

from the energies of the emitted light which are about 2.5–3.5 eV, while direct recombination of a free hole, for example, with an electron in an  $F$  center should result in the emission of about 6 eV.

Finally, mention should be made of the appearance in pairs of the spectral bands in the thermoluminescence. The three pairs: 0.354–0.37, 0.41–0.435, and 0.47–0.50  $\mu$  observed in the present work seem to have a common energy difference of about 0.16 eV within each

pairs. More accurate determination of these separations is necessary before the existence of such a doublet is confirmed. It is of interest to note that a doublet of about 0.15-eV separation has been observed<sup>15</sup> in the exciton-band of NaCl.

The investigation is now extended in our laboratory to include other alkali-halides with the hope that it will lead to better understanding of the effects described.

<sup>15</sup> P. L. Hartman, Phys. Rev. **105**, 123 (1957).

### Antiferromagnetic Linear Chain

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Orbach's integral equation which leads to the value of the ground-state energy of an anisotropic antiferromagnetic linear chain of spins,  $S = \frac{1}{2}$ , has been solved. The result is then expanded in powers of the anisotropy parameter. In this form it corresponds to the result of a perturbation calculation, the transverse part of the Hamiltonian being the perturbation. The rapid convergence of the energy series even for the isotropic case and the adequate convergence of that for the short range order, suggests that the result given by perturbation theory for the sublattice magnetization may also be satisfactory.

ORBACH<sup>1</sup> has recently considered the antiferromagnetic linear chain with an Ising type of anisotropy. The Hamiltonian of the system is taken to be, for a chain of  $N$  spins with  $S = \frac{1}{2}$ ,

$$H = 2J \sum_i (S_i^z S_{i+1}^z + \beta (S_i^z S_{i+1}^x + S_i^y S_{i+1}^y)) \\ = 2J \sum_i (S_i^z S_{i+1}^z + (\beta/2)(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)), \\ 1 \leq i \leq N.$$

If  $E$  is the ground-state energy and a quantity  $\epsilon$  is defined by

$$\epsilon = -(1/2J)(E - \frac{1}{2}JN), \quad (1)$$

Orbach shows that

$$\epsilon = -\frac{N}{2} \int_0^{2\pi} (1 - \beta \cos k) A(k) dk, \quad (2)$$

where  $A(k)$  is a solution of the integral equation

$$A(k) = \frac{1}{\pi} \frac{1}{2\pi} \int_0^{2\pi} dk' \\ \times \frac{(1 - \beta \cos k') A(k')}{1 - \beta(\cos k + \cos k') + \beta^2 \cos[(k+k')/2]}. \quad (3)$$

This equation he solved numerically. By a suitable change of variables (3) may be solved by a Fourier expansion.

<sup>1</sup> R. Orbach, Phys. Rev. **112**, 309 (1958).

We define  $\lambda$  by the relation  $\beta = \text{sech} \lambda$ , with  $\lambda > 0$ , introduce an angle  $\psi$  related to  $k$  by the equation

$$e^{i\psi} = \frac{e^\lambda - e^{ik}}{1 - e^{\lambda+ik}},$$

and replace  $A(k)$  by  $B(\psi)$ , where

$$B(\psi)(e^{i\psi} - e^\lambda)(e^{i\psi} - e^{-\lambda}) = A(k).$$

The integral equation (3) becomes

$$B(\psi) = [\pi(e^{i\psi} - e^\lambda)(e^{i\psi} - e^{-\lambda})]^{-1}$$

$$-\frac{e^{2\lambda} - e^{-2\lambda}}{\pi} \int_0^{2\pi} \frac{e^{2i\psi} B(\psi') d\psi'}{(e^{-\lambda+i\psi'} - e^{\lambda+i\psi})(e^{-\lambda+i\psi} - e^{\lambda+i\psi'})},$$

and has a solution in the form of a series of powers of  $e^{i\psi}$ . The expression for  $B(\psi)$  is

$$B(\psi) = -\frac{1}{\pi} \frac{2}{e^\lambda - e^{-\lambda}} \sum_{-\infty}^{+\infty} \frac{e^{im\psi}}{\cosh |m+1| \psi},$$

or

$$A(\psi) = -\frac{1}{2\pi} \frac{\cos \psi - \cosh \lambda}{\sinh \lambda} \sum_{-\infty}^{+\infty} \frac{e^{im\psi}}{\cosh m\psi}.$$

When this form is introduced into (2) the ground-state energy is found to be given by

$$E = NJ \left[ \frac{1}{2} - \tanh \lambda \left( 1 + \sum_1^{\infty} \frac{4}{e^{2n\lambda} + 1} \right) \right]. \quad (4)$$

For the isotropic case,  $\lambda=0$ ,  $\beta=1$ , this reduces to the well-known value found by Hulthén. It is interesting to note that according to (4)  $\beta$  cannot exceed unity, since  $E$  considered as a function of  $\beta$  has a pole in every interval, however small, of the open segments,  $|\beta| > 1$ .

It is instructive to consider the expansion of Eq. (4) in powers of  $\beta$ , since this corresponds to a perturbation calculation of the energy in which the transverse part of the Hamiltonian is the perturbation.<sup>2</sup> The expansion is given by

$$E/NJ = \frac{1}{2} - (1-\beta^2) \sum_{m=0}^{\infty} \binom{\beta}{2}^{2m} \times \left[ \binom{2m}{m} + 4 \sum_{p=1}^m \binom{2m}{m+p} \varphi_p \right],$$

where  $\varphi_p$  is the difference between the number of odd and of even divisors of  $p$ . The first few terms are

$$E/NJ = -\frac{1}{2} - \frac{1}{2}\beta^2 + \frac{1}{8}\beta^4 - (1/128)\beta^8 - (1/256)\beta^{10} - (1/1024)\beta^{12} + (1/4096)\beta^{14} + \dots \quad (5)$$

This series represents  $E$  excellently even at  $\beta=1$ , presumably in an asymptotic sense. The convergence rests upon the factor of  $\frac{1}{2}$  which precedes the transverse terms. The series, however, is markedly "noisy"; no obvious regularity being apparent in the signs, for example. This can be attributed to fluctuations in the summation over the relatively small number of processes contributing to a given order in perturbation theory. Equation (5) has been checked by a direct perturbation calculation

<sup>2</sup> Such perturbation calculations have been made to estimate the ground-state sublattice magnetization of  $\text{MnF}_2$ . See V. Jacarino and L. R. Walker (to be published).

up to and including sixth order terms. The associated series for the short range order is found to be

$$-(4/N) \langle \sum_i S_i^z S_{i+1}^z \rangle = 1 - \beta^2 + \frac{3}{4}\beta^4 - (14/128)\beta^8 - (18/256)\beta^{10} - (22/1024)\beta^{12} + (26/4096)\beta^{14} \dots \quad (6)$$

This has poorer convergence than (5), but gives an adequate representation at  $\beta=1$ . The latter fact suggests that perturbation theory may give a good value for the sublattice magnetization,  $\sum_i S_i^z$ . It is difficult to obtain any such measure of long range order from Orbach's exact solution. Up to the sixth order one finds

$$(2/N) \langle \sum_i S_i^z \rangle = 1 - \beta^2 - \frac{1}{4}\beta^4 - \frac{1}{16}\beta^6 + \dots \quad (7)$$

If the higher order terms fell off in roughly the same way as those of (6) it would appear that the long range order vanishes when  $\beta^2$  is more than about 0.8. The exact ground-state wave function would lead to a vanishing value, since it must be impartial between the up and down orientations of the sublattices. However, it was pointed out by Anderson<sup>3</sup> that the system will take a very long time (perhaps years) to migrate from a configuration with one preferred orientation of the sublattices to one in which they are inverted. It seems probable that the sublattice magnetization calculated from perturbation theory will correspond to what might be measured experimentally.

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<sup>3</sup> P. W. Anderson, Phys. Rev. **86**, 694 (1952).