Comments and Addenda

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Comment on the ground-state energy of the dilute antiferromagnet

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It is shown that the argument given by Anderson to obtain a lower bound on the ground-state energy of a Heisenberg antiferromagnet can also be used for dilute antiferromagnets. In the limit of extreme dilution it gives the exact ground-state energy.

The ground-state energy of the Heisenberg antiferromagnet described by the Hamiltonian

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \quad (1)$$

is only known exactly for the \( S = \frac{1}{2} \) linear chain.\(^1\)

In this Hamiltonian \( J > 0 \) and connects nearest neighbors which are counted once in the sum as indicated by the angular brackets. It was shown by Anderson,\(^2\) 25 years ago, that for a lattice which can be divided into two sublattices such that the nearest neighbors of atoms in one sublattice lie in the other, the ground-state energy \( E_g \) can be written

$$E_g = -\frac{1}{2} NJ S^2 (1 + \gamma / Sz), \quad (2)$$

where

$$0 < \gamma < 1. \quad (3)$$

The upper bound on the energy \( (\gamma = 0) \) is obtained by using the Néel state as a variational ground state. The lower bound \( (\gamma = 1) \) is obtained by writing

$$H = \sum_{\alpha} H_{\alpha}, \quad (4)$$

where the cluster Hamiltonian \( H_{\alpha} \) describes an atom and its \( z \) neighbors and the summation goes over the \( \frac{1}{2} N \) clusters centered on one sublattice. The ground-state energy is then greater than the sum of the individual cluster ground-state energies which are easily found by writing

$$H_{\alpha} = J \vec{S} \cdot \vec{S}, \quad (5)$$

where \( \vec{S} \) is the central spin of the cluster and \( \vec{S} \) is the vector sum of the spins on the \( z \) neighbors. The ground state energy of the cluster \( E_{\alpha} \) is obtained by maximizing \( \vec{S} \) (i.e., \( \vec{S} = Sz \)) and then coupling \( \vec{S} \) and \( \vec{S} \) antiparallel to give

$$E_{\alpha} = JS(Sz + 1). \quad (6)$$

Results (2) and (3) follow immediately.

In this comment we point out that these arguments can easily be extended to the dilute antiferromagnet where only a fraction \( c \) of sites, chosen randomly, are occupied. The Néel state can be used as a variational ground state leading to an energy as in (1) with \( \gamma = 0 \) but with an extra prefactor \( c^2 \). The Hamiltonian can be expressed as a sum over clusters [as in Eq. (4)]. To contribute to the energy a cluster must have a central atom and \( z \) nearest neighbors where \( 1 < r < 2z \). The ground-state energy of such a cluster is given by (6) with \( z \) replaced by \( r \). The total number of such clusters is \( \frac{1}{2} J c c^{-1} (1 - c)^{3-r} c^r \). The lower bound to the ground-state energy is now given by

$$E_g > -\frac{1}{2} NJ c S(1 - c)^{3-r} c^r, \quad (7)$$

that is,

$$E_g > -\frac{1}{2} NJ c [c Sz + 1 - (1 - c)^r].$$

Putting both bounds together, we obtain

$$E_g = -J S^2 (1 + \gamma / Sz), \quad (8)$$

where

$$0 < \gamma < (1 - (1 - c)^r) / c. \quad (9)$$

This result for \( \gamma \) is shown in Fig. 1. for a simple cubic lattice \((z=6)\). Note that the bounds on \( \gamma \) are

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still spin independent and the Anderson result\(^2\) is recovered as \(c = 1\).

In the limit of extreme dilution, the exact ground-state energy can be found as a power series in the concentration by simply adding up the energy of pairs, triples, etc., with the correct weighing factors. The result for \(\gamma\) up to the term linear in \(c\) (that is counting just pairs and triples) is

\[
\gamma = \varepsilon - \varepsilon (c - 1)c + \cdots, \tag{10}
\]

which is also plotted in Fig. 1. It can be seen that the lower bound on the energy (upper bound on \(\gamma\)) approaches the exact result as \(c \to 0\) but that the slopes differ by a factor 2 for small \(c\). This is because all pairs are assigned to a single cluster but half of the triples are divided between two clusters.

For bond dilution, in which only a fraction \(c\) of the bonds remain, we still obtain the result (9) but the prefactor \(c^2\) is replaced by \(c\) in Eq. (8). The exact expansion (10) is also the same to \(O(c)\) although there would be differences in the next term.

It is interesting to look at the predictions of spin-wave theory.\(^3,4\) When \(c = 1\), we get \(\gamma = 0.58\) and for small \(c\); the exact result \(O(c)\) as given in Eq. (10) (i.e., pairs and triples give the exact ground-state energy within the spin-wave approximation, but some quartets do not). Of course this does not necessarily mean that spin-wave theory is reliable in the dilute limit for other quantities. Indeed the sublattice magnetization is divergent within the spin-wave approximation for any finite cluster with no net moment (equal numbers of up and down spins). In view of this it is perhaps surprising that the neutron scattering law \(S(k, \omega)\) as computed numerically and utilizing the spin wave approximation agrees very well with experiments on \(\text{Rb}_2\text{Mn}_4\text{Mg}_6\cdot\text{Fe}_2\text{F}_{18}\).\(^5,6\) The only substantial error was in the integrated intensity. This is probably another manifestation of the problem with the sublattice magnetization (the addition of a small anisotropy field gets rid of the divergences but the problem remains). More work needs to be done in this area and it is clear that spin-wave theory can only be applied to dilute antiferromagnets if great care is taken.

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\(^4\)A small anisotropy field \(H_A\) must be included in order to remove the degeneracy from the ground state of small clusters. This can be taken to zero after the zero-point correction to the ground-state energy has been calculated.