTO 1
      RETURN
      END
C
```

```
C
      SUBROUTINE LITER
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 L,LOLD
      COMMON A(8192),U(4096),V(4096),W(4096),E,ERR,L,N,M,MBY2
      LOLD=0.
      DONE=0.
1     CALL LMUL
      L=W(1)
      ERL=DABS((L-LOLD)/(L+LOLD))
      LOLD=L
      IF(ERL.GT.ERR) GOTO 3
      ERA=0.
          DO 2  I=2,M
                ERB=DABS(W(I)-L*V(I))/(W(I)+L*V(I)))
                IF(ERB.GT.ERA) ERA=ERB
2         CONTINUE
      IF(ERA.LT.ERR) DONE=1.
          DO 4  I=2,M
4             V(I)=W(I)/L
      IF(DONE.EQ.0.) GOTO 1
      RETURN
      END
C
C
      SUBROUTINE SETUP1
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 L
      COMMON A(8192),U(4096),V(4096),W(4096),E,ERR,L,N,M,MBY2
      DIMENSION BITS(12)
          DO 4  I=1,M
                J1=2*I-2
                IF(J1.GE.M) J1=J1-M
                K=MBY2
                    DO 1  J=1,M
                          BITS(N-J+1)=-1.
                          IF(J1.lt.K) GOTO 1
                          BITS(N-J+1)=1.
                          J1=J1-K
1                   K=K/2
                X=0.
                    DO 2  J=1,N
2                   X=X+BITS(J)
                Y=X+2
                IF(I.GT.MBY2) GOTO 3
                X=-X
                Y=-Y
3               A(2*I-1)=X*DEXP(E*X/N)/N
                A(2*I)=Y*DEXP(E*Y/N)/N
4         CONTINUE
      RETURN
      END
C
```

```
C
      SUBROUTINE RMUL
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON A(8192),U(4096),V(4096),W(4096),E,ERR,L,N,M,MBY2
      MBY2P1=MBY2+1
          DO 1  I=1,MBY2
                W(I)=A(2*I-1)*U(2*I-1) + A(2*I)*U(2*I)
1         CONTINUE
          DO 2  I=MBY2P1,M
                W(I)=A(2*I-1)*U(2*I-M-1) + A(2*I)*U(2*I-M)
2         CONTINUE
      RETURN
      END
C
C
      SUBROUTINE LMUL
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON A(8192),U(4096),V(4096),W(4096),E,ERR,L,N,M,MBY2
          DO 1  I=1,MBY2
                W(2*I-1)=A(2*I-1)*V(I) + A(2*I+M-1)*V(I+MBY2)
                W(2*I)=A(2*I)*V(I) + A(2*I+M)*V(I+MBY2)
1         CONTINUE
      RETURN
      END
C
```

FOOTNOTES AND REFERENCES

1   A review of the Ising model and its subsequent history is given
        by S. G. Brush, Rev. Mod. Phys. $\underline{39}$, 883 (1967). This reference
        contains an extensive bibliography.

2   L. Onsager, Phys. Rev. $\underline{65}$, 117 (1944)

3   G. A. Baker, Phys. Rev. $\underline{112}$, 1477 (1961)

4   S. Katsura, Prog. Theor. Phys. $\underline{13}$, 571 (1955)

5   J. F. Nagle and J. C. Bonner, J. Phys. C $\underline{3}$, 352 (1970)

6   A proof is included in Alston S. Householder, The Theory of
        Matrices in Numerical Analysis (Blaisdell Publishing Company,
        New York, 1964), pp. 48-50.

7   I. M. Ryzhik and I. S. Gradshteyn, 4th ed., rev. Yu. V. Geronimus
        and M. Yu. Tseytlin, Table of Integrals, Series, and Products,
        trans. Scripta Technica, Inc. (Academic Press Inc., New York,
        1965), p. 307.

8   A. Zygmund, Trigonometrical Series, Monografje Mathematyczne,
        (M. Garasinski, Warsaw, 1935), vol. 5, p. 66, quoted by M. B.
        Lewis and A. J. F. Siegert, Phys. Rev. $\underline{101}$, 1227 (1956).

9   See, for example, E. Isaacson and H. B. Keller, Analysis of
        Numerical Methods (John Wiley & Sons, Inc., New York, 1966),
        pp. 147-150.

10   For a discussion on norms, see, for example, reference 9.

BIOGRAPHICAL NOTE

The writer was born September 1, 1952, to James C. and Agnes I. Green. After graduating from the public school in Auburn, Kentucky, he attended Western Kentucky University and graduated cum laude in May, 1975, with a B. S. in Physics. From August, 1976, he has been a graduate student at the same institution.