



# Relationship between coupling constants in Heisenberg exchange Hamiltonian and Ising model



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## ABSTRACT

We show that the coupling constant involved in the Heisenberg exchange Hamiltonian is related to the coupling constant calculated in the Ising model by a simple expression of the form  $J(\text{Hei}) = J(\text{Ising})/N$  where  $N$  is the average number of equivalent magnetic sites per cell taken for calculation. This relation is demonstrated by DFT calculations on the crystallographic geometry of MnSb alloy in different magnetic phases, and on the optimized geometries of polymers of meta-xylene and the silicon substituted counterparts.

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## 1. Introduction

It is well-known that the Heisenberg exchange Hamiltonian serves as the effective spin Hamiltonian for ferromagnetic (FM) and antiferromagnetic (AFM) solids, though in practice the Hamiltonian in Ising approximation is often used for calculations and to obtain qualitative theoretical guidance [1–3]. It is desirable to have a clearly defined relationship between the coupling constants in Heisenberg Hamiltonian and those calculated from Ising Hamiltonian, and whenever possible, compare these with the coupling constants that can be estimated from experiment. This question is addressed here. A relationship is obtained, and it is illustrated by exemplary calculations on three systems.

## 2. Theoretical background

The treatment of ferromagnetism in solids in the absence of an external magnetic field is generally based on the Heisenberg effective spin Hamiltonian,

$$\mathbf{H}_{\text{Hei}} = E_0 - 2 \sum_{\mathbf{j}} \sum_{\varepsilon}^{\text{site axis}} J_{\varepsilon}^{\text{H}} \mathbf{S}_{\mathbf{j}} \cdot \mathbf{S}_{\mathbf{j}+\hat{\mathbf{n}}_{\varepsilon}} \quad (1)$$

In the above  $J_{\varepsilon}^{\text{H}}$  is the exchange coupling constant in Heisenberg model between the neighbouring magnetic sites joined by the unit vector  $\hat{\mathbf{n}}_{\varepsilon}$  along the crystal axis  $\varepsilon$ , and  $\mathbf{S}_{\mathbf{j}}$  is the operator for the spin angular momentum at site  $\mathbf{j}$ . The Ising model, often applied to

metallic or alloy systems [4], relies on a special case of Heisenberg spin exchange in Eq. (1), with all spins considered as directed along a specific ( $z$ ) axis:

$$\mathbf{H}_{\text{Ising}} = E_0^{\text{Ising}} - 2 \sum_{\mathbf{j}} \sum_{\varepsilon}^{\text{site axis}} J_{\varepsilon}^{\text{I}} (S_{\mathbf{j}})_z (S_{\mathbf{j}+\hat{\mathbf{n}}_{\varepsilon}})_z \quad (2)$$

Here  $J_{\varepsilon}^{\text{I}}$  is the magnetic exchange coupling constant in Ising model between neighbouring sites along crystal axis  $\varepsilon$ , and  $(S_{\mathbf{j}})_z$  is the operator for the  $z$ -component of spin angular momentum. The coupling constant  $J_{\varepsilon}^{\text{I}}$  involves the interaction only between the  $z$ -components of spin, and therefore, differs from  $J_{\varepsilon}^{\text{H}}$  that is used in the general exchange Hamiltonian with  $\mathbf{S}_{\mathbf{j}} \cdot \mathbf{S}_{\mathbf{j}}$  term. Ising model has often been used for periodic systems to investigate qualitative trends in properties [4].

### 2.1. Coupling constants

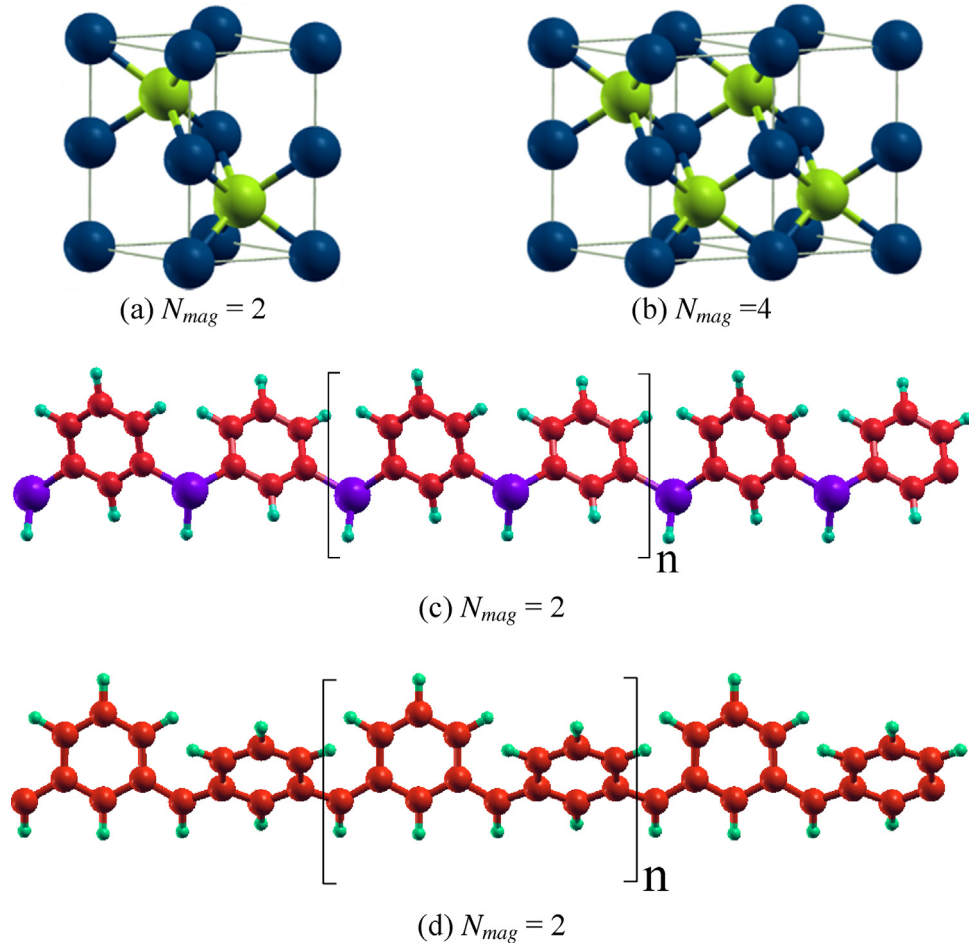
Let us write the number of sites as  $N_{\text{site}} = N_{\text{uc}} N_{\text{mag}}$  where  $N_{\text{uc}}$  is the number of unit cells per unit volume and  $N_{\text{mag}}$  is the number of 'equivalent' magnetic sites per unit cell. The 'equivalent' magnetic sites are sites of same type of atoms in same chemical environment and carrying the same spin, but they may appear at different relative topological positions in the repeating unit as illustrated by Figure 1.

The total spin operators are given by

$$\mathbf{S}_{\text{total}} = \sum_{\mathbf{j}}^{\text{site}} \mathbf{S}_{\mathbf{j}}, \quad S_{\text{tot},z} = \sum_{\mathbf{j}}^{\text{site}} S_{\mathbf{j}z} \quad (3)$$

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**Figure 1.** (a) Elementary unit cell for MnSb ( $N_{mag} = 2$ ); (b) the supercell for MnSb ( $N_{mag} = 4$ ); (c) unit cell for silicon substituted 1-D meta-xylylene polymer ( $N_{mag} = 2$ ) and (d) unit cell for 1-D meta-xylylene polymer ( $N_{mag} = 2$ ). Atoms are coloured as follows: Mn (dark blue), Sb (light green), C (red), Si (purple), and H (green).

The spin state vectors  $|\{m_i\}\rangle$  where  $m_i$  varies over all possible eigenvalues of  $(S_i)_z$  for every site  $i$  form a complete basis set for the common eigenstates of  $S_{total}^2$  and  $S_{tot,z}$ . We note

$$S_{tot,z}|\{m_i\}\rangle = M|\{m_i\}\rangle, \quad M = \sum_j^{\text{site}} m_j \quad (4)$$

and

$$\langle\{m_i\}|S_{total}^2|\{m_i\}\rangle = S_{\max}(S + 1) + M^2 - \sum_j^{\text{site}} m_j^2, \quad S_{\max} = N_{\text{site}}S. \quad (5)$$

For the FM state,  $m_j = S$  for every site  $j$  so that  $M = S_{\max} = N_{\text{site}}S$ , and  $\langle S_{total}^2 \rangle = S_{\max}(S_{\max} + 1)$ . This also yields the spin per cell  $S_{\max}/N_{uc} = N_{mag}S$  so that  $\langle S^2 \rangle_{\text{cell}} = N_{mag}S(N_{mag}S + 1)$ . For any AFM configuration, however,  $M = 0$  that can correspond to any  $S_{total}$  ( $S_{total} = 0, 2S, 4S, \dots, S_{\max}$ ). For any particular AFM arrangement with  $m_j$  alternatively varying as  $S$  and  $-S$  along a particular crystal axis  $\varepsilon'$  while maintaining FM arrangement along all other crystal axes,  $\sum_j m_j^2 = S_{\max}S$  so that  $\langle S_{total}^2 \rangle = S_{\max}$ , and similarly  $\langle S^2 \rangle_{\text{cell}} = N_{mag}S$ . These results are exact.

The total (space-spin) electronic Hamiltonian  $H_{el}$  can be used to calculate the energy of any state with a particular spin configuration under Born–Oppenheimer approximation. This energy can be equated to the energy of a spin Hamiltonian. As there are  $\mathbf{z}_\varepsilon$

nearest neighbours along each direction  $\varepsilon$ , we get from the Ising Hamiltonian

$$E_{\text{FM}} = E_0^{\text{Ising}} - N_{\text{site}}S^2 \sum_{\varepsilon}^{\text{axis}} \mathbf{z}_{\varepsilon} J_{\varepsilon}^I, \quad (6)$$

$$E_{\text{AFM}}^{\varepsilon'} = E_{\text{FM}} + 2N_{\text{site}}S^2 \mathbf{z}_{\varepsilon'} J_{\varepsilon'}^I.$$

where  $\varepsilon$  is a running index and the AFM spin arrangement is present along the specific axis  $\varepsilon'$ .

The energy per cell is written as  $E_c = E/N_{uc}$  such that

$$E_{c,\text{FM}} = E_{c,0}^{\text{Ising}} - N_{mag}S^2 \sum_{\varepsilon}^{\text{axis}} \mathbf{z}_{\varepsilon} J_{\varepsilon}^I, \quad (7)$$

$$E_{c,\text{AFM}}^{\varepsilon'} = E_{c,\text{FM}} + 2N_{mag}S^2 \mathbf{z}_{\varepsilon'} J_{\varepsilon'}^I.$$

This gives

$$2\mathbf{z}_{\varepsilon'} J_{\varepsilon'}^I = \frac{E_{c,\text{AFM}}^{\varepsilon'} - E_{c,\text{FM}}}{N_{mag}S^2} \quad (8)$$

for each crystal axis  $\varepsilon$ .

There arises a problem in the calculation of the Heisenberg coupling constant  $J_{\varepsilon}^I$ . The spin state  $M = S_{\max}$  is necessarily a pure spin state representing  $S_{total} = S_{\max}$ , that is, the FM ground state configuration is indeed the exact ground state configuration of the FM solid. As far as an explicit quantum mechanical calculation is concerned, the calculated solution for  $M = 0$  is in general a mixture of states with different values of  $S_{total}$  as observed earlier after Eq. (5). Anderson showed that the true AFM ground state in any solid is a harmonic

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