Exact ground states for a class of antiferromagnetic Heisenberg models with short-range interactions

D J Klein

Department of Marine Sciences, Texas A & M University at Galveston, Galveston, Texas 77553, USA

Abstract. A special class of Heisenberg spin Hamiltonians with short-range antiferromagnetically signed interactions is described. It is demonstrated via a simple group-theoretic argument that the ground states to many of these Hamiltonians are Kekulé states, involving singlet spin-pairing between nearest-neighbour pairs of sites. A number of examples are given and previous related work is indicated. In addition to standard applications to exchange-coupled atomic ions, the relevance of the present work for the simple valence-bond model of conjugated π-electron networks is mentioned.

1. Introduction

The exact ground-state solution of ferromagnetically signed Heisenberg models is an important problem that has long been of interest. In the case of a cycle of spin-$\frac{1}{2}$ sites with nearest-neighbour interactions only, exact ground-state properties were determined by Hulthén (1938); but it was not till later (Yang and Yang 1966) that Hulthén's eigenstate was proved to be the ground state. In the case of an even cycle of spin-$\frac{1}{2}$ sites with a next-nearest-neighbour interaction half the strength of the nearest-neighbour interaction, exact ground states and some of their properties were described by Majumdar and Ghosh (1969) and Majumdar (1970); later a proof that the eigenstates considered were generally ground states was indicated (van den Broek 1980) with special reference to the open chain case. In addition to these two cases exact results are obtained for infinite site-spin models (see e.g. Fisher 1964), various infinite-range 'uniform' interaction models (see e.g. Kittel and Shore 1965, DeVries et al 1973, Bowers and McKerrell 1974, Kventsel and Katriel 1979), several models with exact local permutational symmetries (Klein and Welsher 1981), and numerous small finite systems.

   Here we introduce and describe a special case of antiferromagnetically signed (isotropic) Heisenberg models for which exact ground states are obtained. The class includes both long- and short-range interaction models of various site spins and applies to finite clusters, extended crystals and amorphous solids. Majumdar's model is realised as a particular one-dimensional spin-$\frac{1}{2}$ case, as are many of the examples involving exact local symmetries. Infinite-range uniform interaction models can even be viewed as a special case, which however we do not pursue here.

   We note the well known identity of Dirac (1929) represents a permutation exchanging spin indices i and j as

$$(ij) = 2s_i \cdot s_j + \tfrac{1}{2}. \tag{1}$$

Hence (isotropic) Heisenberg Hamiltonians H are elements of the group algebra of the symmetric group S_N of permutations on spin indices. The class of models we consider involves taking H as a combination of symmetry projectors for various subgroups of S_N such that each (idempotent) projector has a positive coefficient in H. Because these projectors are non-negative definite, such an H is also; that is, H has only non-negative eigenvalues. Then any state having no component for any of the symmetries of these projectors will be a ground state, with ground-state energy 0.

Here we indicate just some of the more interesting examples found in this general class. Rather than using commuting projectors, as in the cases of exact local symmetries or infinite-range uniform interactions, we here consider the non-commuting[†]case. The interactions are limited to a finite range by using just projectors of small symmetric groups S_n for small collections of nearby sites. Moreover we restrict our attention to the case where the ground states are composed of products of singlet-coupled pairs of near-neighbour sites. For spin-$\frac{1}{2}$ sites such states are already recognised to be of special significance in the valence-bond theory of the π-electron networks of conjugated hydrocarbons (see e.g. Pauling 1960, Wheland 1955); there (as here) they are termed *Kekulé states*. On lattices such Kekulé states do not exhibit the ordinary types of long-range magnetic order, though in some cases they exhibit another type of long-range spin-pairing order.

2. Development

Some elementary group-theoretic results and notation are useful (see e.g. Hammermesh 1962). The irreducible representations of S_n are labelled by partitions λ of n, which for the Pauli-allowed case of interest here take the form

$$\lambda = [\tfrac{1}{2}n + S, \tfrac{1}{2}n - S] \tag{2}$$

in correspondence with a coupling of the n spin indices to an overall spin S. The f^λ-dimensional λth irreducible representation has matrix elements $\Gamma_{tu}^\lambda(P)$ for $P \in S_n$. The group algebraic matric basis elements for S_n are then

$$e_{tu}^\lambda = \frac{f^\lambda}{n!} \sum_{P \in S_n} \Gamma_{ut}^\lambda(P^{-1})P. \tag{3}$$

When applied to a state $|\mu v\rangle$ transforming as the vth row of the μth irreducible representation of S_n, one finds

$$e_{tu}^\lambda|\mu v\rangle = \delta_{\mu\lambda}\delta_{uv}|\lambda t\rangle. \tag{4}$$

In particular we utilise the (idempotent) projectors e_{tt}^λ.

Let us first consider the case of N spin-$\frac{1}{2}$ sites and assume that for the system there is a connected graph such that at least one 'dimer covering' is possible, i.e. there is at least one way to colour bonds of the graph such that each site has exactly one coloured bond incident on it. An example is given in figure 1. Then let $S_{n_i}(i)$ denote the symmetric group for the indices of site i and its $n_i - 1$ nearest neighbours. The matric basis element projector for the $\lambda = [n_i]$ totally symmetric irreducible representation with $f^{[n_i]} = 1$ is

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† A single state can be a simultaneous eigenstate to several operators which do not commute (on the whole space); for example an S state is a simultaneous eigenstate to L_x, L_y and L_z. That operators are non-commuting merely implies that there is no complete basis of simultaneous eigenstates.
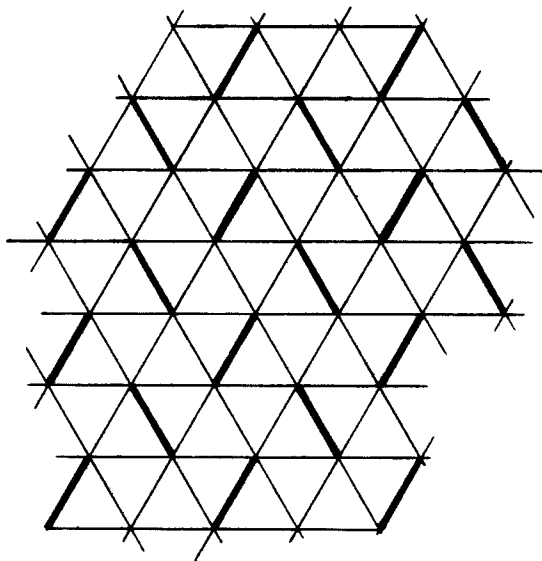
Figure 1. A Kekulé structure shown on a portion of the triangular lattice.

denoted $e^{[n_i]}(i)$, and the Hamiltonian to be considered is

$$H = \sum_i J_i e^{[n_i]}(i) \tag{5}$$

with the J_i being positive exchange parameters. Now associate with each dimer covering Δ of the system graph a Kekulé state $|\Delta\rangle$ such that each dimer (or 'coloured bond') of Δ corresponds to a singlet-coupled pair of spins in $|\Delta\rangle$. Thus each Kekulé state is an overall singlet, and further $e^{[n_i]}(i)|\Delta\rangle = 0$ because a pair of the indices of $S_{n_i}(i)$ are coupled to a singlet so that the whole set can have no maximal spin $\lambda = [n_i]$ component. Hence

$$H|\Delta\rangle = 0 \qquad \forall \Delta \tag{6}$$

and along with the non-negative definite feature of H, this implies that all Kekulé states are ground states to H, with ground-state energy 0.

It is possible to decorate H such that one or more of the Kekulé states remain as ground states. For instance, one could consider the symmetric group $S_{p_i}\{i\}$ of permutations on the p_i indices of site i, its nearest neighbours, and their neighbours. Then the $e_{tu}^{\lambda}\{i\}$ for any λ corresponding to a spin $S \geq (p_i - n_i + 1)/2$ gives 0 when applied to a Kekulé state $|\Delta\rangle$, since $|\Delta\rangle$ involves at least $n_i - 1$ singlet-coupled pairs of sites within those acted upon by $S_{p_i}\{i\}$. Hence if any of the $e_{tt}^{\lambda}\{i\}$ are added† into H with positive coefficients, all the Kekulé states are still ground states. Projectors for various other sets of indices may often be added in while preserving the Kekulé states as ground states; for example, the totally symmetric projector for any site set including the indices of $S_{n_i}(i)$ could be so added. Another type of decoration retains only a subset of the Kekulé states as ground states. For example, consider a subset of bonds every one of

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† More generally, we could add in e_{tu}^{λ} with coefficient a_{tu} such that a_{tu} is the (t, u)th element of a non-negative definite matrix. This is in effect simply using a new choice for the matrix basis, which is undefined up to a unitary transformation.

which is coloured by one special Δ, say Δ_0. Then the $\lambda = [2]$ triplet projectors for each of these bonds give 0 when applied to $|\Delta_0\rangle$; and if these triplet projectors are added into H with positive coefficients, $|\Delta_0\rangle$ remains a ground state.

Even for site spins $s > \frac{1}{2}$, Kekulé states (with neighbour pairs of singlet-coupled sites) may still be ground states to suitable Hamiltonians. One simply identifies $2s$ spin-$\frac{1}{2}$ indices with each site and requires that the spin-$\frac{1}{2}$ indices on each site be coupled to the maximum spin, s. So if we consider site i to have $z_i - 1$ nearest neighbours and take $n_i = sz_i$, then the Hamiltonian of (5) has the Kekulé states as ground states. In fact, since for a Kekulé state $|\Delta\rangle$ two of the $z_i + 1$ sites of $e^{[n_i]}(i)$ are coupled to a singlet, $|\Delta\rangle$ has no component of any spin S for these sites with $S > (z_i - 1)s$; hence any $e^\lambda_{tt}(i)$ for λ with $S > (z_i - 1)s$ can be added on with positive coefficients and still retain such a $|\Delta\rangle$ as a ground state. Various decorations are again possible.

The Hamiltonian of (5) may be recast in terms of exchange operators (ij), or disjoint products thereof, as described elsewhere (Klein 1980). For the special linear combinations of permutations occurring in (5) the reduction to such involutory permutations can be carried out especially simply, as is done in the Appendix here. If desired, these involutary permutations may in turn be recast in terms of spin operators via the Dirac identity of (1). The calculation of the central idempotents

$$e^\lambda \equiv \sum_t e^\lambda_{tt} = \frac{f^\lambda}{n!} \sum_{P \in S_n} \chi^\lambda_P P^{-1} \tag{7}$$

just requires symmetric group characters χ^λ_P, and these are easily computed via Coleman's (1966) rules.

An alternative approach to the various projectors is also possible via Löwdin's (1964) formulation

$$e^\lambda = \prod_T^{\neq S} \frac{\boldsymbol{S} \cdot \boldsymbol{S} - T(T+1)}{S(S+1) - T(T+1)} \tag{8}$$

where S corresponds to λ as in (2). Various e^λ_{tt} could be recovered by multiplying e^λ by central idempotents for subsets of sites, so that the t-labels would identify different spin-coupling paths.

3. Examples

For a cycle of N sites we have $n_i = 3$, and if $J_i = J$ independent of i, then (via the results in the Appendix)

$$H = \tfrac{2}{3}J \sum_i [(i, i+1) + \tfrac{1}{2}(i, i+2)]. \tag{9}$$

For cycles of $N = 4, 6, 8$ and 10 this is essentially the Hamiltonian for which Majumdar and Ghosh (1969) noted that the ground states were Kekulé states. They noted that the Kekulé states remained eigenstates for general even N, as did Majumdar (1970) who also pointed out these states are lacking in the ordinary long-range magnetic order. Majumdar *et al* (1972) studied the low-lying excitation spectrum. That these Kekulé states exhibit a type of long-range spin-pairing order has been pointed out (Klein and García-Bach 1979) and its implications for spin-Peierls-type transitions suggested.

Finally, van den Broek (1980) published a proof that the Kekulé state for a linear chain†
was in fact a ground state, for arbitrary even N.

For the case of a honeycomb or graphite lattice $n_i = 4$. Then on taking $J_i = J$
independent of i, we have (via the results in the Appendix)

$$H = \frac{J}{3} \sum_{i \sim j} (i, j) + \frac{J}{6} \sum_{i \sim \sim j} (i, j) + \frac{J}{12} \sum_i [(i, i')(i'', i''') + (i, i'')(i', i''') + (i, i''')(i', i'') - 3] \qquad (10)$$

where the first sum is over all nearest-neighbour pairs of sites, the second sum is over all
next-nearest-neighbour pairs of sites, and the third sum is over all sites i with i', i'', i'''
denoting the three nearest neighbours to site i. In the simple valence-bond theory of
graphite the system is modelled by the nearest-neighbour Heisenberg Hamiltonian and
the ground-state solution is often viewed (see e.g. Pauling (1960) or Wheland (1955)) in
an approximate manner as a linear combination of the Kekulé states, which are here
exact solutions. Because of the success of such simple views in chemistry, it seems likely
that a model perturbed from the simple nearest-neighbour model in the direction of (9)
might be relevant.

Indeed this last suggestion can be further supported. For graphite and other
conjugated hydrocarbons the Hubbard model, or even better the Parisier–Parr–Pople
model, is commonly presumed to be a 'better' model. (See e.g. Linderberg and Ohrne
1973.) But near the atomic limit of this model degenerate perturbation theory can be
applied (see e.g. Buleavski 1966, Klein and Seitz 1973, Takahashi 1977) to derive
effective Heisenberg models for the lower-lying states. The lowest-order terms yield a
nearest-neighbour Heisenberg model and the next corrections yield terms as we have in
(9), typically with like signs for the interactions. It seems, however, that the non-
nearest-neighbour terms in say (9) or (10) are about twice as strong as those appropriate
for conjugated hydrocarbons; nevertheless they might still serve as good zero-order
models.

In the simple valence-bond model of saturated hydrocarbons (or diamond) each
C atom is represented by a (sp^3-hybridised) tetrahedron of spin-$\frac{1}{2}$ sites, while each
H atom is represented by a single spin-$\frac{1}{2}$ site. The graph we utilise is in close
correspondence with the classical chemical structure; for example, for ethane we have
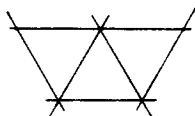the graph of figure 2, where the more heavily drawn edges represent the classical

Figure 2. The graph representing the valence electron system for ethane, C_2H_6.

chemical bonds and also identify a special Kekulé structure Δ_0. Now consider the
Hamiltonian

$$H = J_C \sum_i^C e^{[5]}(i) + J_H \sum_i^H e^{[2]}(i) + J_0 \sum_{i \sim j}^{\Delta_0} e^{[2]}(i, j) \qquad (11)$$

where the first sum is over C-atom sites, the second sum is over H-atom sites, and the

† The model took $J_i = J_N = 0$ and $J_i = J$, $i = 2$ to $N - 1$, with triplet projectors for the end bonds added in with
coefficients $\frac{2}{3}J$. The same proof applies to the cyclic model.

third sum is over interatomic C–C bonds (in Δ_0). Utilising the formulae from the Appendix, one obtains coefficients of $J_C + \frac{1}{2}J_0$ and $\frac{1}{2}(J_C + J_H + J_0)$ for the transpositions of the C–C and C–H bonds, respectively, while all other interactions involve the J_0 as a coefficient. Here $|\Delta_0\rangle$ is the ground state, and moreover $|\Delta_0\rangle$ is retained as the ground state upon decorating H, so as to enhance further the model as a good zero-order description of saturated hydrocarbons. Such decorations include adding on, with non-negative coefficients, projectors $e^{[3]}$ or $e_{tt}^{[2,1]}$ for triples of sites, say i, j, k with i and j on the same C atom and k on another atom bonded to j; here the index t is constrained to identify the [2] subsymmetry for j, k (which is orthogonal to the $[1^2]$ symmetry for j, k present in $|\Delta_0\rangle$); that is,

$$e_{tt}^{[2,1]} = e^{[2,1]}\tfrac{1}{2}\{1 + (jk)\} = \tfrac{1}{3}[1 - 3(ij) - 3(ik) - 2(ij)]. \tag{12}$$

Similar decorations involving e_{tt}^{λ} for [4], [3, 1] and $[2^2]$ as well as various partitions of $n = 5$ are possible, so long as t identifies a subsymmetry of [2] for bonded pairs in Δ_0.

For the case of a triangular lattice, Anderson (1973) and Fazekas and Anderson (1974) have developed arguments and calculations describing the ground state of the nearest-neighbour Heisenberg model in terms of Kekulé states. Again we can construct related models with the Kekulé structures being exact ground states. Making the choice of equation (5) and expanding H in terms of permutations, as in the Appendix, one finds the coefficients of the (nearest-neighbour) transpositions to be ferromagnetically signed. A Hamiltonian more similar to that of Fazekas and Anderson is

$$H = J \sum_a e^{[5]}(a) \tag{13}$$

where the sum is over quintets of sites as in figure 3. Then

$$H = \tfrac{13}{2}J \sum_{i<j}^{\alpha} (ij) + 2J \sum_{i<j}^{\beta} (ij) + J \sum_{i<j}^{\gamma} (ij)$$

$$+ 3J \sum_{i<j<k<l}^{\delta} (ij)(kl) + \tfrac{3}{4}J \sum_{i<j<k<l}^{\varepsilon} (ij)(kl) - \tfrac{3}{2}N_{\text{sites}} \tag{14}$$

where the sums here are for the types of interactions indicated in figure 4. One of the ground states to (14) is indicated in figure 1.
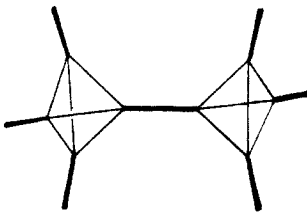

Figure 3. A portion a of the triangular lattice such as referred to in equation (13).

For the case of an even cycle of spin-1 sites, we associate two spin-$\frac{1}{2}$ indices with each site, and we let $e^{\lambda}(i)$ with λ a partition of $n = 6$ denote a central idempotent for a site i and its two nearest neighbours. Then

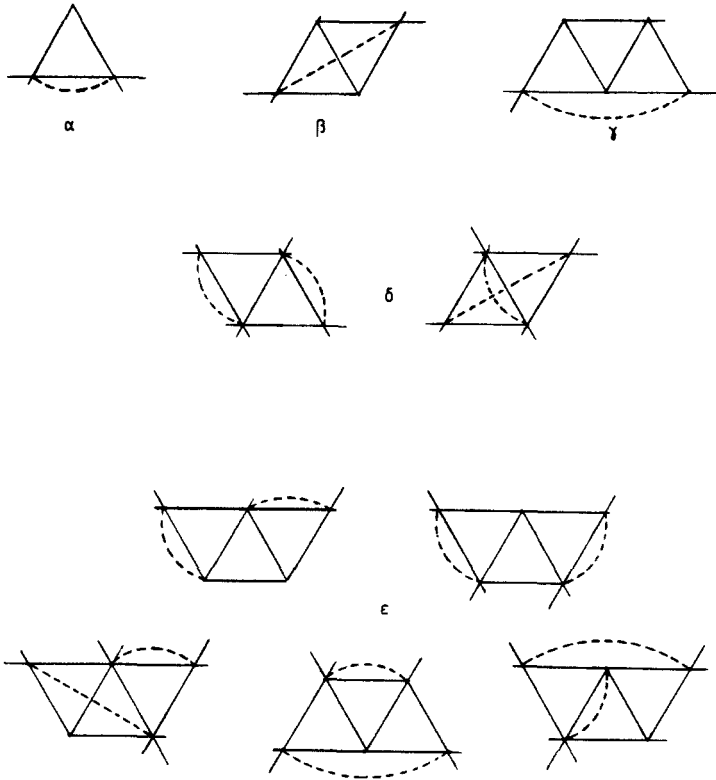$$H = \sum_i [J_0 e^{[6]}(i) + J_1 e^{[5,1]}(i)] \tag{15}$$

Figure 4. A listing of the different interactions referred to in equation (14). Each broken line indicates a transposition between the spins of so-joined sites.

has the two Kekulé states as ground states, with eigenvalue 0. Representing H in terms of permutations via the results of the Appendix, noting the restriction to the space of spin-1 sites, and using the Dirac identity of (1), we obtain H in terms of site spin operators, s_i for site i. If we choose $J_0 = 5J_1$, then the terms triquadratic in spin operators are eliminated, and

$$H = \tfrac{7}{3}J_1 \sum_i s_i \cdot s_{i+1} + \tfrac{7}{6}J_1 \sum_i s_i \cdot s_{i+2} + \tfrac{1}{6}J_1 \sum_i (\Lambda_i + \tfrac{51}{4}) \tag{16}$$

where Λ_i is the sum over the six biquadratic terms formed as a product of any (ordered) pair of distinct quadratic operators $s_{i-1} \cdot s_i$, $s_i \cdot s_{i+1}$ and $s_{i-1} \cdot s_{i+1}$. Additional terms involving $\varepsilon_{ii}^{[5,1]}(i)$ or $\varepsilon^{[32]}(i)$ could also be included in H, while still retaining the Kekulé states as ground states.

Finally we note that there are Hamiltonians for which the Kekulé states are eigenstates but for which it is not necessarily obvious whether they are ground states. One such example for an even cycle of spin-s sites is

$$H = \sum_a \left(\sum_i J_i s_a \cdot s_{a+i} \right) \tag{17}$$

where the exchange parameters J_i for two sites an even distance apart are related to

those an odd distance apart via

$$J_i = \tfrac{1}{2}(J_{i-1} + J_{i+1}), \qquad i = \text{even}. \tag{18}$$

This includes the Hamiltonian of equation (9) as a special case.

4. Properties and conclusions

Ground-state expectation values may be considered. The states are isotropic in spin space so that an expectation value over $s_i^z s_j^z$ is just $\tfrac{1}{3}$ of that over $s_i \cdot s_j$. Now if i and j are other than nearest neighbours, it is quite simple to show that the expectation value of any Kekulé state $|\Delta\rangle$ over $s_i \cdot s_j$ is 0, so that there is no long-range magnetic order of the conventional type in such a $|\Delta\rangle$. However, since the different Kekulé states may be degenerate, linear combinations are also of interest; hence we consider off-diagonal matrix elements between pairs of Kekulé states. This is conveniently done via Pauling's (1933) 'island counting' technique, which generalises (Klein 1979) to sites of arbitrary spin s. In this approach one first considers the overlap

$$\langle\Delta|\Delta'\rangle = \pm(2s+1)^{I(\Delta,\Delta')-N/2} \tag{19}$$

where N is the number of spin-s sites and $I(\Delta, \Delta')$ is the number of islands (i.e. different disjoint pieces) in the superposition graph obtained by superimposing the two graphs for Δ and Δ'. Next one notes that

$$\langle\Delta|s_i \cdot s_j|\Delta'\rangle = f_{ij}^{\Delta\Delta'}\langle\Delta|\Delta'\rangle \tag{20}$$

where the deletion factor $f_{ij}^{\Delta\Delta'}$ is $\pm s(s+1)$ or 0, with the value 0 arising if i and j occur in different islands. Now if i and j are a graph distance m apart, i.e. the shortest path on the lattice between i and j consists of m bonds, then $f_{ij}^{\Delta\Delta'} \neq 0$ implies that i and j are in the same island which must consist of at least $2m$ sites. But in $\langle\Delta|\Delta\rangle$ or $\langle\Delta'|\Delta'\rangle$ these $2m$ sites would be in m different islands, so that $\langle\Delta|\Delta'\rangle$ would have a deficit of $m-1$ islands compared with $\langle\Delta|\Delta\rangle$. Hence $|\langle\Delta|\Delta'\rangle|$ would, from (19), be less than $\langle\Delta|\Delta\rangle = 1$ by a factor of at least $(2s+1)^{-(m-1)}$; so that $s(s+1)(2s+1)^{-(m-1)}$ is an upper bound to $|\langle\Delta|s_i \cdot s_j|\Delta'\rangle|$. Thence for any linear combination $|\psi\rangle$ of Kekulé states, we have

$$|\langle\psi|s_i \cdot s_j|\psi\rangle| \leq s(s+1)(2s+1)^{-(m-1)} \tag{21}$$

where m is the graphical distance between i and j. Thus for this general ground state $|\psi\rangle$ we have no conventional long-range magnetic order, i.e. the expectation value of (21) approaches 0 as $m \to \infty$. In some cases another type of long-range order is known (Klein and García-Bach 1979) to exist.

In conclusion, we see there are numerous examples of short-range antiferromagnetically signed Heisenberg Hamiltonians for which the ground state(s) is (or are) easily and exactly obtained in any dimension. The occurrence of these models is conveniently viewed in terms of simple group-theoretic ideas. Typically the ground states do not exhibit classical magnetic ordering, so that, as pointed out by a referee, the corresponding Heisenberg spin Hamiltonians provide examples of so-called 'frustrated' models. The present models, with exactly soluble ground states, may be used as checks on approximate many-body techniques which are intended for application on related models. Furthermore, these new Hamiltonians may themselves serve as zero-order descriptions upon which many-body perturbation techniques can be applied to treat other models.

Appendix

Here we consider the reduction of class operators, i.e. sums over all permutations of a given conjugacy class of S_n, to a linear combination of those for involutary, i.e. self-inverse, permutations. Of course, such a reduction is limited to the representation of these operators in spin space, but it is known (see e.g. Klein 1980) that it is possible since $P + P^{-1}$ for any $P \in S_n$ can be expressed as a linear combination of involutary permutations. Indeed, these class operators for involutary permutations form a basis for the subalgebra of elements commuting with every element of the group algebra of S_n, because in addition to spanning this centrum these class operators are equal in number to the basis of central idempotents e^Λ.

We label a conjugacy class of S_n by a list of the lengths of its non-unit cycles. If $z \geqslant 2$ disjoint cycles of the same length $l \geqslant 2$ occur in a class abel, this is indicated by l^z rather than z repeated l's. The number of elements in class ρ of S_n is denoted $|\rho|_n$, and the 'normalised' class ρ operator, which is the sum over elements of class ρ divided by $|\rho|_n$, is denoted $\langle \rho \rangle_n$.

We start with the fairly well known result

$$(123) + (132) = (12) + (23) + (13) - 1 \tag{A1}$$

for three-cycles in spin space. In our present notation this is

$$2\langle 3 \rangle_3 = 3\langle 2 \rangle_3 - 1. \tag{A2}$$

Now $|3|_n \langle 3 \rangle_n$ is simply the sum of $|3|_n/2$ different pairs of a three-cycle and its inverse; and via equations like (A1) for each pair this yields, aside from a scalar $-|3|_n/2$, a number of two-cycles whose sum must be a multiple of $\langle 2 \rangle_n$. Since there are just $3|3|_n/2$ of these two-cycles, this evidently is the multiple $3|3|_n/2|2|_n$ of the simple sum $|2|_n \langle 2 \rangle_n$. Hence

$$2\langle 3 \rangle_n = 3\langle 2 \rangle_n - 1. \tag{A3}$$

More generally, we see that the expansion coefficients $(z|\rho)$ for $\langle \rho \rangle_n$ in terms of the $\langle 2^x \rangle_n$, for involutary permutations, are independent of n. Further, the same arguments lead us to conclude that if $\rho = \sigma$, ζ consists of two subsequences σ and ζ with

$$\langle \sigma \rangle_n = \sum_x (x|\sigma) \langle 2^x \rangle_n,$$

$$\langle \zeta \rangle_n = \sum_y (y|\zeta) \langle 2^y \rangle_n, \tag{A4}$$

then

$$\langle \sigma, \zeta \rangle_n = \sum_{x,y} (x|\sigma)(y|\zeta) \langle 2^{x+y} \rangle_n. \tag{A5}$$

Next, to determine the reductions as in (A2) for larger single cycles, we develop an inductive procedure involving products $\langle 2 \rangle_n \langle n - 1 \rangle_n$. Direct multiplication yields a result with a non-zero coefficient for $\langle n \rangle_n$, but first making the presumed-known reduction for $\langle n - 1 \rangle_n$ and then multiplying yields only $\langle \rho \rangle_n$ involving cycles of size no greater length than $n - 1$. Hence $\langle n \rangle_n$ is determined in terms of $\langle \rho \rangle_n$ with cycles no greater than $n - 1$. For instance, for $n = 4$,

$$\langle 2 \rangle_4 \langle 3 \rangle_4 = \tfrac{1}{2} \langle 4 \rangle_4 + \tfrac{1}{2} \langle 2 \rangle_4 \tag{A6}$$

and

$$\langle 2 \rangle_4 \langle 3 \rangle_4 = \tfrac{1}{2} \langle 2 \rangle_4 (3 \langle 2 \rangle_4 - 1) = \langle 3 \rangle_4 + \tfrac{1}{4} \langle 2^2 \rangle_4 - \tfrac{1}{2} \langle 2 \rangle_4 + \tfrac{1}{4}. \tag{A7}$$

But combining (A6) with (A7), then using (A2), we find

$$\langle 4 \rangle_4 = 2\langle 3 \rangle_4 + \tfrac{1}{2}\langle 2^2 \rangle_4 - 2\langle 2 \rangle_4 + \tfrac{1}{2} = \tfrac{1}{2}\langle 2^2 \rangle_4 + \langle 2 \rangle_4 - \tfrac{1}{2}. \tag{A8}$$

Hence a general inductive procedure is established for the reduction of class operators. Applying these methods, we find that

$$\begin{aligned}
2\langle 4 \rangle_n &= \langle 2^2 \rangle_n + 2\langle 2 \rangle_n - 1, \\
4\langle 5 \rangle_n &= 5\langle 2^2 \rangle_n - 1, \\
4\langle 6 \rangle_n &= \langle 2^3 \rangle_n + 6\langle 2^2 \rangle_n - 3, \\
8\langle 7 \rangle_n &= 7\langle 2^3 \rangle_n + 7\langle 2^2 \rangle_n - 7\langle 2 \rangle_n + 1,
\end{aligned} \tag{A9}$$

which along with (A3) and (A5) determines the reduction for any class of S_7.

Finally, to obtain the desired totally symmetric projector in terms of involutary permutations we use

$$e^{[n]} = \frac{1}{n!} \sum_\rho |\rho|_n \langle \rho \rangle_n. \tag{A10}$$

Then utilising (A9), we find

$$\begin{aligned}
e^{[3]} &= \langle 2 \rangle_3, \\
4e^{[4]} &= \langle 2^2 \rangle_4 + 4\langle 2 \rangle_4 - 1, \\
4e^{[5]} &= 3\langle 2^2 \rangle_5 + 2\langle 2 \rangle_5 - 1, \\
8e^{[6]} &= \langle 2^3 \rangle_6 + 9\langle 2^2 \rangle_6 - 2, \\
8e^{[7]} &= 4\langle 2^3 \rangle_7 + 8\langle 2^2 \rangle_7 - 3\langle 2 \rangle_7 - 1.
\end{aligned} \tag{A11}$$

These formulae yield directly several Hamiltonians for which the exact ground state is known, including those of equations (9), (10), (11), (13) and (14) here. Also utilising Coleman's (1966) character formulae, we find that

$$8e^{[5,1]} = -5\langle 2^3 \rangle_6 - 15\langle 2^2 \rangle_6 + 20\langle 2 \rangle_6 \tag{A12}$$

which is used in (14). Likewise formulae for other central idempotents can be generated.

References

Anderson P W 1973 *Mat. Res. Bull.* **8** 153–60
Bowers R G and McKerrell A 1974 *J. Phys. C: Solid State Phys.* **5** 2392–404
van den Broek P M 1980 *Phys. Lett.* **77A** 261–2
Buleavski L N 1966 *Zh. Eksp. Teor. Fiz.* **51** 230–40 (Engl. transl. 1967 *Sov. Phys.–JETP* **24** 154–60)
Coleman A J 1966 *Induced Representations with Applications to S_n and $GL(n)$* (Kingston, Ontario: Queen's University Press)
DeVries A S, Vertogen G and Kroak J 1973 *Physica* **63** 619–25
Dirac P A M 1929 *Proc. R. Soc.* A **123** 714–33
Fazekas P and Anderson P W 1974 *Phil. Mag.* **30** 423–40
Fisher M E 1964 *Am. J. Phys.* **32** 343–6
Hammermesh M 1962 *Group Theory* (Reading, Mass.: Addison-Wesley)
Hulthén L 1938 *Arkiv. Mat. Astron. Fysik* **26** No 11
Kittel C and Shore H 1965 *Phys. Rev.* **138** A1165–9

Klein D J 1979 *Phys. Rev.* B **8** 870–6
—— 1980 *J. Phys. A: Math. Gen.* **13** 3141–6
Klein D J and García-Bach M A 1979 *Phys. Rev.* B **19** 877–86
Klein D J and Seitz W A 1973 *Phys. Rev.* B **8** 2236–47
Klein D J and Welsher T L 1981 *J. Stat. Phys.* **24** 555–81
Kventsel G F and Katriel J 1979 *J. Appl. Phys.* **50** 1820–1
Linderberg J and Ohrne Y 1973 *Propagators in Quantum Chemistry* (New York: Academic)
Löwdin P O 1964 *Rev. Mod. Phys.* **36** 966–76
Majumdar C K 1970 *J. Phys. C: Solid State Phys.* **3** 911–5
Majumdar C K and Ghosh D K 1969 *J. Math. Phys.* **10** 1388–402
Majumdar C K, Krishnan K and Mubayi V 1972 *J. Phys. C: Solid State Phys.* **5** 2896–901
Pauling L 1933 *J. Chem. Phys.* **1** 280–3
—— 1960 *The Nature of the Chemical Bond*, 3rd edition (Ithaca, NY: Cornell University Press)
Takahashi M 1977 *J. Phys. C: Solid State Phys.* **10** 1289–301
Wheland G W 1955 *Resonance in Organic Chemistry* (New York: Wiley)
Yang C N and Yang C P 1966 *Phys. Rev.* **150** 321–7