The Icosahedral Symmetry Antiferromagnetic Heisenberg Model

N.P. Konstantinidis

*Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011*

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Abstract

The antiferromagnetic Heisenberg model on icosahedral symmetry $I_h$ fullerene clusters exhibits unconventional magnetic properties, despite the lack of anisotropic interactions. At the classical level, and for number of sites $n \leq 720$, the magnetization has two discontinuities in an external magnetic field, except from the dodecahedron where it has three, emphasizing the role of frustration introduced by the pentagons in the unusual magnetic properties. For spin magnitudes $s_i = \frac{1}{2}$ there is a discontinuity of quantum character close to saturation for $n \leq 80$. This common magnetic behavior indicates that it is a generic feature of $I_h$ fullerene clusters, irrespectively of $n$.

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The antiferromagnetic Heisenberg model (AHM) is a prototype for strongly correlated electronic behavior, and the combination of low dimensionality, quantum fluctuations and frustration produces unconventional magnetic behavior. This includes non-magnetic excitations in the low-energy spectrum, non-trivial dependence of the specific heat and the susceptibility on temperature, and magnetization plateaux and discontinuities in a magnetic field. Here the model is investigated for spins sitting on vertices of clusters of the fullerene type, with icosahedral spatial symmetry. Fullerene molecules have been found to superconduct when doped with alkali metals. An electronic mechanism for superconductivity was suggested based on perturbation theory calculations on the one-band Hubbard model on doped \(C_{60}\), the fullerene with sixty carbon atoms and \(I_h\) point group symmetry, which geometrically corresponds to the truncated icosahedron. Diagonalization of the Hubbard model is prohibitive due to limitations imposed by the dimensionality of the Hilbert space of this molecule. As a first step, the model is considered on its strong on-site repulsion limit at half-filling, the AHM, on clusters of \(I_h\) symmetry with number of sites \(n\) up to 720. We look for correlations between the magnetic properties and spatial symmetry at the classical and quantum level. The presence of such correlations could open the possibility of studying smaller clusters to gain insight on larger ones of the same symmetry, which are intractable with present day computational means. This approach could as well be used for the Hubbard model to investigate superconducting correlations.

Fullerene molecules are three-fold coordinated and consist of 12 pentagons and \(\frac{n}{2} - 10\) hexagons. For \(I_h\) symmetry the number of sites is given by \(n_1 = 20i^2\) (to be called type I molecules) or \(n_2 = 60i^2\) (type II), with \(i\) an integer. These clusters belong to the class of Goldberg polyhedra. The smallest is the dodecahedron with \(n = 20\) and no hexagons, and the largest considered here has \(n = 720\). Frustration is introduced by the pentagons, with each surrounded only by hexagons for \(n > 20\). The dodecahedron is the only cluster where pentagons are neighboring each other, hence frustration is maximal. As the number of hexagons increases with the number of sites, frustration on the average decreases. It has already been shown that there are strong similarities in the low energy spectra, the specific heat and the magnetic susceptibility of the dodecahedron and the icosahedron, a five-fold coordinated cluster with the same spatial symmetry and 12 sites consisting only of triangles. Here we extend the investigation to the larger molecules and show that spatial symmetry determines to a large extent the behavior in a magnetic field. We conclude that...
significant insight can be gained on more complicated fermionic models on large $I_h$ fullerene molecules from their solution on smaller molecules of the same symmetry.

The AHM is isotropic in spin space, and the total magnetization is usually a smooth function of an external magnetic field at the classical level for unfrustrated systems. Coffey and Trugman showed that it has a discontinuity for the dodecahedron and the truncated icosahedron \cite{13}. It was also shown that for individual spin magnitudes $s_i = \frac{1}{2}$ and 1 the magnetization curve is discontinuous and the total spin changes by $\Delta S = 4s_i$ for the dodecahedron, twice as much as the change between adjacent $S$ sectors, with a particular sector never including the ground state in the field \cite{12}. The icosahedron also has a magnetization jump for classical spins and for higher $s_i$ \cite{14}. The icosidodecahedron is another molecule with $I_h$ symmetry, four-fold coordinated and consisting of triangles and pentagons, with a similar property at high magnetic fields for the lowest $s_i$ \cite{15}. Here the magnetic response of the AHM is calculated at the classical limit, $s_i \rightarrow \infty$, and the full quantum limit, $s_i = \frac{1}{2}$. We find that the response to an external magnetic field is discontinuous for all the $I_h$ fullerene clusters, showing the correlation between magnetic behavior and spatial symmetry. For classical spins, there are two discontinuities, one at relatively small magnetic fields and the second at high fields close to saturation. For the dodecahedron, another discontinuity precedes the low-field one, bringing the total number to 3, a rather uncommon feature in the absence of anisotropic magnetic interactions. At the opposite limit, $s_i = \frac{1}{2}$, there is a jump with $\Delta S = 2$ for the three smallest clusters ($n \leq 80$), where the lowest state of the sector with five flipped spins from saturation and $S = \frac{n+5}{2}$ is never the ground state in a field. The mechanism of the jump is the same in all cases. For higher $n$’s memory requirements prohibit the calculation of the magnetization curve down to the appropriate fields. These common properties of the $I_h$ fullerenes point out the importance of symmetry and frustration for the determination of magnetic behavior.

The antiferromagnetic Heisenberg Hamiltonian for spins $\vec{s}_i$ on the vertices $i$ of the clusters is

$$H = J \sum_{<i,j>} \vec{s}_i \cdot \vec{s}_j - hS^z$$

where $<>$ denotes nearest neighbors, and $J$ is positive and is set equal to 1, defining the unit of energy. $h$ is the strength of an external magnetic field in units of energy and $S^z$ the projection of the total spin along the field direction $z$.  

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For classical spins, \(|\vec{s}_i|\) is taken equal to 1, and the Hamiltonian is a function of the spin polar and azimuthal angles. The critical fields for the magnetization discontinuities are listed in Table I. In the absence of a field the spins are non-coplanar in the dodecahedron ground state \[13\]. With increasing field, they turn gradually to its direction, and are distributed around the \(z\) axis at 4 different polar angles in groups of 5, as shown in figure II. This phase is called I. Above the first critical field, the spins share a common polar angle in pairs and the azimuthal angles of these pairs add up to the same field-dependent value \(c\), except from two pairs which have different polar angles but the same azimuthal angle, equal to \(\frac{c}{2}\) and \(\frac{c}{2} + \pi\) respectively. This phase (Ia) is unique to the dodecahedron and appears for a very small window of the magnetic field. In the following phase (II), all the spins have now negative magnetic energy, with polar angles not differing very much from each other that assume 5 different values, each corresponding to 4 spins (figure II). For higher fields there is a third transition to a more symmetric phase III around the field, where the spins form only 2 polar angles with the \(z\) axis in groups of 10 until the magnetization saturates. The magnetization curves of the other clusters differ only in the lack of phase Ia, and they go directly from phase I to phase II at the first transition. All the magnetization jumps are characterized by a discontinuous derivative of the energy with respect to the field. The number of different polar angles can be expressed in terms of the integer \(i\) that gives the number of sites \(n_1\) and \(n_2\). For phase I it is \(4i\), each corresponding to a group of 5 spins, plus \(2i(i - 1)\), each representing 10 spins for clusters of type I. For type II there are \(6i^2\) different polar angles, each corresponding to 10 spins. For phase II there are \(\frac{n}{4}\) different polar angles each including 4 spins for both types. For phase III the corresponding numbers are \(2i\), each having 10 spins, plus \(i(i - 1)\), each having 20 spins for type I. For type II there are \(2i\) different polar angle values each corresponding to 10 spins, plus \((3i - 1)i\) values each representing 20 spins.

Table II shows that as frustration decreases with \(n\), phase II, the least symmetric around the \(z\) axis, becomes the ground state for a wider range of fields. In contrast, phase I is suppressed to lower fields, and phase III appears just before saturation. The change in the magnetization \(\Delta M\) over the saturation magnetization \(n\) is decreasing with \(n\) for both transitions. These results indicate that the discontinuities will occur for any value of \(n\), albeit closer to \(h = 0\) and \(h = h_{sat}\) and with smaller \(\frac{\Delta M}{n}\) as \(n\) increases. The role of the pentagons, which introduce frustration in the system, is not diminished even when the
hexagons strongly prevail in number. It is also noted that hysteresis curves were calculated by slowly increasing the field from zero to saturation and then switching it off to zero in the same manner. In both cases the magnetization curve is the same and no hysteresis is observed. All the clusters are in phase I for low fields, and in phase III for higher fields, with a transition having discontinuous magnetic susceptibility between the two phases.

In the extreme quantum case \( s_i = \frac{1}{2} \), the magnetization curve typically follows a step-like structure with \( \Delta S = 1 \) between adjacent \( S \) sectors. However, frustration can lead to magnetization discontinuities. It has been found for the dodecahedron that the spin sector \( S = \frac{n-5}{2} \) with five flipped spins from saturation never includes the ground state in a field, resulting in a step \( \Delta S = 2 \) [12]. For \( s_i = 1 \) a similar discontinuity was found, along with a second one for lower \( S \). The calculation is here extended to the truncated icosahedron and the \( n = 80 \) cluster, where memory requirements permit Lanczos diagonalization for at least \( S^z = \frac{n-6}{2} \). Similarly to the dodecahedron, there is a magnetization discontinuity for both clusters with a step \( \Delta S = 2 \) between sectors on the sides of \( S = \frac{n-5}{2} \) (figure 2). The discontinuities are accompanied by magnetization plateaux. The mechanism of the jump is the same in all three cases. The ground state below and above the transition is non-degenerate. It switches from the \( A_g \) to the \( A_u \) one-dimensional irreducible representation of the \( I_h \) symmetry group as the field increases, changing its spatial symmetry from symmetric to antisymmetric [6].

For the dodecahedron, the magnetization curve has also been calculated for higher quantum numbers up to \( s_i = \frac{5}{2} \) close to saturation, and there are no discontinuities related to the sector with five flipped spins for \( s_i > 1 \). The same is true for the truncated icosahedron when \( s_i = 1 \) or \( \frac{3}{2} \). In these cases there are only magnetization plateaux. This indicates that the jump is not related to the classical limit, but rather is a purely quantum effect. Similarly to the classical case, the discontinuities appear closer and closer to the saturation field with increasing \( n \).

The common magnetic properties of the AHM for all the \( I_h \) fullerene clusters investigated for \( s_i \rightarrow \infty \) and \( s_i = \frac{1}{2} \) suggest that they are shared by all the clusters of this class, independently of \( n \). Frustration, spatial symmetry and the presence of pentagons result in magnetization discontinuities which are uncommon for a model lacking magnetic anisotropy. Combined with the similarities in the low energy spectra and thermodynamic properties of \( I_h \) clusters found in [12], the results presented here show that predictions for the behavior of fermionic models on \( I_h \) clusters can be made by studying smaller clusters of the same
symmetry. In particular, comparison of the energy of neutral $C_{60}$ plus two electrons to the total energy of two separate molecules of neutral $C_{60}$ where one electron has been added to each, shows if there is an effective attractive interaction between the two electrons, favoring superconductivity \[16\]. This calculation is much more tractable in the Hilbert space of the dodecahedron, than the one of the truncated icosahedron.

In summary, the magnetization of the AHM for fullerene clusters of spatial symmetry $I_h$ has been shown to exhibit discontinuities in a field ranging up to 3 at the classical level. The results indicate that the discontinuities are a feature of any $I_h$ fullerene cluster, even though phase II is strongly predominant with increasing $n$. For $s_i = \frac{1}{2}$, there is also a jump for higher fields for $n \leq 80$, which is of purely quantum character. Again it is anticipated that this is a generic feature of the AHM on fullerene molecules with $I_h$ symmetry. These effects are non-trivial in the absence of anisotropic magnetic terms from the Hamiltonian. The common spatial symmetry of the $I_h$ fullerenes leads to similar magnetic behavior. It is of interest to examine correlations between spatial symmetry and magnetic properties for other types of symmetry, as well as investigate correlations between electronic behavior and spatial symmetry for more complicated models with orbital degrees of freedom. The findings of this article show that insight on the superconducting properties of the truncated icosahedron can be gained from considering the significantly smaller Hilbert space of the dodecahedron.

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TABLE I: Magnetic fields over their saturation value $\frac{h_c}{h_{sat}}$ with a magnetization discontinuity for $n$ sites, and reduced magnetization values on the sides of the discontinuity $\frac{M^-}{n}$ and $\frac{M^+}{n}$. For the dodecahedron ($n = 20$), the numbers in the left part of the table correspond to the phase Ia to phase II transition. The corresponding numbers for the phase I to phase Ia transition are 0.26350, 0.22411 and 0.22660.

|   | $n$ | $\frac{h_c}{h_{sat}}$ | $\frac{M^-}{n}$ | $\frac{M^+}{n}$ | $\frac{h_c}{h_{sat}}$ | $\frac{M^-}{n}$ | $\frac{M^+}{n}$ |
|---|-----|------------------------|------------------|------------------|------------------------|------------------|------------------|
| 20 | 0.26982 | 0.23688 | 0.27518 | 0.73428 | 0.74766 | 0.75079 |
| 60 | 0.14692 | 0.11723 | 0.14790 | 0.94165 | 0.94574 | 0.94651 |
| 80 | 0.12596 | 0.10003 | 0.12702 | 0.95134 | 0.95465 | 0.95527 |
| 180 | 0.08275 | 0.06438 | 0.08325 | 0.98013 | 0.98208 | 0.98234 |
| 240 | 0.07139 | 0.05525 | 0.07176 | 0.98541 | 0.98697 | 0.98716 |
| 320 | 0.06161 | 0.04749 | 0.06190 | 0.98902 | 0.99027 | 0.99041 |
| 500 | 0.04910 | 0.03765 | 0.04928 | 0.99301 | 0.99386 | 0.99396 |
| 540 | 0.04722 | 0.03618 | 0.04738 | 0.99355 | 0.99434 | 0.99443 |
| 720 | 0.04082 | 0.03120 | 0.04094 | 0.99516 | 0.99577 | 0.99584 |
FIG. 1: Unique polar angles $\theta_i$ in units of $\pi$ in the ground state of the classical AHM on the dodecahedron, as a function of the magnetic field over its saturated value. The four phases are divided

FIG. 2: Difference $\Delta S = S - S_{sat}$ between the total spin in the ground state of the $s_i = \frac{1}{2}$ AHM, $S$, and its saturated value $S_{sat} = \frac{n}{2}$, with $n$ the number of sites, as a function of the magnetic field over its saturation value $\frac{h}{h_{sat}}$. Solid line: $n = 20$, dotted line: $n = 60$, dashed line: $n = 80$. The discontinuities occur at $\frac{h_c}{h_{sat}} = 0.75177$, 0.94179 and 0.96142 respectively.