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A Class of Energy Levels for the Heisenberg Linear Chain. I.

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Abstract

The highest and lowest energies as a function of the total spin are computed for the class of "unbound" states in the Bethe formalism for the linear chain of spin $\frac{1}{2}$ atoms with a Heisenberg exchange interaction between nearest neighbors. In addition, the magnetization as a function of magnetic field is calculated in the limit of zero temperature for an infinite antiferromagnetic chain.

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I. Introduction

The properties of antiferromagnetic insulators are often discussed on the basis of the Heisenberg model of exchange between neighboring atoms. Calculations for two and three dimensional lattices invariably proceed by means of approximations whose validity is difficult to judge. Hence there is still some interest in examining the one dimensional case, for which a certain amount of progress has been made toward an exact solution.

Bethe[1] showed that the eigenvalue problem for a chain of N spin $\frac{1}{2}$ atoms with Hamiltonian

$$\mathcal{H} = 2J \sum_{i=1}^{N} \underset{\sim}{S}_i \cdot \underset{\sim}{S}_{i+1}$$

$$\underset{\sim}{S}_{N+1} \equiv \underset{\sim}{S}_1 \qquad (1)$$

where $\underset{\sim}{S}_i$ is the spin operator for the i'th atom and J the "exchange integral," could be reduced to that of finding the solutions to a set of coupled transcendental algebraic equations. Using this procedure, Hulthén[2] calculated the exact ground state energy for an infinite antiferromagnetic ($J > 0$) chain; and des Cloizeaux and Pearson[3] have recently calculated the energies of the lowest-lying excitations or "spin waves."

A certain subset of the eigenstates in the Bethe formalism are "unbound"; this nomenclature is made more precise in Section II below. The unbound states are of particular importance in discussing the properties of the antiferromagnetic chain, since they include the antiferromagnetic ground state and the des Cloizeaux and Pearson "spin waves."

The present report is concerned entirely with the unbound states. In particular we compute in Sections III B, C, and D the minimum and maximum energies for unbound states having a given total spin S, as a function of S. The minimum energies are of particular interest since there is good reason to believe that they also represent the minimum energies of all states in the chain (for a given S). This permits a calculation (in Section IV) of the magnetization of the antiferromagnetic chain as a function of magnetic field at zero temperature.

The Bethe formalism for treating the eigenvalue problem is summarized and discussed in Section II. A small contribution towards the formidable task of making the formalism fully rigorous is contained in an existence proof in Appendix A. The derivation of the Hulthén integral equation, upon which the work in Section III B, C, and D depends, is summarized in Section III A.

The results of our computations do not agree with a previous calculation by Ledinegg and Urban.[4] The reason for the discrepancy, which we believe to be an error in their computations, is discussed in Appendix B.

By considering the detailed energy level structure of the class of "unbound" states, one can also say something about the free energy of the antiferromagnetic chain at low temperatures. This discussion will be deferred to another report.

II. The Bethe Equations

Consider a linear chain of N spin $\frac{1}{2}$ atoms, closed upon itself, with Hamiltonian (1). Assume that J is positive, that is, the interaction is antiferromagnetic. The largest eigenvalue of $\mathcal{H}$, corresponding to the ferromagnetic ground state, is

$$E_F = \tfrac{1}{2} N J , \tag{2}$$

while the lowest eigenvalue, the energy of the antiferromagnetic ground state, is[2]

$$E_{AF} = NJ \left(\tfrac{1}{4} - 2 \log 2 \right) \tag{3}$$

in the limit of very large N.

Choose as basis vectors states for which all spins in the chain are either "up" or "down" with respect to the z axis. Let $\Psi_{n_1 n_2 \cdots n_r}$ be a state for which the spins n_1, n_2, . . ., n_r are down and all other spins are up. Any state with z component of spin equal to N/2 - r may be written as a linear combination of such states:

$$\Psi = \sum a(n_1, n_2, \cdots, n_r) \, \Psi_{n_1 n_2 \cdots n_r} \tag{4}$$

where the summation extends over all sets of r (distinct) indices n_j.

The eigenfunctions discussed by Bethe[1] are of the form:

$$a(n_1, n_2, \cdots, n_r) = \sum_{p=1}^{r!} \exp i \left(\sum_{j=1}^{r} k_{p_j} n_j + \tfrac{1}{2} \sum_{j<l} \phi_{p_j, p_l} \right) \tag{5}$$

where the summation extends over all r! permutations of the integers 1, 2, . . ., r among themselves; Pj is the image of j under the P'th permutation. The "wavevectors" k_j satisfy the equations:

$$N k_j = 2\pi \lambda_j + \sum_{l(\phi_j)} \phi_{jl} \qquad j = 1, 2, \ldots, r \tag{6}$$

where the λ_j's are integers between 0 and N-1, and the ϕ's are defined by:

$$\cot \tfrac{1}{2}\phi_{jl} = \tfrac{1}{2}\left(\cot \tfrac{1}{2} k_j - \cot \tfrac{1}{2} k_l\right)$$

$$-\pi \le \phi_{jl} \le \pi \tag{7}$$

Let E be the energy of the eigenstate, and define the "normalized energy" ϵ by:

$$\epsilon = (E_F - E)/(2JN), \tag{8}$$

a quantity which is obviously non-negative.[5] Similarly define ϵ_1 by:

$$\epsilon_1 = \log 2 - \epsilon = (E - E_{AF})/(2JN). \tag{9}$$

The energy of the state (5) is given by

$$\epsilon = N^{-1} \sum_{j=1}^{r} (1 - \cos k_j) \tag{10}$$

With each eigenstate of the form (5) there is associated a set of

integers λ_j through (6). The order of the λ_j is obviously unimportant. Furthermore, a state with some of the λ_j equal to zero has the identical energy and total spin (though not the same z component of spin) as the corresponding state for which all the zero λ's have been eliminated.[2] Thus without loss of generality we can restrict the discussion to sets of integers such that

$$0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_r < N \quad . \tag{11}$$

Since the chain is closed upon itself, each eigenstate may be characterized by a wave number q given by:

$$q = 2\pi N^{-1} \sum_j \lambda_j \pmod N = \sum_j k_j \pmod{2\pi}. \tag{12}$$

(Note that $\phi_{j\ell} = -\phi_{\ell j}$.)

Although the sum of all the k_j is real, individual k values may be real or complex. This fact, among others, makes the discussion of the existence of roots of Eq. (6) rather difficult. The following questions have not been discussed (to the best of our knowledge) in any adequate sense: For what choices of sets of integers λ_j does (6) possess a solution? If there is a solution, is it unique? Given a solution to (6), what are the conditions such that the wave function (5) does not vanish? Are the wave functions corresponding to different sets of λ_j linearly independent? Can all, or at least almost all, the eigenfunctions of the chain be written in the form (5)?[6]

It is convenient to divide the eigenstates of the form (5) into two categories, the "bound" states and the "unbound" states. The latter category contains the states for which all the k_j are real, the former the states for which at least some of the k_j are complex. There is a corresponding division of the sets of integers $\{\lambda_j\}$. The reason for the terminology "bound" and "unbound" is to be found in Bethe's discussion[7] of the case r = 2. He shows that complex k values correspond to a state in which $|a(n_1,n_2)|^2$ decreases exponentially as $|n_2-n_1|$ increases; i.e., two spin waves interact with each other to form a bound state.

In particular Bethe's calculations indicate that the class C[8] consisting of those sets of integers for which

$$\lambda_{j+1} \geq \lambda_j + 2 \tag{13}$$

is satisfied are unbound. We shall denote by B the class of all states for which (13) is not satisfied. Class B also contains some unbound states, although Bethe's computations suggest that the relative number of such states is small.

In our calculations below we shall be concerned entirely with states of class C. We shall assume that each set of integers satisfying (11) and (13) gives rise to a single state (or, rather, a multiplet of degeneracy 2S+1, where S is the total spin of the state) for which all the k values are real, and that states corresponding to different sets of integers in class C are linearly independent. A certain (but far from complete!) justification for these assumptions is to be found in the calculations of

des Cloizeaux and Pearson[3] and the author[9] on finite chains; and in a proof of the existence of solutions to Eq. (6) which will be found in Appendix A.

The importance of the states in class C for the problem of the antiferromagnetic chain comes from the following "theorem": For a given total spin S, the state with the lowest energy (for antiferromagnetic coupling) belongs to class C. The "theorem" has not been proved, although it is supported by the aforementioned calculations in references 1 and 3, and also by the results of this paper (see Section III D and Fig. 1).

Some insight into the structure of Eq. (6), at least for real values of the k_j, is provided by regarding it as a non-linear transformation of the vector $(k_1, \ldots, k_r)$ into another vector with components:

$$k_j' = 2\pi N^{-1} \lambda_j + N^{-1} \sum_{\ell(\neq j)} \phi(k_j, k_\ell) , \qquad (14)$$

where for $\phi_{j\ell}$ we have written $\phi(k_j, k_\ell)$. A solution to (6) is a fixed point of the transformation (14). Suppose that we attempt to solve (14) by iteration. A sensible starting value for k_j is:

$$k_{j0} = 2\pi N^{-1} \lambda_j \qquad (15)$$

which lies within the interval $(0, 2\pi)$. If k_j and k_1 are both in the interval $(0, 2\pi)$ and k_1 is greater than k_j, then $\varphi(k_j, k_1)$ is positive. Hence the second term on the right hand side of (14) represents an "attractive force" between pairs of wavevectors. Thus if, for example, the initial

values k_{jo} are distributed uniformly over the interval $(0, 2\pi)$, successive iterations of (14) will lead to an increase in the density of the k_j's near π and a decrease at the end points of the interval, 0 and 2π.

If the starting values for k_j and k_{j+1} are too close together, successive iterates of (14) may eventually lead to a "collision" in which $k_{j+1} = k_j$. But a solution of (6) for which two of the k_j's coincide is trivial in the sense that the corresponding wavefunction (5) vanishes identically. A possible remedy for this situation is to make the two k_j's complex, with imaginary parts of opposite sign, resulting in a "bound state." Condition (13) for states in class C insures that the initial values of adjacent k_j are far enough apart so that no "collisions" will occur. These considerations are further developed in Appendix A.

As a first step in examining the energy level structure of class C we shall investigate the highest and lowest energies for a given value of S, the total spin. If the value of r (and thus S) is fixed, Eq. (10) indicates that ϵ will be a maximum when the k_j are near the center of the interval $(0, 2\pi)$ and a minimum when they are distributed at the two ends of the interval. On the basis of (15) and the discussion following that equation, it is reasonable to assume (although we have no proof) that the former condition is achieved when the λ_j are near the center of the interval (0,N) and the latter when they are distributed at the two ends of the interval. Further recall that ϵ measures the energy

from the ferromagnetic ground state, whereas we are interested in maximum and minimum energies for antiferromagnetic coupling. The foregoing argument leads to the following choices for a given value of $S = \frac{1}{2}N-r$:

Minimum energy:

$$\lambda_1 = \tfrac{1}{2}N-r+1,\ \lambda_2 = \lambda_1+2,\ \lambda_3 = \lambda_1+4,\ \dots,\ \lambda_r = \tfrac{1}{2}N+r-1\ . \qquad (16)$$

In particular, the antiferromagnetic ground state (S=0) corresponds to:

$$\lambda_1 = 1,\ \lambda_2 = 3,\ \lambda_3 = 5,\ \dots,\ \lambda_{N/2} = N-1\ . \qquad (17)$$

Maximum energy:

$$\lambda_1 = 1, \lambda_2 = 3, \dots, \lambda_{r/2} = r-1,$$
$$\lambda_{r/2+1} = N-(r-1),\ \lambda_{r/2+2} = N-(r-3),\ \dots,\ \lambda_r = N-1\ . \qquad (18)$$

We have tacitly assumed in writing (16), (17), and (18) that N and r are even; minor modifications are required if one or the other is odd.

III. The Hulthén Integral Equation

A. The Antiferromagnetic Ground State

Consider the antiferromagnetic ground state which corresponds to the set of integers (17). For large N it is reasonable to replace Eq. (6) by an integral equation in the following manner:[2] Let x be a continuous variable on the interval (0,1). Replace λ_j by Nx, k_j by $k(x)$, and Eq. (6) by

$$N k(x) = 2\pi N x + \tfrac{1}{2} N \int_0^1 \phi(x,y)\, dy \tag{19}$$

where

$$\cot \tfrac{1}{2}\phi(x,y) = \tfrac{1}{2}\left[\cot \tfrac{1}{2} k(x) - \cot \tfrac{1}{2} k(y)\right]$$
$$-\pi \le \phi < \pi . \tag{20}$$

The normalized energy ϵ (see Eq. (10)) is given by:

$$\epsilon_0 = \tfrac{1}{2} \int_0^1 [1 - \cos k(x)]\, dx . \tag{21}$$

In place of the non-linear Eq. (19), Hulthén obtained a linear equation by first differentiating both sides of (19) with respect to x and then introducing dx/dk as the new unknown function and k as the new independent variable, resulting in the equation:

$$1 = \pi \frac{dx}{dk} + \frac{1}{\sin^2 \frac{1}{2} k} \int_0^{2\pi} \frac{(dx/dk')\, dk'}{4 + (\cot \frac{1}{2} k - \cot \frac{1}{2} k')^2} \tag{22}$$

Still another change of variables:

$$\xi = \cot \tfrac{1}{2} k$$

$$f_0(\xi) = -dx/d\xi \tag{23}$$

permits (22) to be rewritten in the form:

$$f_0(\xi) = g_0(\xi) - \int_{-\infty}^{\infty} K(\xi-\eta)\, f_0(\eta)\, d\eta \tag{24}$$

where

$$g_0(\xi) = (2/\pi)(1+\xi^2)^{-1} \tag{25}$$

$$K(\xi-\eta) = (2/\pi)\left[4 + (\xi-\eta)^2\right]^{-1}, \tag{26}$$

and, furthermore,

$$\epsilon_0 = \int_{-\infty}^{\infty} f_0(\xi)(1+\xi^2)^{-1} d\xi. \tag{27}$$

Hulthén solved (24) by successive iteration. For our purposes it is convenient to write the solution in the form

$$f_0(\xi) = g_0(\xi) - \int_{-\infty}^{\infty} R(\xi-\eta)\, g_0(\eta)\, d\eta \tag{28}$$

where the resolvent kernel R(x) may be written as an infinite sum:

$$R(x) = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{2n\,(-1)^{n+1}}{(2n)^2 + x^2} \tag{29}$$

or as an integral:

$$R(x) = \frac{1}{4\pi} \int_{-\infty}^{\infty} \frac{\operatorname{sech}(\pi y/2)}{1 + (y+x)^2}\, dy\,. \tag{30}$$

The following is an important relationship between the kernel K and its resolvent R:

$$\int_{-\infty}^{\infty} K(\xi - \eta) R(\eta - \tau)\, d\eta = K(\xi - \tau) - R(\xi - \tau) \tag{31}$$

The solution to (24) is:

$$f_0(\xi) = \tfrac{1}{2} \operatorname{sech} \tfrac{1}{2}\pi\xi \tag{32}$$

and the corresponding energy is:

$$\epsilon_0 = \log 2\,. \tag{33}$$

B. States of Minimum Energy

Hulthén's procedure outlined above (with some changes in notation) may be applied with only minor modifications to the more general problem of finding the energies associated with states corresponding to the sets of λ values in (16) and (18). Consider first the states of minimum energy, (16). Equations (19) and (21) must be replaced by:

$$k(x) = 2\pi x + \tfrac{1}{2}\int_{\frac{1}{2}-a}^{\frac{1}{2}+a} \phi(x,y)\,dy \tag{34}$$

$$\epsilon = \tfrac{1}{2}\int_{\frac{1}{2}-a}^{\frac{1}{2}+a} [1-\cos k(x)]\,dx \quad , \tag{35}$$

with a determined by the requirement that

$$\tfrac{1}{2}N - S = r = Na \quad . \tag{36}$$

In place of r and S it is convenient to introduce the abbreviations:

$$\rho = r/N$$

$$\rho_1 = S/N = \tfrac{1}{2} - \rho. \tag{37}$$

Equation (34) may be transformed by the same procedure used with (19). Define

$$\xi = \cot \tfrac{1}{2}k$$

$$f(\xi) = -dx/d\xi \quad . \tag{38}$$

The resulting linear integeral equation is[2]:

$$f(\xi) = g_0(\xi) - \int_{-\alpha}^{\alpha} K(\xi-\eta) f(\eta)\, d\eta , \tag{39}$$

with limits of integration determined by the requirement:

$$\rho = a = \frac{1}{2}\int_{\frac{1}{2}-a}^{\frac{1}{2}+a} dx = -\frac{1}{2}\int_{-\alpha}^{\alpha} (dx/d\xi)\, d\xi = \frac{1}{2}\int_{-\alpha}^{\alpha} f(\xi)\, d\xi . \tag{40}$$

The normalized energy ϵ is equal to:

$$\epsilon = \int_{-\alpha}^{\alpha} f(\xi)\,(1+\xi^2)^{-1}\, d\xi \tag{41}$$

The quantity of interest is, of course, ϵ regarded as a function of ρ. The most convenient procedure to follow in deducing this function, however, is to choose a value of α, solve (39), and then obtain ρ and ϵ by means of (40) and (41).

In Eqs. (39)-(41), only the values of $f(\xi)$ for $|\xi| \le \alpha$ are employed. However, $f(\xi)$ may be defined for values of $|\xi| > \alpha$ by means of (39) and thus extended to a function on the entire real axis. This extended function also satisfies a different integral equation. Multiply the right and left hand side of (39) by $R(\zeta - \xi)$ and integrate with respect to ξ from $-\infty$ to $+\infty$. By interchanging the order of integration on the right hand side and utilizing the relations (31), (28), and (39), one obtains the equation:

$$f(\xi) = f_0(\xi) + \left(\int_{-\infty}^{-\alpha} + \int_{\alpha}^{\infty}\right) R(\xi-\eta)\, f(\eta)\, d\eta . \tag{39a}$$

Similarly, in place of (40) and (41) one has:

$$\rho_1 = \frac{1}{2} - \rho = \frac{1}{2}\int_{\alpha}^{\infty} f(\xi)\, d\xi \tag{40a}$$

$$\epsilon_1 = \epsilon_0 - \epsilon = \pi \int_{\alpha}^{\infty} f_0(\xi)\, f(\xi)\, d\xi \quad . \tag{41a}$$

Equation (40a) is obtained by integrating both sides of (39) from $-\infty$ to $+\infty$, noting that

$$\int_{-\infty}^{\infty} g_0(\xi)\, d\xi = 2 \; ; \; \int_{-\infty}^{\infty} k(\xi)\, d\xi = 1 \quad . \tag{42}$$

To obtain (41a), multiply the right and left hand sides of (39a) by

$$(1+\xi^2)^{-1} = \frac{1}{2}\pi g_0(\xi)$$

and integrate from $-\infty$ to $+\infty$. By interchanging the order of integration on the right hand side and utilizing (27), (28), and (41), one arrives at the result (41a).

The equations (39a)-(41a) are particularly useful in the problem of obtaining the asymptotic behavior of ϵ_1 and ρ_1 when α is large; i.e., when ϵ_1 and ρ_1 are small. This asymptotic behavior is of particular interest since it determines the magnetic susceptibility in small magnetic fields when the temperature is zero, as shown below in Section IV. An investigation of this problem by Ledinegg and Urban[4] utilizing Eqs. (39)-(41) appears to be in error due to some unjustified approximations. We shall discuss their calculation further in Appendix B.

Since $f(\xi)=f(-\xi)$, (39a) may be rewritten as:

$$f(\xi) = f_0(\xi) + \int_\alpha^\infty [R(\xi-\eta)+R(\xi+\eta)]\, f(\eta)\, d\eta. \qquad (43)$$

Furthermore, since

$$e^{-\frac{1}{2}\pi\xi} - e^{-\frac{3}{2}\pi\xi} < f_0(\xi) < e^{-\frac{1}{2}\pi\xi} \quad , \qquad (44)$$

we are clearly justified in replacing $f_0(\xi)$ by $\exp(-\frac{1}{2}\pi\xi)$ in (43) and (41a) in order to obtain an asymptotic solution for large α. Note that only values of ξ and η greater than α come into consideration in solving the integral equation and evaluating ϵ_1 and ρ_1. For large values of z,

$$R(z) = R(-z) \sim (2\pi z^2)^{-1} \quad ; \qquad (45)$$

therefore, provided α is very large, it should be possible to neglect $R(\xi + \eta)$ relative to $R(\xi - \eta)$ in (43).

Next define:

$$p(\xi) = e^{\frac{1}{2}\pi\alpha}\, f(\xi+\alpha) \qquad (46)$$

and rewrite (43), using the approximations introduced in the preceding paragraph, in the form:

$$p(x) = e^{-\frac{1}{2}\pi x} + \int_0^\infty R(x-y)\, p(y)\, dy \quad . \qquad (47)$$

The quantities ϵ_1 and ρ_1 are given by:

$$\rho_1 \approx e^{-\frac{1}{2}\pi\alpha}\left(\tfrac{1}{2}\int_0^\infty p(x)\,dx\right) = a\,e^{-\frac{1}{2}\pi\alpha} \tag{48}$$

$$\epsilon_1 \approx e^{-\pi\alpha}\left(\pi\int_0^\infty e^{-x}\,p(x)\,dx\right) = b\,e^{-\pi\alpha} \quad . \tag{49}$$

Numerical solutions of (39) confirm the exponential variation of ρ_1 and ϵ_1 predicted by (48) and (49), with coefficients which are slowly varying functions of α. A numerical solution of (47), though not to a very high accuracy, yields the following values for a and b:

$$\begin{aligned} a &= .484 \pm .0005 \\ b &= 1.156 \pm .001 \quad . \end{aligned} \tag{50}$$

On the basis of a model we plan to discuss in a subsequent report, we expect the ratio b/a^2 to be equal to $\frac{1}{2}\pi^2$, and this is in agreement with (50) within the precision of our calculations. Hence we write:

$$\epsilon_1 \sim \frac{1}{2}\,\pi^2\rho_1^{\,2} \tag{51}$$

for very small ρ_1.

It is also useful to consider the states of minimum energy for the case where α is small, and hence ρ and ϵ are both small. Equations (39)-(41) yield immediately the asymptotic limits:

$$\rho \sim 2\alpha/\pi$$
$$\epsilon \sim 2\rho \qquad (52)$$

provided ρ or α is very small.

C. States of Maximum Energy

For a given value of total spin S, we expect the states with the maximum energy in class C to be associated with sets of integers of the form (18). The calculation of energy as a function of S may be carried out in complete analogy with the procedure in Section III B above. Thus Eq. (34) must be replaced by:

$$k(x) = 2\pi x + \tfrac{1}{2}\left(\int_0^b + \int_{1-b}^{1}\right) \phi(x,y)\,dy \tag{53}$$

and Eqs. (39)-(41) by:

$$f(\xi) = g_0(\xi) - \left(\int_{-\infty}^{-\alpha} + \int_{\alpha}^{\infty}\right) k(\xi-\eta)\, f(\eta)\, d\eta \tag{54}$$

$$\rho = \int_{\alpha}^{\infty} f(\xi)\, d\xi \tag{55}$$

$$\epsilon = 2\int_{\alpha}^{\infty} f(\xi)\,(1+\xi^2)^{-1}\, d\xi \,. \tag{56}$$

In analogy with (39a)-(41a), it is possible to derive an equivalent set of equations where the integrals run from $-\alpha$ to α :

$$f(\xi) = f_0(\xi) + \int_{-\alpha}^{\alpha} R(\xi-\eta)\, f(\eta)\, d\eta \tag{54a}$$

$$\rho_1 = \tfrac{1}{2}\int_0^{\alpha} f(\xi)\, d\xi \tag{55a}$$

$$\epsilon_1 = \pi \int_0^{\alpha} f_0(\xi) f(\xi)\, d\xi . \tag{56a}$$

When α is small, we have, approximately,

$$\begin{aligned} \rho_1 &\sim \tfrac{1}{4}\alpha \\ \epsilon_1 &\sim \tfrac{1}{4}\pi\alpha \end{aligned} \tag{57}$$

or

$$\epsilon_1 \sim \pi \rho_1 \tag{58}$$

provided ρ_1 is small.

The asymptotic values of ϵ and ρ when α is large may be obtained as follows using (54)-(56). First rewrite (54) in the form:

$$f(\xi) = g_0(\xi) - \int_{\alpha}^{\infty} [K(\xi-\eta) + K(\xi+\eta)]\, f(\eta)\, d\eta. \tag{59}$$

Since $K(z)$ decreases as $1/z^2$ for large values of z, it is reasonable to neglect $K(\xi + \eta)$ relative to $K(\xi - \eta)$ on the right hand side of (59), provided α is large and we are only interested in values of ξ greater than α. Thus for large α we have, approximately,

$$f(\xi) \approx 2(\pi \xi^2)^{-1} - \int_{\alpha}^{\infty} K(\xi-\eta)\, f(\eta)\, d\eta . \tag{60}$$

Let $\xi = \alpha x$, $\eta = \alpha y$, and $f(\alpha x) = p(x)$. Equation (60) becomes:

$$p(x) \approx 2(\pi \alpha^2 x^2)^{-1} - \int_{1}^{\infty} \alpha\, K(\alpha x - \alpha y)\, p(y)\, dy. \tag{61}$$

Now as α becomes very large, the kernel $\alpha K(\alpha x - \alpha y)$ approaches a Dirac delta function, $\delta(x - y)$. If we replace it with a delta function inside the integral, the solution of (61) is:

$$p(x) = (\pi \alpha^2 x^2)^{-1} \quad . \tag{62}$$

Thus $p(x)$ is a function of α, but only through a multiplicative constant; otherwise it is a smoothly varying function of x. This provides an <u>a posteriori</u> justification for replacing the kernel in (61) with a delta function. Finally we obtain for ρ and ϵ the results:

$$\begin{aligned} \rho &\sim 1/(\pi \alpha) \\ \epsilon &\sim 2/(3 \pi \alpha^3) \end{aligned} \tag{63}$$

and

$$\epsilon \sim \tfrac{2}{3} \pi^2 \rho^3 \tag{64}$$

when ρ is small.

D. Numerical Solutions of the Integral Equations

The integral equations (39) and (54a) were approximated by a set of 41 coupled linear algebraic equations, and these were solved on a high speed digital computer. The results are shown in Fig. 1. The normalized energies ϵ, measured from the ferromagnetic ground state, and ϵ_1, measured from the antiferromagnetic ground state, are plotted as a function of $\rho_1 = S/N$, where S is the total spin of the state, and $\rho = \frac{1}{2} - \rho_1$. Note that $\epsilon_1 = .693 - \epsilon$. The lower curve, computed by means of (39)-(41), represents not only the lowest energy for a given ρ_1 for states in class C, but should also, according to the discussion in Section II, be the lowest energy for all states in the antiferromagnetic chain. The open circles in Fig. 1 are the lowest energies for an antiferromagnetic chain containing 9 spins, while the solid circles are the corresponding energies for a chain containing 10 spins. These energies, computed directly from the Hamiltonian (1)[9] and therefore independently of the Bethe formalism, fall surprisingly close to the solid curve--which should represent the limit as N becomes infinite--and thus provide additional support for the "theorem" of Section II.

The numerical calculations provide some confirmation for the asymptotic estimates contained in (48), (49), (50), and (51). For $\alpha = 3.0$, the numerical results are:

$$\begin{aligned} \rho_1 &= 1.531 \times 10^{-3} = .504\, e^{-1.5\pi} \\ \epsilon_1 &= 9.39 \times 10^{-5} = 1.163\, e^{-3\pi} \\ \epsilon_1 &= 4.57\, \rho_1^2 = .926 \left(\tfrac{1}{2}\pi^2 \rho_1^2\right) \end{aligned} \tag{65}$$

Equation (52) is also borne out by numerical calculations. For instance, at $\alpha = .2$:

$$\rho = .1182 = .928\,(2\alpha/\pi)$$
$$\epsilon = .2333 = 1.97\rho \quad . \tag{66}$$

The upper curve in Fig. 1 represents the maximum energy for states in class C and was computed by means of (54a)-(56a). The calculations were supplemented by the use of (54)-(56) for larger values of α. It must be emphasized that this curve has significance only for the class C and not for the entire energy level spectrum, as in general (except, perhaps, for ρ very close to 0 or $\frac{1}{2}$) there will be states in class B lying both above and below the curve. Once again, the numerical calculations confirm the asymptotic behavior for small and large α values given by (57), (58), (63), and (64). Thus for $\alpha = .2$

$$\rho_1 = .05145 = 1.029\,(\alpha/4)$$
$$\epsilon_1 = .1591 = .984\,(\pi\rho_1) \tag{67}$$

and for $\alpha = 10$.

$$\rho = .03369 = 1.058\,(\pi\alpha)^{-1}$$
$$\epsilon = 2.521\times10^{-4} = 1.002\,(2\pi^2\rho^3/3). \tag{68}$$

IV. Magnetic Moment and Susceptibility at Zero Temperature

In the presence of a magnetic field H along the positive z axis, there is, in addition to the exchange energy (1), a Zeeman energy:

$$\mathcal{H}_z = g\mu H \sum_i S_{iz} \tag{69}$$

where μ is the Bohr magneton, g the electron g factor, and S_{iz} the z component of spin for the i'th atom. The lowest energy level of the chain for a given value of total spin S in the presence of a magnetic field will be:

$$E_{min}(S) = E(S) - g\mu HS \tag{70}$$

where E(S) is the lowest energy in the absence of a magnetic field, and thus equal to:

$$E(S) = 2NJ\,\epsilon_1(S/N) + E_{AF} \,. \tag{71}$$

By $\epsilon_1(S/N) = \epsilon_1(\rho_1)$ we mean the function corresponding to the lower curve in Fig. 1 and determined by Eqs. (39a)-(41a). Next, let us choose among all the values of S the value S_o for which (70) is a minimum. This can be done by differentiating the right hand side of (70) with respect to S and setting the derivative equal to zero, with the result:

$$2J\,\epsilon_1'(S_o/N) = g\mu H \,. \tag{72}$$

At zero temperature the free energy of the chain, F, is equal to $E_{min}(S_o)$. From this one can calculate the average magnetization per spin:

$$M = -N^{-1}\, dF/dH = g\mu S_o/N. \tag{73}$$

The magnetization as a function of applied field is plotted in Fig. 2. At fields in excess of $4J/g\mu$, the magnetization is completely saturated. There is a well defined susceptibility for values of H much less than $J/g\mu$:

$$\chi = g^2\mu^2/(2\pi^2 J) \quad . \tag{74}$$

The numerical constant appearing on the right side of (74) is determined by the asymptotic expression (51), and is only known to a precision of about one-half percent, as indicated in the discussion preceding (51).

Strictly speaking, the result (74) holds only for the infinite antiferromagnetic chain. For chains containing a finite number of atoms the susceptibility at zero temperature in the limit of zero magnetic field is either zero (for N even) or infinite (for N odd). Calculations at finite temperatures for short chains containing up to 11 spins[10] indicate that (74) is probably not an unreasonable limit for the infinite chain.

Hulthén[11] derived, by means of a "statistical model," an approximate value for χ, identical with (74) except that the constant $(2\pi^2)^{-1} = .0506$ is replaced by .0593. The "self consistent" procedure used by Fain[12] yields in place of $(2\pi^2)^{-1}$ the constant .0556, only 10% larger than the exact value.

Acknowledgments

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Appendix A. Existence of Solutions of Equation (6) for States in Class C

We shall prove that the transformation (14), under suitable restrictions, possesses a fixed point, and hence Eq. (6) a solution. Let V be the real r-dimensional space of vectors of the form $(k_1, k_2, \ldots, k_r)$ and let K be the subset of V consisting of those vectors whose components satisfy the inequalities:

$$\begin{aligned} k_1 &\geq 2\pi N^{-1} \\ k_r &\leq 2\pi (1 - N^{-1}) \\ k_{j+1} - k_j &\geq 2\pi N^{-1} \end{aligned} \qquad \text{(A1)}$$

The function $\phi(k_j, k_\ell)$ (see (7)) is positive for $k_\ell > k_j$, negative for $k_\ell < k_j$ and continuous for all k_j, k_ℓ in the interval $(0, 2\pi)$ except at the points $k_j = k_\ell$. Hence the transformation (14) restricted to the subset K is continuous. Furthermore the function $\phi(k_j, k_\ell)$ in either the region $k_j < k_\ell$ or the region $k_j > k_\ell$ is monotone increasing in the first argument and monotone decreasing in the second. Utilizing this fact one obtains the inequality:

$$k'_{j+1} - k'_j \geq 2\pi N^{-1} (\lambda_{j+1} - \lambda_j) - 2N^{-1} \phi(k_j, k_{j+1}). \qquad \text{(A2)}$$

For states in class C we have the inequality (13) which together with the fact that $|\phi| < \pi$ implies that

$$k'_{j+1} - k'_j \geq 2\pi N^{-1} \qquad \text{(A3)}$$

The aforementioned properties of ϕ together with condition (11) guarantee

the inequalities:

$$k_1' \geq 2\pi N^{-1}$$

$$k_r' \leq 2\pi(1-N^{-1}) \qquad \text{(A4)}$$

A comparison of (A3) and (A4) with (A1) shows that the transformation (14) carries the set K into itself. The set K is closed, convex, and bounded; this together with the continuity of (14) on the set K implies the existence of at least one fixed point by Brouwer's theorem.[13]

Appendix B. The Ledinegg-Urban Calculation

For convenience, we shall enclose equation numbers from the paper by Ledinegg and Urban[4] in square brackets, and transcribe the equations in our notation. Their paper is concerned with the problem of obtaining asymptotic values for ρ and ϵ (or ρ_1 and ϵ_1) as a function of α in the limit of large α, using (39)-(41). Their results are:

$$\rho_1 \sim .518\, e^{-\frac{1}{2}\pi\alpha} \qquad [38d]$$

$$\epsilon_1 \sim .398\, e^{-\frac{1}{2}\pi\alpha}/\alpha^2 \qquad [37]$$

The result [38d] is not much different from our calculations--see (48) and (50)--except we obtain a smaller value for the numerical constant. However, a comparison of [37] with (49) shows a very important difference: The exponent which appears in the latter is twice the value in the former, and the factor α^{-2} is missing. The numerical solutions to Eqs. (39)-(41) support (49) rather than [37].

Ledinegg and Urban obtain their asymptotic estimate as follows. The function $f(\xi)$ in (39) (their Eq. [23]) is set equal to:

$$f(\xi) = f_0(\xi) + \phi(\xi) \qquad [24a]$$

where $f_0(\xi)$ is the solution of (24) given by (32). Next they assume that

$$|\phi(\xi)| / f_0(\xi) \ll 1, \qquad [24c]$$

stating that this inequality will be justified through an explicit calculation of the function ϕ. It is not stated whether the inequality [24c] is to hold for $|\xi| < \alpha$ or for $|\xi| > \alpha$. They make explicit use of [24c] for $|\xi| > \alpha$ in deducing the approximate integral equation for ϕ:

$$\phi(\xi) = \left(\int_{-\infty}^{-\alpha} + \int_{\alpha}^{\infty} \right) k(\xi - \eta)\, f_0(\eta)\, d\eta - \int_{-\infty}^{\infty} k(\xi - \eta)\, \phi(\eta)\, d\eta . \qquad [26b]$$

Their justification for [24c], however, is contained in the equation:

$$\phi(\xi) = (4\pi)^{-1}\, e^{-\frac{1}{2}\pi\alpha} \left[\Phi(\alpha + \xi) + \Phi(\alpha - \xi) \right] \qquad [33a]$$

where Φ is a relatively slowly varying function of its arguments. This shows, indeed, that the inequality [24c] is justified--but <u>only</u> for $|\xi| < \alpha$. It is easy to prove, using their expression [33d] for Φ, that for $|\xi| \gg \alpha$, [24c] is not only incorrect, but the reverse inequality holds, since for large ξ,

$$f_0(\xi) \sim e^{-\frac{1}{2}\pi\xi} . \qquad (44)$$

However, it is for the region $|\xi| > \alpha$ that the inequality [24c] must be invoked in order to justify [26b]. Thus we infer that their treatment is not internally consistent.

It is, in fact, very difficult to attack (39) by a straightforward perturbation approach, since ϵ_1, which is of the order of $\exp(-\pi\alpha)$, turns

out to be the difference between two much larger terms, both of order $\exp(-\frac{1}{2}\pi\alpha)$. The advantage of (39a)-(41a) over (39)-(41) for the case of large α consists precisely in the fact that no such near cancellation occurs in calculating either e_1 or o_1. Even the zeroeth order approximation to (39a)--replacing $f(\xi)$ by $f_o(\xi)$--leads to the correct functional form for the asymptotic values (48) and (49), although not to the correct numerical coefficients.

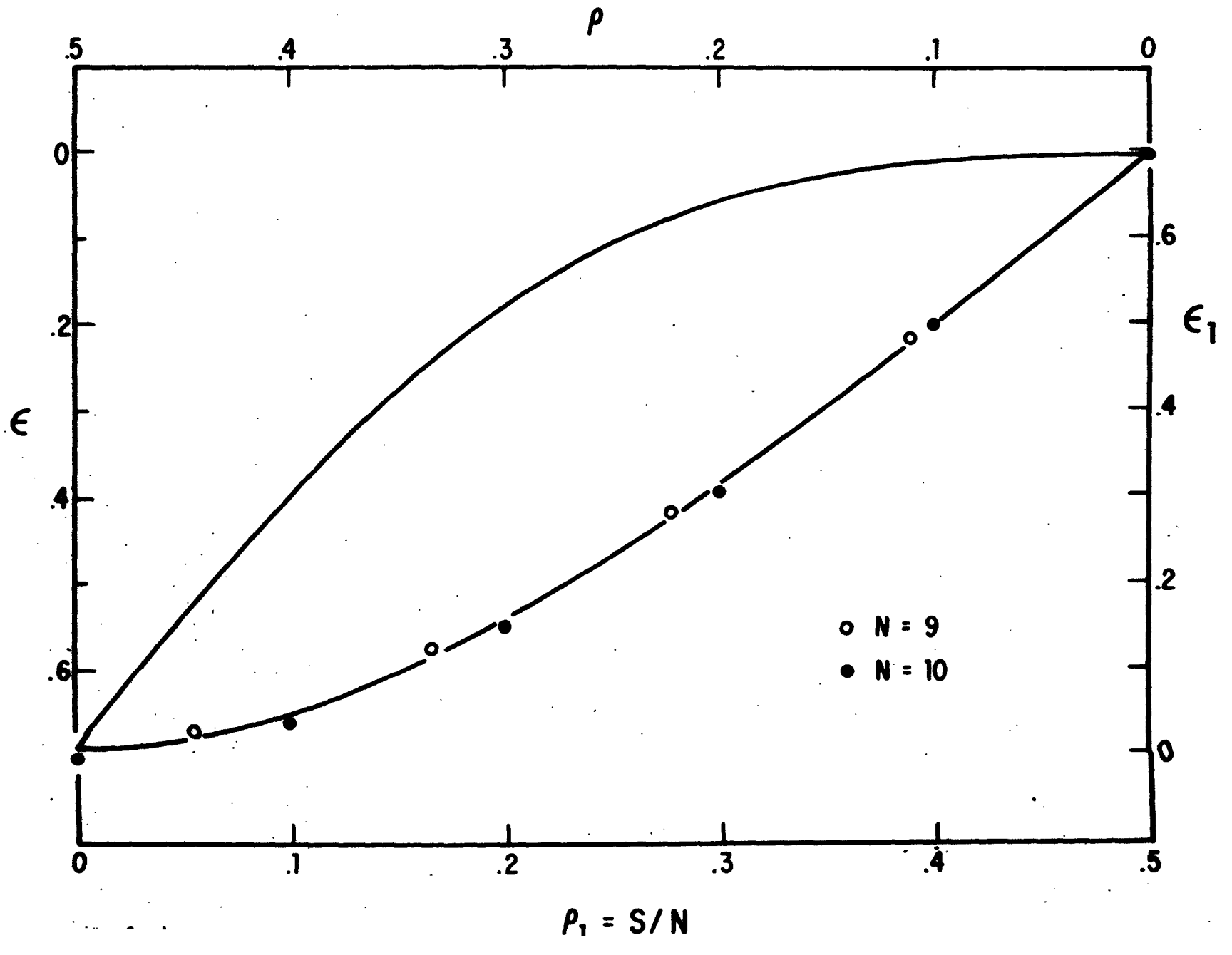
Figure Captions

Fig. 1. Highest and lowest energies for states in class C as a function of the total spin S. The circles represent the lowest energies for finite chains containing 9 and 10 atoms.

Fig. 2. The magnetization as a function of field for the antiferromagnetic linear chain at zero temperature.

Footnotes

1. H. Bethe, Z. Physik 71, 205 (1931).
2. L. Hulthén, Arkiv Mat. Astron. Fysik 26A, No. 11 (1938).
3. J. des Cloizeaux and J. J. Pearson, Phys. Rev. 128, 2131 (1962).
4. E. Ledinegg and P. Urban, Acta Physica Austriaca 6, 257 (1953).
5. Our definition of ϵ is smaller than that given in references 1, 2, and 3 by a factor N^{-1}.
6. It is known that there are certain eigenstates of (1) which cannot be expressed in the form (5) except, perhaps, as limiting cases. See reference 1, p. 214, and reference 3.
7. Reference 1, p. 214.
8. Notation of reference 3.
9. R. B. Griffiths (unpublished).
10. J. C. Bonner and M. E. Fisher (to be published).
11. Reference 2, p. 78.
12. Reported in V. L. Ginzburg and V. M. Fain, J. Exptl. Theoret. Phys. (U.S.S.R.) 42, 183 (1962) [Soviet Phys. JETP 15, 131 (1962)].
13. G. T. Whyburn, Analytic Topology, Amer. Math. Soc. Colloquium Publications, Vol. XXVIII (American Mathematical Society, New York, 1942), p. 243.


ρ
.5
.4
.3
.2
.1
0
0
.2
.4
.6
ε
ε1
.6
.4
.2
0
o N = 9
• N = 10
0
.1
.2
.3
.4
.5
ρ1 = S/N

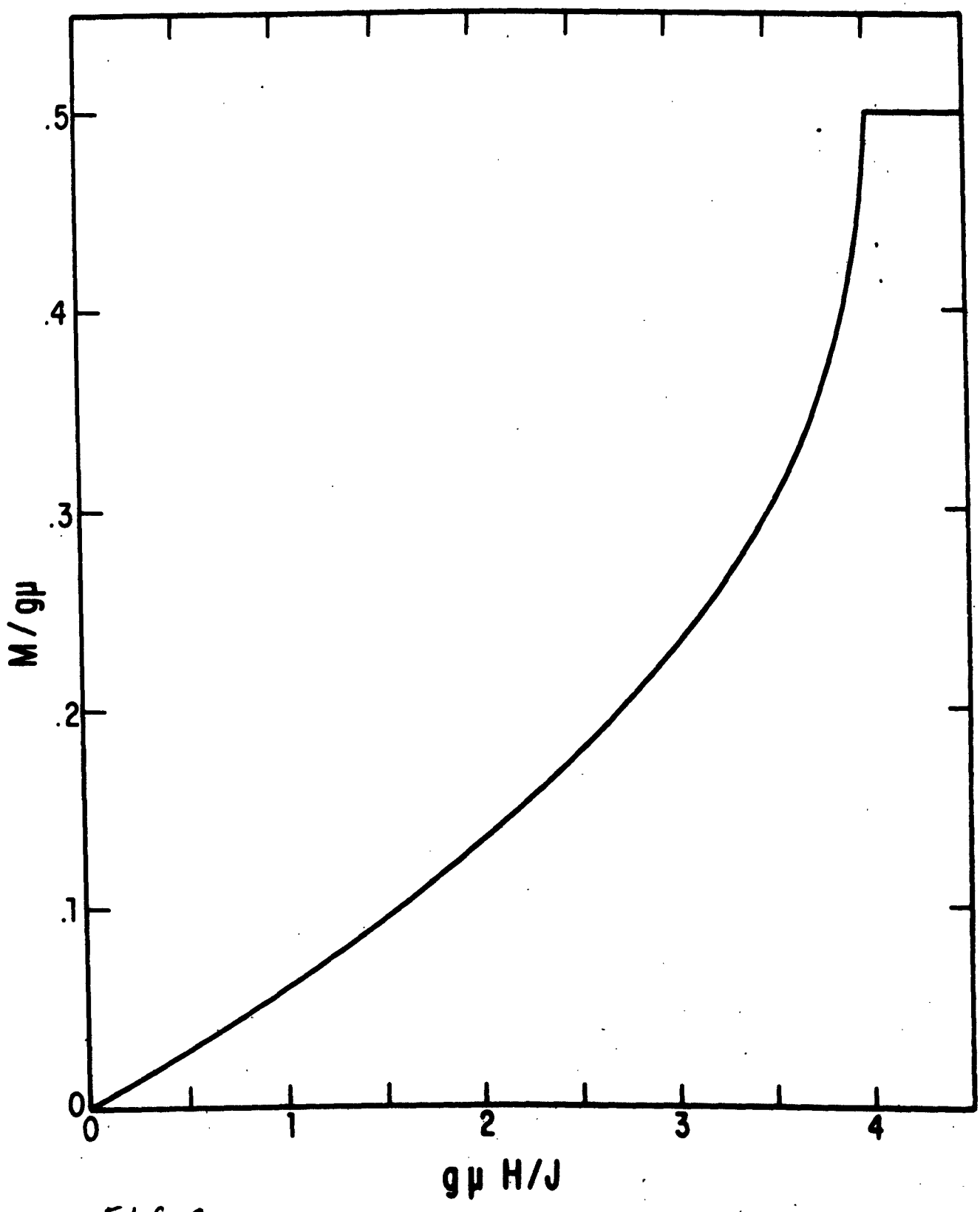


FIG 2