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# An exactly soluble two-dimensional quantum mechanical Heisenberg model: quantum fluctuations versus magnetic order

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Abstract. Using some simple geometries composed solely of interconnecting 'diamonds', we study the competition between long-range magnetic order and quantum fluctuations. Since a four-atom 'diamond' is formed from two-edge sharing triangles, a 'diamond' is topologically frustrated, and hence magnetic order is energetically less favourable than usual. The classical limit yields a ferrimagnetic state with equally large ferromagnetic and antiferromagnetic moments. Symptomatic of the topological problems, there are some zero energy 'spin wave' modes in the classical limit. For low-spin systems these low energy modes become excited in the ground state, which has none of the properties predicted by the classical solution. For spin  $\frac{1}{2}$ , the ground state has only short-range correlations, a broken translational symmetry, and a gap to localised spin- $\frac{1}{2}$  excitations, which also have a topological quantum number.

#### 1. Introduction

One of the most interesting gaps in our understanding of the behaviour of electronic motion in solids, is strong-coupling paramagnetism. The physical materials which exhibit this behaviour are epitomised by heavy fermions [1] and high-temperature superconductors [2]. It may simply be that the underlying physical cause remains a mystery, but there is a more disturbing possibility. The materials are easily modelled by simple tight-binding Hamiltonians which include: chemical bonding, short-range Coulomb repulsion and Pauli exclusion. These models may well *predict* the strange behaviour associated with these strong-coupling paramagnets. The problem then becomes a technical problem of deducing the required behaviour from these simple models. It is our belief that all the relevant physics is encapsulated in these simple tight-binding models, *provided* that the topology of the connectivity is taken seriously.

The main difficulty encountered in studying tight-binding Hamiltonians in strong coupling limits is that the low-energy spectrum may bear no resemblence to the weakcoupling solution that we know and understand. Indeed, the first time that this fact is usually encountered is in the study of magnetic insulators. One starts out with fermions and one expects charged excitations carrying spin half. In fact, at low energies, these systems have chargeless exitations carrying spin 1 which exhibit bosonic properties; the spin waves. For this case it is now understood how this change occurs, in terms of a mapping of the original description onto an effective spin interaction at low energies [3]. This idea seems relevant even for the cases of present interest, where for one of the atoms in the system the charge degrees of freedom become 'frozen out' leaving only a residual spin in interaction with its neighbours. Usually the effective interaction between spins leads to some form of magnetic coherence at low temperatures, and one way to interpret our problem is that we are asking why no magnetic coherence exists in strong-coupling paramagnets. In this article we explore the possibility that *topological frustration* might be responsible for the lack of order. We present an exact ground state to a two-dimensional quantum mechanical spin half Heisenberg model which involves symmetry breaking but exhibits no long-range magnetic phase coherence.

A second crucial aspect of the interesting strong-coupling paramagnets is the existence of low-energy charged excitations. Experimental strong-coupling paramagnets carry a current at low temperatures, and some are even superconducting. It is generally believed that the charge motion is in some way linked to the spin fluctuations and we will employ a model where the charge motion requires a spin interaction; the t-J model.

The charge degrees of freedom show two puzzling phenomena of fundamental interest; Firstly, at very low temperature but before long-range coherence intervenes, the effective mass of the charge carriers is orders of magnitude larger than that found in weak-coupling systems. This is known as 'heavy-fermion' behaviour. Secondly, at even lower temperatures, the long-range coherence which sometimes occurs is superconductivity. Superconductivity involves a gap in the spectrum and is usually associated with charged bosons, normally Cooper pairs. These intriguing properties of strong-coupling paramagnets have led to some interesting conjectures for the characteristics of the energy excitations in such systems. The characteristics of interest are: firstly the statistics of the excitations, bosons or fermions or even something worse, secondly the quantum numbers of the excitations, namely the charge and spin of a single excitation and thirdly whether or not the relevant excitation spectrum has a gap. As well as the weak-coupling assignation of gapless spin- $\frac{1}{2}$  charge e fermions and the spin fluctuation assignation of gapless spin-1 chargeless bosons, there have been recent conjectures of gapless spin- $\frac{1}{2}$  chargeless fermions, 'spinons', and spin zero charge e bosons, 'holons' [4]. These excitations are contraversial and the only relevant exactly solvable models that we can analyse are the one-dimensional Hubbard chain [5] and the more recent but very similar supersymmetric t-J model [6]. For this model we find gapless spin- $\frac{1}{2}$  chargeless bosons and spin zero charge e fermions, 'spinless fermions', although actually in the strict limit the statistics of the charge carriers is indeterminate. There is no evidence of any long-range order, other than power law decay of 'Néel' correlation functions. These power law correlations are, however, strong enough to support the gapless 'spin waves', and this suggests that the system is exhibiting a form of latent magnetism and not something more exotic. Attention should be drawn however to the possible interpretations of the quantum mechanical excitations [7], which are not necessarily classical spin waves.

In this article we will present an exactly solvable quantum mechanical t-J model which exhibits only short-range spin correlations. The lack of magnetic coherence is enforced by our choice of geometry, which is topologically frustrated and rather contrived. Although the particular geometry considered is unlikely to be realised in nature, we feel that since it belongs to the class of strong-coupling paramagnets, it is quite likely to yield the *generic* answers to the fundamental characteristics of the low-energy excitations. The statistics and quantum numbers of these excitations are the objectives of this article.

The one-dimensional Hubbard chain and our own solvable one-dimensional 'sawtooth' topology [8] suffer from the usual one-dimensional ailments caused by the virulence of quantum fluctuations in low dimensional systems. Another distressing aspect of solvable one-dimensional problems is the fact that particles must be brought together to be exchanged and this leads to the previously mentioned difficulty in deciding the statistics of the excitations. These problems are so worrying that it is not unnatural to consider one-dimensional problems as *pathological*. One of the great strengths of the model considered in this article is that it is *two-dimensional* and is therefore only plagued by the lesser two-dimensional pathologies.

The model itself is built from the ideas presented in our earlier analysis of the 'diamond' topology [8]. The previous analysis of the Heisenberg model on this topology, which used finite size scaling to suggest that the ground state is that of an infinite chain of alternating spin  $\frac{1}{2}$  and spin-1 atoms, is re-examined with larger clusters. In section 2 we use our numerical work to deduce the Heisenberg ground states of the 'diamond' connectivities depicted in figure 1; the one-dimensional chain and the two-dimensional honeycomb. We also deduce the existance of a *gap* in the spin excitation spectrum to a localised spin- $\frac{1}{2}$  'spinon'. A little time is then spent on the topological properties of this excitation which displays the properties of a 'soliton'. In section 3 we conclude our investigations, leaving the charge degrees of freedom to a future publication.



Figure 1. The two geometries central to the article. The vertices represent atoms and the lines represent equal Heisenberg interactions. (a) The linear chain; (b) the honeycomb lattice.

#### 2. Exact quantum mechanical Heisenberg ground states

The Heisenberg model is that of simple isotropic interactions between spins situated on a lattice. For a system dominated by superexchange, namely where the dominant spin interactions are caused by motion of the electrons making up the localised spins themselves, the interactions are short ranged and we will assume that only nearest neighbour interactions are non-zero. The Hamiltonian is

$$H = J \sum_{[ij]} \mathbf{S}_i \cdot \mathbf{S}_j \tag{2.1a}$$

$$\boldsymbol{S}_i \cdot \boldsymbol{S}_i = S(S+1) \tag{2.1b}$$

where J is the interaction strength, [ij] denote the relevant bonds (for our purpose the connections in figure 1), the square of the total spin is assumed fixed (the constraints of (2.1b)) and  $S_i$  are quantum mechanical operators satisfying the commutation relations

$$[S_i^{\alpha}, S_j^{\beta}] = \delta_{ij} \epsilon^{\alpha\beta\gamma} S_i^{\gamma}$$
(2.1c)

The connectivities of interest to us are depicted in figure 1 and are composed of interconnecting 'diamonds'. There are various ways to arrange the terms for our geometry that demonstrate different ways to study the problem. We will use *i* to denote the atoms on the longer diagonal of the diamonds, *j* to denote the atoms on the shorter diagonal,  $S_B = S_{j_1} + S_{j_2}$  to denote the total spin of the pair of spins which make up the bond on the shorter diagonal,  $S_T = S_B + S_i$  to denote the total spin of the triangle containing the bond *B* and the site *i* and finally  $S_D = S_B + S_i + S_{i'}$ to denote the total spin of the diamond containing the bond *B* and the sites *i* and *i'*. The different ways of writing the Hamiltonian are

$$H = J \sum_{[ij]} \boldsymbol{S}_{i} \cdot \boldsymbol{S}_{j} + \frac{J}{2} \sum_{B} \boldsymbol{S}_{B} \cdot \boldsymbol{S}_{B} - N_{D} J S(S+1)$$
(2.2)

$$H = J \sum_{[iB]} \boldsymbol{S}_i \cdot \boldsymbol{S}_B + \frac{J}{2} \sum_{B} \boldsymbol{S}_B \cdot \boldsymbol{S}_B - N_D J S(S+1)$$
(2.3)

$$H = \frac{J}{2} \sum_{T} \boldsymbol{S}_{T} \cdot \boldsymbol{S}_{T} - \frac{J}{2} \sum_{B} \boldsymbol{S}_{B} \cdot \boldsymbol{S}_{B} - 2N_{D} J S(S+1)$$
(2.4)

$$H = -J \sum_{[ii']} \boldsymbol{S}_{i} \cdot \boldsymbol{S}_{i'} + \frac{J}{2} \sum_{D} \boldsymbol{S}_{D} \cdot \boldsymbol{S}_{D} - 2N_{D} J S(S+1)$$
(2.5)

where  $N_D$  is the number of diamonds, [ij] denote nearest neighbours on the edge of a diamond, [iB] denote nearest neighbour sites and bonds and [ii'] denote all the long diagonals of the diamonds which are *not* bonds in the model.

Our first observation is that (2.3) shows that  $[\mathbf{S}_B \cdot \mathbf{S}_B, H] = 0$  for each bond and so the total spin of each bond is conserved and the ground state may be chosen to be simultaneously an eigenstate of each total bond spin. It is not clear which value of total spin each bond should have. Equation (2.3) suggests a small bond spin, whereas (2.4) suggests a large bond spin should be preferred. In fact, each breakdown indicates that there is a competition at work. In equation (2.3), the first term is minimised by making  $\mathbf{S}_B$  large and antiparallel to  $\mathbf{S}_i$  whereas the second term is minimised when the bond spin vanishes. In equation (2.4), it is clear that high bond spins and low triangle spins are preferred, but since each triangle is composed of one bond spin and one other spin, these constraints are not independent. Equation (2.5) is the easiest to think about and yields the classical solution to the problem.

#### 2.1. The classical limit

The classical limit is that of large spin,  $S \mapsto \infty$ . In this limit the components of the spin commute to leading order, since the commutator on the left-hand side of (2.1c) is O(S), one order of S less than the right hand side. All the spins become conserved quantities and the problem reduces to finding their preferred orientations. Each term in (2.5) can be simultaneously minimised, if we let all the  $S_i$  be parallel and let the  $S_B$  be maximal and antiparallel to the  $S_i$ . All the  $S_D$  then vanish and the second term disappears, while the first term is clearly minimised when  $S_i$  are parallel. The classical ground state energy is  $E = -3N_D JS^2$  and the ground state has both long-range Néel order and long-range ferromagnetism; namely ferrimagnetism.

It is also possible to determine the low-energy excitations in the classical limit; the spin waves. Employing the Holstein-Primakoff transformation to first order, we find

$$H = -3N_D JS^2 + 2JSZ_B \sum_{i} b_i^{\dagger} b_i + 2JS \sum_{B} b_B^{\dagger} b_B - \sqrt{2}JS \sum_{[iB]} [b_i^{\dagger} b_B^{\dagger} + b_B b_i]$$
(2.6)

where  $Z_B$  is the number of bonds neighbouring an *i*-site,  $b_i^{\dagger}$  is a bosonic operator creating a spin fluctuation on an *i*-site and  $b_B^{\dagger} = (1/\sqrt{2})(b_{j_1}^{\dagger} + b_{j_2}^{\dagger})$  is a bosonic operator creating a spin fluctuation on a bond direction B.

The spectra for the two cases of figure 1 are

$$E_{k} = JS\left(\sqrt{[5-4\cos ak]} \pm 1\right) \tag{2.7a}$$

for the chain of diamonds and

$$E_{k} = 2JS$$
  $E_{k} = JS(\sqrt{[10 \pm 6C]} \pm 2)$  (2.7b)

where

$$C = \frac{1}{3} \left[ \left( 2\cos\frac{ak_x}{2} + \cos\frac{\sqrt{3}ak_y}{2} \right)^2 + \sin^2\frac{\sqrt{3}ak_y}{2} \right]^{1/2}$$
(2.7c)

for the honeycomb of diamonds. These spectra are depicted along restricted directions in figure 2. As well as the excitations presented, there are the operators  $\bar{b}_B^{\dagger} = (1/\sqrt{2})(b_{j_1}^{\dagger} - b_{j_2}^{\dagger})$  which correspond to a drop in total bond spin. At the order we are analysing, these excitations have zero energy, and they only achieve 'dispersion' at higher orders in 1/S. It is these modes that play a rather different role in the spin- $\frac{1}{2}$ 



Figure 2. The spin wave spectra for the classical ferrimagnetic ground state of our two geometries. (a) the linear chain; (b) the honeycomb lattice.

problem. The simple picture presented, of long-range magnetic order combined with gapless bosonic excitations, the spin waves, is the *usual* picture for magnetism. This picture is even being used for the spin- $\frac{1}{2}$  square lattice, where long-range Néel order is thought to survive the inclusion of strong quantum fluctuations. We will later go on to solve the spin- $\frac{1}{2}$  version of these diamond geometries and show that their character is quite different from this classical limit.

In the classical limit, the spins have fixed directions and fluctuations in direction make up the excitation spectrum: the spin waves. For smaller spin magnitudes, the effects of quantum fluctuations are present even in the ground state: zero-point motion. The picture that is generally believed, is that the directions found in the classical limit survive the inclusion of quantum mechanics on average. The expectation value of the spin  $\langle S_i \rangle$  is expected to be parallel to the classical direction but reduced in length to take account of the configurations where the spin direction fluctuates. Even for spin  $\frac{1}{2}$ , where the fluctuations are huge, involving a complete reversal of direction, the residual moment is still large; being about  $\frac{2}{3}$  the maximum for the two-dimensional square lattice for example. The long-range order is thought to support spin waves and the basic physical picture is that of the classical limit with only minor modifications.

Our interest is in systems where the energy gain from long-range antiferromagnetic order is weakened by topological frustration. In some systems the quantum fluctuations are so strong that the long-range order is completely lost. For such systems we may ask: what replaces the long-range order and what is the excitation spectrum?

As well as in topologically frustrated systems, long-range order is weakened in low dimensional systems. In one dimension, the quantum fluctuations destroy the longrange order, but there are residual long-range spin-spin correlations. Although the long-range order has disappeared, power law decay of the spin-spin correlations are sufficient to support 'spin wave'-like excitations and the overall physical picture is not dissimilar to the classical limit. We believe that the effects of topological frustration are quite different and do *not* support long-range correlations. We believe that the model presented in this article is more representative of the behaviour to be expected in frustrated antiferromagnetic topologies such as the triangular lattice and the facecentred cubic (FCC) lattice, where the basic building block is the triangle.

For our diamond connectivities, it is the fluctuations in the length of the bond spins on the short diagonal of the diamonds which become active in the ground state. In the classical limit these modes are at zero energy, but for low-spin systems these modes become excited in the ground state.

### 2.2. A soluble limit with some ferromagnetic bonds

Although our main concern is with antiferromagnetic coupling, we can gain some insight into certain elements of the problem by studying the case where most of the bonds are ferromagnetic. The case of some interest is when all but the bonds on the short diagonal are ferromagnetic, because this system is *totally* solvable and shows some of the characteristics of the system with antiferromagnetic coupling.

For this problem the various representations of the Hamiltonian are

$$H = -J \sum_{[ij]} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \frac{J}{2} \sum_{B} \boldsymbol{S}_B \cdot \boldsymbol{S}_B - N_D J S(S+1)$$
(2.8)

$$H = -J \sum_{[iB]} \boldsymbol{S}_i \cdot \boldsymbol{S}_B + \frac{J}{2} \sum_{B} \boldsymbol{S}_B \cdot \boldsymbol{S}_B - N_D J S(S+1)$$
(2.9)

$$H = -\frac{J}{2} \sum_{T} \boldsymbol{S}_{T} \cdot \boldsymbol{S}_{T} + \frac{(3J)}{2} \sum_{B} \boldsymbol{S}_{B} \cdot \boldsymbol{S}_{B}$$
(2.10)

$$H = -J \sum_{[ii']} S_i \cdot S_{i'} + \frac{J}{2} \sum_{D} (S_i + S_{i'} - S_B)^2 - 2N_D J S(S+1) \quad (2.11)$$

where once again the bond spins  $S_B \cdot S_B$  are conserved quantities. The classical limit is deduced from (2.11) to be a saturated *ferromagnet*, since each term is independently optimised. Once again we can determine the spin waves from the quadratic Hamiltonian

$$H = -3N_{D}JS^{2} + 2JSZ_{B}\sum_{i}b_{i}^{\dagger}b_{i} + 2JS\sum_{B}b_{B}^{\dagger}b_{B} - \sqrt{2}JS\sum_{[iB]}[b_{i}^{\dagger}b_{B} + b_{B}^{\dagger}b_{i}]$$
(2.12)

The spectra for the two cases of figure 1 are

$$E_{k} = JS(3 \pm \sqrt{[5+4\cos ak]})$$
(2.13a)

for the chain of diamonds and

$$E_{k} = 2JS$$
  $E_{k} = JS(4 \pm \sqrt{[10 \pm 6C]})$  (2.13b)



Figure 3. The spin wave spectra for the classical ferromagnetic ground state of our two geometries when all the bonds connecting long diagonal sites to short diagonal sites are turned ferromagnetic. (a) The linear chain; (b) the honeycomb lattice.

for the honeycomb of diamonds, depicted in figure 3.

The fact which leads to insight into the system with antiferromagnetic coupling, is that the excitations which reduce the bond spins, namely  $\bar{b}_B^{\dagger}$ , remain at zero energy. This can be attributed to the fact that the triangles *remain* topologically frustrated when the two bond signs are reversed, and these soft modes correspond to the expected degeneracy. The present problem with ferromagnetic bonds is exactly solvable for *all* possible values of the spins, and suggests the effect to be expected from the soft modes at low spin.

The fact which allows the quantum mechanical ground-state solution is that Heisenberg ferromagnets do not suffer from quantum fluctuations and have fully saturated moments. The first term in (2.9) may be optimised by ferromagnetically aligning all the relevant spins, both  $S_i$  and  $S_B$ , and since  $S_B \cdot S_B$  is a conserved quantity, the energy of this ferromagnetic state is simply

$$E = -3JN_D S^2 + \frac{J}{2} \sum_B (2S - S_B)(2S - 1 - S_B)$$
(2.14)

where  $S_B \cdot S_B = S_B(S_B + 1)$  and  $S_B$  takes only integer values. The second term is positive definite for integer values of  $S_B$  and vanishes, yielding the ground state, when either  $S_B = 2S$  or 2S - 1. The zero energy soft modes are manifested in this ground state degeneracy and may be expected also in the case of real interest with antiferromagnetic coupling. From spin 1 through to spin  $\infty$  (the classical limit), the system has long-range ferromagnetic order, but spin  $\frac{1}{2}$  holds a privileged position, since long-range order is *not* necessary.

For spin  $\frac{1}{2}$  there are only two possible values of each bond spin,  $S_B = 0, 1$ . A ground state is obtained by either choice for each diamond, provided that the triplet bonds occur in diamonds with saturated ferromagnetism. It is important to understand the role of singlet bonds in this analysis; a singlet bond spin is locally an eigenstate of *all* the bonds in the relevant diamond. When a bond spin is singlet, the bonds

on the diamond become irrelevant and, further, the two spins on the long diagonal are independently free to point in whatever direction the rest of the diamonds want them to. The class of ground states is now fairly easy to describe; Any configuration of singlet bond spins mixed with triplet bond spins leads to a ground state. Given a configuration of singlet bond spins, the remaining spins split into clusters for which each spin is connected to each other spin in the cluster, by a path of bonds which does not pass across a singlet bond. Each cluster has saturated ferromagnetism in a ground state, but each cluster is independently free to point in any direction. It is this breakup into clusters that can kill the long-range order. One such ground state has all bond spins singlet, and then all the long diagonal spins are independently free to point in any direction. A very similar situation pertains to the spin- $\frac{1}{2}$  limit of the system with antiferromagnetic coupling that we will now move on to.

## 2.3. Antiferromagnetic coupling for the linear chain

Although the topological frustration is similar for the ferromagnetically and antiferromagnetically coupled systems, there is a crucial difference which complicates the antiferromagnetic case. For a ferromagnet, the Heisenberg interaction yields saturated moments and there are no residual quantum fluctuations in the ground state. For antiferromagnets, quantum fluctuations can be strong and a low-spin state is likely to be stabilised from amongst the degeneracy found in the ferromagnetic case. Two important types of coherence are present in the classical limit: both ferromagnetism and antiferromagnetism. The quantum fluctuations will affect these correlations in different ways, so both types of correlations must be studied.

Quantum fluctuations in antiferromagnets may be understood as neighbouring spins exchanging spin quanta. Since  $S_i \cdot S_j$  conserves the total spin of the pair of spins involved, a quantum fluctuation involves only a change in quantisation *direction* for the total spin of the pair; a rotation of the local quantisation direction. Long-range coherence is lost when it is preferable for the system to explore local orientations independently from more distant spins. One would naively expect quantum fluctuations to prefer low spin locally, and indeed this is precisely what is found. For our own case, we might expect the quantum fluctuations to stabilise a low-spin state from amongst the degenerate ground states found in our study of the ferromagnetic problem.

Now let us consider the case of  $spin-\frac{1}{2}$  atoms on a diamond geometry interacting via the antiferromagnetic Heisenberg model. The fact which allows a solution, is that diamonds with singlet bond spins locally disconnect the spins on the long diagonal of the relevant diamond, leaving them uncorrelated. If sufficient bonds are singlet in the ground state, then the remaining spins may become disconnected into clusters and these small clusters may be exactly solved yielding the ground state. The difficulty is to show that a disconnected solution is relatively stable, and the only way we have so far discovered to demonstrate this is by numerical solutions of clusters, combined with finite-size scaling to show that the infinite disconnected clusters are higher in energy than the connected clusters.

The one-dimensional chain of diamonds is our first concern and yields the ideas applicable to the two-dimensional case. Clusters are simply finite numbers of diamonds connected in chain segments. We have solved numerically all segments which involve up to *eight* diamonds using the Lanczos algorithm, and the results are presented in table 1. Systems with more than 25 atoms are too large to be easily solved, and do not yield sufficient new insight to be worth tackling. The ground state may be deduced from figure 4. Extrapolating the energy per diamond for the infinite chain of

Table 1. Tabulated ground state energies and sublattice magnetisations for our cluster calculations with free boundary conditions. The excitations of the true ground state with alternating spin-0 and spin-1 bond spins are composed of regions of the chain with precisely these states.

N <sub>D</sub>	Total spin	Sublattice spin squared	Sublattice spin squared	Ground-state energy
1	0	2.0000	1.0000	-1.7500
1	0, 1			-0.7500
1	0	2.0000	1.0000	-0.7500
2	1/2	3.2821	5.3590	-2.8815
2	1/2	3.0380	1.5434	-1.7728
3	1	4.6457	9.7874	-4.0692
3	0	3.8964	3.8964	-3.5906
4	3/2	6.1386	15.3342	-5.2705
4	1/2	4.9044	6.8774	-4.9634
4	1/2	5.4678	7.4563	-4.5181
5	2	7.7926	22.0938	-6.4743
5	1	6.1066	11.0883	-6.2711
5	0	5.1222	5.1222	-6.0083
6	5/2	9.6168	30.1007	-7.6783
6	3/2	7.5090	16.4323	-7.5370
6	1/2	6.1781	8.0244	-7.3649
7	3	11.6122	39.3615	-8.8824
7	2	9.1035	23.0519	-8.7795
7	1	7.4063	12.0966	-8.6589
7	2	9.6746	24.2162	-8.5546
7	0	6.5364	6.5364	-8.5125
7	1	7.5460	12.2392	-8.4437
8	7/2	13.7779	49.8692	-10.0865
8	5/2	10.8830	30.9468	-10.0087
8	3/2	8.8146	17.4172	-9.9197
8	5/2	11.4409	32.1610	-9.8263
8	1/2	7.5810	9.3029	-9.8152
8	3/2	9.0268	17.7950	-9.7463

alternating spin  $\frac{1}{2}$  and spin-1 bonds, we find about -1.2041J per diamond which is more than the ground-state energy of -1.25J per diamond, which is achieved when singlet and triplet bonds are alternated. The ground state has only very short-range singlets, with spin correlations restricted to lie in the same diamond and spins on different diamonds being completely uncorrelated. The ground state clearly breaks translational symmetry with a doubling of the unit cell from one diamond to two diamonds. The two different types of diamond have very different wavefunctions. A diamond with a singlet bond has energy -0.75J, which all comes from the singlet bond itself, the other bonds being uncorrelated. A diamond with a triplet bond has energy -1.75J and has a short-range antiferromagnetic state. The four spins have total spin zero and the bond spin points in the opposite direction to the other two spins which are parallel in a local triplet state. The quantum fluctuations are huge for this state, and yield a larger contribution than the Néel energy of -0.75J. It is this very stable arrangement which is the cause of the loss of long range order, with the large quantum fluctuation energy dominating the Néel energy.



Figure 4. (a) Finite-size scaling analysis of the energy per diamond of a linear chain of diamonds. The lower data sets are with free boundary conditions, the upper three with periodic boundary conditions. Curves correspond to the ground state. The rest are for the quantum analogue of the classical ground state. The two limit points are -1.2500 J and -1.2041 J. (b) Finite-size scaling analysis of the magnetisation fraction for the states of (a). The lowest four data sets are for the ground state, the upper four for the quantum analogue to the classical ground state. The former clearly tend to zero, the latter remaining unclear. The corresponding analysis for the spin- $\frac{1}{2}$ chain is known to tend to zero logarithmically. Short diagonal magnetisation fractions are shown for for periodic (\*) and free (O) boundary conditions. The system is ferrimagnetic, so these curves should not tend to zero: a lower limit of a quarter seems natural. Long diagonal magnetisation fractions are shown for periodic (+) and free (x) boundary conditions. (c) Short diagonal bond spin correlations for the ground and first excited states of the quantum analogue to the classical ground state for a chain of length 8 diamonds and a loop of length 9 diamonds. Symmetric data sets are for the loop, showing a spin wave. The other two are for free boundary conditions, showing a spin spiral. (d) As (c), but showing long diagonal spin correlations (comments on curves in (c) also apply here).

Although the ground state has lost long-range order, it is important to realise that there is a state which exhibits the correlations that one expects from an unfrustrated one-dimensional antiferromagnet. The state with the lowest energy subject to all its bond spins being triplet seems to exhibit the properties to be expected from the lowspin analogue of the classical ground state. The relevant chain segment states look to be converging to an unsaturated ferromagnet. The total spin is precisely that predicted by the classical ferrimagnetic state of  $\frac{1}{2}(N_D-1)$ , and would appear to become long range order for the infinite chain. The second correlation of interest is whether or not there are residual Néel correlations also present in this state. In order to study this issue we have calculated the spin correlation functions for the ground states and first excited states of our chains. In figure 4 we present the correlation functions, and there is clearly a slowly decaying parallel component. In table 1 and figure 4 we give the square of the total spin of the 'sublattices' as a fraction of the maximum possible, and it is not clear to the order calculated, whether or not the Néel order survives into the infinite chain. The solved example of the infinite chain of identical spin- $\frac{1}{2}$  spins, which exhibits no long-range order and power law decay of correlations, suggests that long-range order probably does not survive, but it also suggests that the state still probably exhibits most of the behaviour to be expected from a state with Néel order. in that correlations extend over long distances and can support gapless 'spin waves'. The correlations presented in figure 4 substantiate this claim, where the excitations are seen to involve long range spirals as is found for the spin- $\frac{1}{2}$  chain.



Figure 5. The lowest two gaps to excitations for the quantum analogue of the classical ferrimagnetic ground state. The stars and plusses are for periodic boundary conditions and the circles and crosses are for free boundary conditions. This state is probably gapless.

In figure 5 we depict the gap to the first two excited states, when all the bond spins in the relevant clusters are constrained to be triplets. The gaps appear to vanish in the limit of infinite chain length, suggesting that an infinite chain of alternating spin- $\frac{1}{2}$ and spin-1 atoms is gapless and has behaviour more reminiscent of the spin- $\frac{1}{2}$  chain which is also gapless, than the spin-1 chain which has a gap. It must be borne in mind, however, that an analogous treatment for the spin-1 chain can also suggest *no* gap. The spin-1 chain with free boundary conditions yields *two* degenerate ground states, although with periodic boundary conditions the Haldane gap is observed. The results strongly suggest that this system is gapless although the issue remains unresolved.

## 2.4. Antiferromagnetic coupling for the honeycomb lattice

Although we have essentially proved that the chain of diamonds has the ground state with bond spins alternating between spin 0 and spin 1, we also believe that the twodimensional honeycomb of diamonds exhibits similar behaviour with four-atom Néel ordered clusters which are separated from each other by singlet bond spins. One might hope to be able to prove this result in a similar manner to the method employed for the chain, but the small size of the clusters that we can diagonalise makes such a technique dubious. We have performed such calculations on the clusters depicted in figure 6. The slightly wider chain clearly has a ground state with no long-range coherence, but the honeycomb is still not clear. In order to convince oneself that this lattice too has the ground state with only short-range correlations, a rather different argument needs to be employed.

The cause of our difficulty may be traced to our choice of 'free' boundary conditions. This choice vigorously favours triplet bond spins, since any diamond which has



Figure 6. The clusters for which we have performed exact diagonalisation analysis. (a) The linear chain with both free and periodic boundary conditions; (b) the augmented chain with free boundary conditions; (c) the 'flower' arrangement; (d) the honeycomb lattice with periodic boundary conditions.

a disconnected end will have a triplet bond in the ground state. The triangle containing the disconnected end has topological degeneracy, and its ground state is achieved with both singlet and triplet bond spins. If the bond spin is singlet, then the triangle is disconnected from the other spins, whereas if the bond spin is triplet, then there is a matrix element connecting it to the other spins which forces it to be relatively stable. The clusters depicted in figure 6(c) are clearly composed of diamonds with disconnected ends and the ground states all have triplet bond spins for each diamond. One way to avoid the fact that edge triangles favour triplet bonds spins, is to use boundary conditions which involve no edges. Indeed, the calculations with periodic boundary conditions *all* suggest the ground state with disconnected clusters.

In fact the ground state is suggested by a special class of eigenstates; those with disconnected clusters. If we focus on the atoms which sit on the long diagonals, then the clusters are sets of these points which are connected by paths passing only over triplet bond spins. The clusters are surrounded by singlet bond spins, which disconnect them. The states of interest for comparison, are states where all the points on the long diagonals are involved, and further where all the clusters are the same. For these states it is easy to calculate the energy gain per diamond, and the crucial point to observe, is that all the long diagonal points like to be involved in non-trivial clusters, but the larger the cluster the *worse* the energy per diamond.

There is one complication in the comparison: that is the diamonds with singlet bonds. For any given type of cluster, the number of singlet bonds required to separate a plane of such clusters varies. The contribution from the singlet bonds is therefore not directly comparable. Fortunately there is a way to compare each cluster directly, and further, the comparison has a physical interpretation.

It is convenient to measure energies from a different zero. The best reference



Figure 7. The quantum fluctuation energy per long diagonal site for our various clusters. The plusses and crosses are the linear chain with periodic and free boundary conditions respectively. The squares are the augmented chain with free boundary conditions, the stars are the 'flowers' and the circles are the honeycomb lattice with periodic boundary conditions. All these clusters are worse than the Néel ordered diamond which yields precisely -0.5 J per long diagonal site.

is to compare with an energy of -0.75 J per diamond, rather than the usual zero, since then all the diamonds with singlet bonds contribute nothing and we can make a direct measure of a cluster's contribution. Coincidentally, the Néel contribution is also -0.75 J, and so we are calculating the quantum fluctuation energy in this calculation. The final comparison between different clusters can then be performed by measuring these residual energies per long diagonal site, since we are assuming that all such spins are involved. The clusters of figure 6 yield the contributions depicted in figure 7 and it is clear that a single diamond gains the most energy from quantum fluctuations. All the clusters that we have analysed always break up into subclusters of the form of those in figure 6(c), and so eigenstates are either higher in energy or contained within the presented results. We believe that whatever the geometry or number of diamonds, the quantum mechanical ground state finds the spins on the long diagonals paired up, with as many diamonds as possible forming the four spin Néel state, and all the other bond spins either being singlet, if they are internal, or forming one of the clusters depicted in figure 6(c) if they are external. This includes the honeycomb lattice arrangement, which has multiply degenerate ground states, two of which are depicted in figure 8. It is important to realise that loops constitute a significant change in basic topology, and all our clusters with loops also satisfy this hypothesis.



Figure 8. A pictorial representation of two of the possible ground states for the honeycomb lattice. The diamonds marked 'N' have the Néel state while all the unmarked diamonds have a singlet bond spin.

When we consider the magnetic coherence inherent in our clusters, we find an important fact. Calculations of the sublattice magnetisation suggest that the worse the quantum fluctuation energy the stronger the magnetic order. One can view the two effects as being in direct competition and the low-energy excitations as being a trade off between the two.

The clusters depicted in figure 6 were chosen to exhibit the way different geometric considerations affect the quantum fluctuation energy. The most important calculations are those for the 'flower' arrangements of figure 6(c). As the number of 'petals' is increased, the amount of quantum fluctuation energy per long diagonal site in the ground state is reduced. In tessalated structures these configurations will never be stable, and the quantum analogue of the classical solution will be further away in energy for systems with higher coordination number of diamonds. This indicates that higher dimensional systems exhibit only minor remnants of their original dimensionality and show almost identical behaviour to the one-dimensional chain. A comparison between the free and periodic boundary conditions on the chain is also important. The loops are clearly relatively stable, and this can be attributed to the fact that there is one less long diagonal site to share the Néel energy with. Loops clearly promote Néel order, but the fact that the quantum fluctuation energy is reduced as the loops increase means that the ordered state can never be stable. The two-dimensional calculations suggest that the quantum analogue to the classical ground state is not stable for the honeycomb lattice. The fact that each long diagonal site has a coordination number of three suggests that the eventual limit for this state will be above the result found for the three petal flower, much less stable than the corresponding state for the chain.

The above argument is by no means rigorous, but we find it convincing.

# 2.5. A soluble limit with antiferromagnetic coupling

One point which seems surprising at first sight, is that the solution that we are suggesting does not depend on  $Z_B$ , the coordination number of bond spins for a site on a long diagonal. For the chain,  $Z_B = 2$ , while for the honeycomb,  $Z_B = 3$ , and one consequence of this is that the fraction of singlet bond spins is different for the ground states of these two lattices. In order to justify this claim, and to achieve further insight into the problem with antiferromagnetic coupling, we now present another exactly solvable geometry. The problem we consider is that of a collection of diamonds which all have identical long diagonal spins. This pair of spins then want to be antiparallel to each and every bond spin and the complication of the general case, where the two long diagonal spins have different connecting bond spins and conflicting directions to point in, is avoided.

The Hamiltonian for this case is simply

$$H = J(\boldsymbol{S}_{i_1} + \boldsymbol{S}_{i_2}) \cdot \sum_{B} \boldsymbol{S}_{B} + \frac{J}{2} \sum_{B} \boldsymbol{S}_{B} \cdot \boldsymbol{S}_{B} - JN_{D}S(S+1)$$
(2.15)

where  $S_{i_1}$  and  $S_{i_2}$  denote the spins on the long diagonals. This expression may be rewritten as a sum of the squares of the spin operators

$$H = \frac{J}{2} \left( \mathbf{S}_{i_1} + \mathbf{S}_{i_2} + \sum_B \mathbf{S}_B \right)^2 - \frac{J}{2} (\mathbf{S}_{i_1} + \mathbf{S}_{i_2})^2 - \frac{J}{2} \left( \sum_B \mathbf{S}_B \right)^2 + \frac{J}{2} \sum_B \mathbf{S}_B \cdot \mathbf{S}_B - J N_D S(S+1)$$
(2.16)

which are all conserved quantities. If we set the total spin of the sum of the bond spins to be  $S_X$ , then provided that  $S_X \ge 2S$ , the first two terms are minimised by letting  $S_{i_1}$  and  $S_{i_2}$  be parallel to each other and antiparallel to the sum of the bond spins, namely  $\sum_B S_B$ . The energy then reduces to

$$E = -2JS(S_X + 1) + \frac{J}{2}\sum_B S_B(S_B + 1) - JN_DS(S + 1)$$
(2.17)

This energy is clearly minimised by choosing  $S_X$  to be the maximum allowable for a given choice of  $S_B$ , namely  $S_X = \sum_B S_B$ , from which we deduce that

$$E = \frac{J}{2} \sum_{B} S_B(S_B + 1 - 4S) - 2JS - JN_D S(S + 1)$$
(2.18)

which must finally be minimised over integer values of  $S_B$ , namely  $0 \le S_B \le 2S$ . It is easy to see that  $S_B = 2S$  or 2S - 1 minimises (2.18) to yield a final ground-state energy of

$$E = -3JN_D S^2 - 2JS (2.19)$$

where the ground state is multiply degenerate with each bond spin being either 2S or 2S-1 and all such spins being both parallel to each other and antiparallel to the long diagonal spins. This result is true provided that the total spin of the sum of bond spins,  $S_X$ , is greater than or equal to the total spin on the long diagonal, 2S. The first term is simply the Néel contribution and so the second term corresponds to the quantum correction attributable solely to the fluctuations. This particular geometry may be considered the most favourable to Néel order, since there is no conflict of interests for the long diagonal spins. For this case the short-range correlation state is degenerate with the higher bond spin states, and only awaits a few more distant diamonds in order to become stable. The simplest periodic cluster depicted in figure 6 is an example of this geometry with  $Z_B = N_D = 3$ . The degeneracy found for this case is an example of our result and the larger clusters then show the stabilisation of the required ground state.

One interpretation of these results is, that quantum mechanically,  $S_B = 2S$  or 2S - 1 are both energetically equivalent, provided that the local Néel order for the interaction with the long diagonal spins is achieved. The effect of quantum fluctuations is to stabilise the state with the lowest total spin on a local level. For spin- $\frac{1}{2}$  systems, all the long diagonal spins become tied into four-atom Néel states, which have zero total spin and triplet bond spins, in order to achieve the Néel order. All other bond spins are zero, achieving the lowest total spin on a local level.

Each long diagonal spin gains the maximum quantum fluctuation energy when in interaction with only one large bond spin. It can be chosen to have more large bond spins, provided that it is coherent with all the spins at the other ends of the long diagonals, an almost impossibly difficult constraint to achieve.

Our next major task is to think about excitations in these systems and to try to deduce the quantum numbers of the excitations and whether or not they are gapped.

## 2.6. The excitation spectrum

The excitation spectrum of all the possible diamond geometries exhibits similar behaviour, and it suffices to study only the chain of diamonds in order to deduce the basic physical picture. As might be expected from the classical limit, the changes in bond spin magnitudes remain the lowest energy modes, and constitute the low temperature excitation spectrum. Unlike the classical limit, where changes in bond spin magnitudes were degeneracies, now a change in bond spin involves a loss in quantum fluctuation energy. The discrete short-range nature of the correlations forces these losses to be discrete, and we find a gap to the lowest lying excitation.

The lowest lying excitations may be chosen to be localised in real space. If we use the representation where all the squares of bond spins are diagonal, then the excitations are restricted to sit on the bond spins which are excited from the ground state configuration, together with any triplet bond spin diamond which happens to be connected to them. The excitations are therefore simply isolated clusters with modified spin configurations, and the energies quoted in table 1 readily provide the low-energy excitation spectrum. The physical interpretation of the excitations is surprising and at first sight seems unphysical. An excitation corresponds to a finite region of the system for which the classical order has been reinstated. At first sight the excitations have more order than the ground state, and the usual view of order being found in the ground state which is destroyed as the temperature is increased seems reversed. The resolution of this 'paradox' is that for this system, magnetic order does *not* mean lower energy. Quantum fluctuations involve energy even at zero temperature; zero-point motion. The excitations in the system involve a gain in Néel ordering energy but a larger loss in quantum fluctuation energy. The spin correlations between spins on different diamonds increase at first as the temperature rises. The disorder which is physically necessary is restricted initially to the loss of the non-magnetic order associated with the regular alternation of types of diamonds.

The lowest energy excitation is seen to be an isolated pair of triplet bonds (TT), which from the five diamond cluster which splits up into two, is seen to reside at energy 0.1185 J each. The most interesting aspect to this excitation, is that it has topological properties. For the linear chain, there is a broken symmetry (akin to Peierls distorted polyacetylene) and two degenerate ground states. A phase boundary between these two ground states constitutes an excitation with a conserved topological quantum number. For the present system this excitation, which is usually called a *soliton*, is precisely the pair of excited triplet bonds. In order for the topological quantum number to be conserved, these objects must be created and destroyed in pairs, and so in most experiments the observed gap to such excitations would be 0.237 J, and two would be excited. The quantum numbers of a single excitation are zero charge and spin  $\frac{1}{2}$ , and therefore two can have either spin 0 or 1 and could be excited with a non-magnetic probe. Although such states might be hard to find with spectral probes, the single soliton gap might be expected to play the dominant role in the low-energy thermodynamics.

The lowest lying non-topological excitation involves a three diamond cluster and finds the central singlet bond being excited to a triplet, forming a three diamond long 'ferrimagnetic' state. The excitation has total spin 1 and so can only be excited by a magnetic probe, but at 0.1808 J, it would be excited before two topological excitations. The remaining low lying excitations of the chain are ennumerated in table 2.

The honeycomb lattice exhibits all the excitations found in the linear chain, together with two types of excitations peculiar to the two-dimensional characteristics. The lowest lying excitation involving the three diamond cluster of figure 6(c), is total spin 1 and is not topological, although it does require the reorganisation of the correlations on at least one loop. At energy 0.2426 J, it may be relevant at low temperatures. The other new excitation of some interest is that involving a six diamond loop. This excitation of spin 3 at energy 0.2746 J may also play a role at low temperatures, and is the quantum analogue of the classical ferrimagnet restricted to the loop.

# 2.7. Diamonds composed of spin-1 atoms

The next question we found of interest was: is the spin- $\frac{1}{2}$  system truly different from the higher spin systems, or does a transition occur at some higher value of spin? In order to gain some insight into this problem, we performed some cluster calculations on some spin-1 systems. Our motivation was analagous to that for spin  $\frac{1}{2}$  and the corresponding results will be more fully analysed at a later date.

First let us summarise the predictions of our exactly soluble geometries and our conjectures. The system with most bonds being ferromagnetic suggests that all the

ND	Bond spins	Total spin	Topological quantum No	Energy				
Linear chain								
2	TT	1/2	1	0.1185				
3	TTT	1	0	0.1808				
4	TTTT	3/2	1	0.2295				
5	TTTTT	2	0	0.2757				
6	TTTTTT	5/2	1	0.3217				
7	TTTTTTT	3	0	0.3676				
8	TTTTTTTT	7/2	1	0.4135				
6	TTTTTT	3/2	1	0.4630				
7	TTTTTTT	2	0	0.4705				
5	TTTTT	1	0	0.4789				
8	TTTTTTTT	5/2	1	0.4913				
4	TTTT	1/2	1	0.5366				
8	TTTTTTTT	3/2	1	0.5803				
7	TTTTTTT	1	0	0.5911				
6	TTTTTT	1/2	1	0.6351				
3	TTT	o	0	0.6594				
7	TTTTTTT	2	0	0.6954				
7	TTTTTTT	0	0	0.7375				
5	TTTTT	0	0	0.7417				
Honeycomb								
3	TTT	1	0	0.2426				
6	TTTTTT	3	0	0.2746				
4	TTTT	3/2	1	0.2842				

Table 2. The low-energy excitations of our geometries together with their quantum numbers.

bonds are expected to be either  $S_B = 1$  or 2 in the absence of quantum fluctuations. The geometry with only two long diagonal sites suggests that both  $S_B = 1$  and 2 will yield the same amount of quantum fluctuation energy, provided that the long diagonal spins see *coherent* bond spins. Finally we are conjecturing that spin fluctuations stabilise the lowest value of the spin locally.

The energy scale for the fluctuations is very much smaller than that for spin  $\frac{1}{2}$ . To our surprise finite-size scaling suggests that for the chain, the analogue of the classical ground state is also the quantum ground state. We have no understanding of this result which further suggests that spin-1 systems can behave in anomalous ways.

#### 2.8. The quantum analogue of classical spin waves

We finally consider the quantum analogue of the classical spin waves. There seems a general belief that including spin waves into a classical description yields an acceptable description of the quantum system, including even zero-point motion.

In figure 9 we plot the lowest lying spin-wave branch calculated from our finite linear chain of diamonds with periodic boudary conditions. These excitations do *not* constitute the lowest lying excitations, since it is cheaper to create many spin-waves at small wavevectors due to the quadratic nature of the dispersion. The excitations presented are the lowest energy excitations subject to the constraint that there is a change in total spin of only one.



Figure 9. The lowest lying spin wave branch calculated from our finite loops. The dispersion is very similar to that predicted by the classical limit and depicted in figure 2(a).

The dispersion depicted in figure 9 is directly comparable with the classical spin wave spectrum of figure 2(a) and agrees quite accurately when the curve is renormalised by the factor of  $S = \frac{1}{2}$ . It seems likely that the quantum analogue of the classical ground state *is* well described by the classical ground state with classical spin waves included.

## 3. Conclusions

The physical ideas suggested by this article are conceptually simple. The normal ground state for Heisenberg magnets is a state with long-range magnetic coherence, even for low-spin systems. There are other types of spin state with quite different physics, but these states must be stabilised by some other phenomenon. When the energy gain from long-range magnetism is severely weakened by topological frustration, then for low-spin systems, quantum fluctuations can stabilise a new kind of ground state without any long range order. Although we have only studied topological ways of destroying magnetism in this paper, we believe that charge carriers which are strongly coupled to the spin system can also destroy the magnetism and replace it with a state very similar to that presented in this article, a more common cause of strong-coupling paramagnetism in nature.

The ground states stabilised by quantum fluctuations in this article exhibit several different characteristics from the classical magnetically ordered states, and we believe that the basic properties are generic to the class of strong-coupling paramagnets and are indicative of very special and interesting physical behaviour. The spin correlations decay very rapidly in our calculations, vanishing between spins on distinct diamonds. The precipitous decay is probably special to our model, but we expect exponential decay in less contrived systems. There is a gap to the first excitation in the system, unlike the classical ordered states, and we believe that this too is generic. The excitations are localised and small, in contrast to the long-range mobile spin waves. We also find that the excitations are spin  $\frac{1}{2}$ , unlike the spin-1 bosons which make classical spin

waves. We believe that these exotic excitations are also generic to strong-coupling paramagnets, although the topological aspects may be restricted to the present case.

Although the spin- $\frac{1}{2}$  systems are quite different to the classical limit, with quantum fluctuations stabilising the strong-coupling paramagnet over the magnet by an energy of about 0.04 J per diamond and with local excitations about 0.2 J away, the corresponding spin-1 systems appear to be well described by the classical ideas, with the excitations only removed from the ground state on an energy scale of 0.01 J. The present ideas seem only likely to be relevant to spin- $\frac{1}{2}$  systems.

The crucial feature of the present system is that the quantum fluctuation energy of a long diagonal site is optimised when it pairs up in a triplet with one other such site, and when the resulting triplet also forms a local singlet with a *single* bond spin. This state is the spin zero ground state of an isolated diamond. Whatever the configuration or dimensionality of diamond connectivity, we believe that the long diagonal sites will pair off, as far as they are able, leaving all the remaining bond spins as singlets. The only proviso is that any diamond with a disconnected end will have a triplet bond spin, yielding the possibility of some of the 'flower' arrangements of figure 6(c) in the ground state.

The ground state has only short-range magnetic order with spin correlations restricted to lie within individual diamonds. Surprisingly, as the temperature is raised, the spin correlations initially *increase* in range.

The lowest lying excitation is a topological soliton for both the one dimensional chain and the honeycomb lattice, and exciting these solitons is associated with the loss of the unit cell doubling order.

Finally we would like to point out that quantum fluctuations and magnetic order are in *competition* in general and that the quantum fluctuation energy dominates for our geomety. The excitations exhibit this competition involving a gain in ordering energy but a larger loss in quantum fluctuation energy. This effect has recently been observed in the spin-1 chain [9].

Note added in proof. Due to the excessive length of this article, the charge motion aspects have been relegated to a subsequent article. The charge motion is also exactly soluble at the one hole level, and is *much* more interesting at the many hole level than the Heisenberg problem.

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