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Conceptual Paper

Thermodynamics of the Dzyaloshinskii-Moriya (DM) interaction

Abstract

Bohr-van Leeuwen theorem dictates that a collection of interacting classical charged particles in an external magnetic field under thermal equilibrium is non-magnetic in nature. Indeed, the so called dipole-dipole interaction between the magnetic moments of electrons is too weak to account the observed magnetic order at high temperatures. The responsible interaction is identified by Heisenberg as the well-known Coulomb repulsion between the electrons, independent of spins is suitably strong enough to showcase the magnetism. The spin selectivity appears however from quantum mechanics via the famous Pauli Exclusion Principle. Two electrons with parallel (ferromagnetism) for antiparallel spins (antiferromagnetism) behave differently, even though the fundamental interaction is the same. The observation of weak ferromagnetic in antiferromagnetic crystals prompted Dzyaloshinskii and Moriya (DM) to propose a special type anisotropic spin interaction for the system. In this pedagogical article, we indicate the origin of such DM interaction from the relevant symmetry and indicate a simple two-spin toy model leading to an exact dispersion relation of the magnetic system.

Keywords: Magnetic Moments, Ferromagnetism, Antiferromagnetism, Dzyaloshinskii-Moriya Interaction, Dipole-dipole Interaction

Volume 9 Issue 2 - 2025

Debnarayan Jana
Department of Physics, University of Calcutta, India

Correspondence: Debnarayan Jana, Department of Physics, University of Calcutta, 92 A P C Road, Kolkata - 700009, West Bengal, India

Received: January 30, 2025 | **Published:** April 7, 2025

Introduction

Magnetisation is the equilibrium response property of a system under the magnetic field applied externally. However, Bohr-van Leeuwen theorem dictates that we cannot obtain equilibrium ferromagnetism in a classical theory.[1] Understanding of magnetism needs a full quantum theory. The contribution of magnetisation comes from the orbital motion and spin of the electron in a solid.[2] The diamagnetism is due the situation where total spin is zero and only the orbital motion of electrons is taken into account. Diamagnetism being present in all substances is a universal feature characteristic of the core electrons. However, the magnetic properties other than diamagnetism emerge from the involved interactions/interplay of spins of the unpaired electrons. These properties are very common in natural science with transition metals, lanthanides, and their respective compounds due to the presence of unpaired d and f electrons.

The so called magnetic orders can be broadly classified into major three types of magnetic spin alignments. In the paramagnetic phase, the unpaired electrons are randomly arranged and showcase Curie law $\left(\chi \propto \frac{1}{T}\right)$. On the other hand, when the unpaired electrons are all aligned we call it a ferromagnetic state. Further antiferromagnetism is expected when the unpaired electrons line up opposite of one another. The ferromagnetic state has more ordered but less symmetry while the paramagnetic state has the reverse of it. On the other hand, the ferrimagnetic involves antiparallel spin arrangements to each other with an unbalanced length of the spins in each orientation leading to an overall magnetic moment. Besides, there are some peculiar ferromagnetic substances (known as spin-glass-like) in which antiferromagnetic materials possess small regimes of aligned spins. In Figure 1, we schematically illustrate the common spin arrangements observed in materials as a result of optimization of energy between various spins.

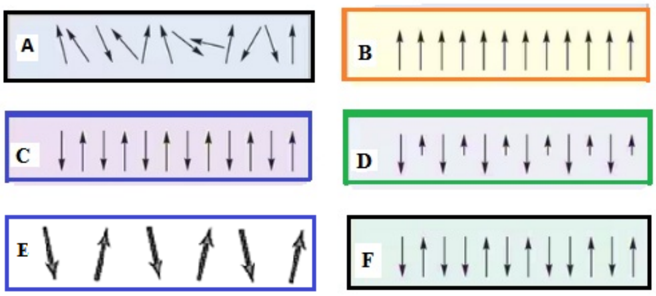

Figure 1 Generic spin arrangements are depicted here (A) Paramagnetism $(\langle M \rangle = 0)$ (B) Ferromagnetism (Spontaneous as well as saturation magnetisation $(\langle M \rangle \neq 0)$ (C) Antiferromagnetism $(\langle M \rangle = 0)$ but staggered $(\langle M_s \rangle \neq 0)$ (D) Ferrimagnetism $(\langle M \rangle \neq 0)$ (E) Canted Antiferromagnetism (saturation magnetisation $(\langle M \rangle \neq 0)$ as well as staggered $(\langle M_s \rangle \neq 0)$ (F) Enforced ferromagnetism (spin-glass behavior).

Dzyaloshinskii-Moriya interaction[3-7] is generated in a solid having a lack of inversion symmetry of the compound and a strong spin-orbit coupling. Since the origin of spin emerges from Dirac's relativistic theory unlike Schroedinger one, the spin-orbit coupling (SOC) has its root in a relativistic electron in atoms occurring in high Z elements and via this interaction, the spin-space and real-space are tied together. The typical SOC term in atomic system is noted as $\lambda(r)\vec{L}.\vec{S}$, where $\lambda(r)$ is the spin-orbit coupling constant dependent on the atomic number Z. For example, in MnSi (manganese silicide) the inversion symmetry is broken in its unit cell. Besides, MnSi has a strong spin-orbit coupling due to large value of atomic number Z. This special type interaction is indeed very essential in case of multiferroic materials. Instead of the superexchange interaction mediated by connected oxygen atoms, the excited state is created here by the spin-orbit interaction. Consequently, an exchange interaction between the excited state of one ion and the ground state of the other ion is taken into account. Physically, suppose an atom with a spin is moving in time δt towards another vacant site situated at a distance a under an external electric field $\vec{E}$. The relevant speed is roughly $a/\delta t$. As a result, a magnetic field $\vec{B} = -\left(\vec{v} \times \vec{E}\right)$ emerges in this situation. Consequently, the spin will twist in an angle $\delta\varphi \sim B \times \delta t$. This feature is captured by the DM interaction for two spins given by the following form

$$H_{DM} = -\overrightarrow{D_{12}} \cdot \left(\overrightarrow{S_1} \times \overrightarrow{S_2}\right) \qquad (1)$$

It is to be noted that $\overrightarrow{S_1}$ and $\overrightarrow{S_2}$ are nothing but the atomic spins. As a result, it is obvious that DM interaction points outwards from the plane of the atoms. The source of $\overrightarrow{D_{12}}$ is the reduced crystal symmetry. It is well-known that in a ferromagnetic state the ground state is where all spin are aligned $\overrightarrow{S_1} \parallel \overrightarrow{S_2}$ and then a strong SOC present in that material will induce this DM interaction. The emerging magnetic structure as a result will depend on the direction of D-vector. Interestingly, this direction is highly dependent on the way the crystal symmetry is broken in a magnetic material. The significance in DMI has been reviewed in the field of modern spintronics.[8]

Heisenberg spin Hamiltonian has been serving the key role in understanding the features in magnetism in solid.[1,9] For the symmetric type of exchange interaction, the Heisenberg Hamiltonian reads as

$$H = -J\left(\overrightarrow{S_1} . \overrightarrow{S_2}\right) \qquad (2)$$

which contains the scalar product of two spins that $\overrightarrow{S_1}$ and $\overrightarrow{S_2}$. The lowest energy is possible only if they possess a collinear orientation. In case of ferromagnetic situation we must have $J > 0$ while for the antiferromagnetic case we need to have $J < 0$. It is interesting to note that any deviation from either parallel or antiparallel configuration will necessarily involve a cost in energy. Let us assume that $\overrightarrow{S_1}$ is held fixed, while $\overrightarrow{S_2}$ makes an angle with $\overrightarrow{S_1}$. Then, it is easy to notice that the cost involved in the energy of spin configuration remains the same, regardless if the deviation from collinearity is to this side or the other. This fact essentially indicates that the interaction is indeed symmetric in nature. Note that this type of interaction is unable to explain the differences observed between Bloch walls of different rotational sense arising from non-relativistic effect.

On the other hand, unlike other interactions, the DMI is a pseudo-scalar containing the cross product $\left(\overrightarrow{S_1} \times \overrightarrow{S_2}\right)$ times DM vector $\overrightarrow{D_{12}}$. As a result, one can argue that that the energy of the system can be acquired by inserting an angle between $\overrightarrow{S_1}$ and $\overrightarrow{S_2}$. But, the deviation from collinearity has to be fixed in the right direction while the opposite direction is energetically costly. As a result, only one particular sense of spin rotation is supported. This fact inherently indicates that DMI is indeed an asymmetric interaction. We call this part of exchange interactions antisymmetric (not just asymmetric) as the vector product $\left(\overrightarrow{S_1} \times \overrightarrow{S_2}\right)$ changes its sign after $\overrightarrow{S_1}$ and $\overrightarrow{S_2}$ are exchanged. Although Heisenberg interaction is the leading term in most magnetic materials, however, there arise situations where DMI can make significant contribution in deciding the ground state of the system. Sometimes, the crystal symmetry does not allow this term. It is treated as a small relativistic correction to the main interaction. The profound difference between the Heisenberg type of interact and DM interaction in terms of the minimization as function of the angle between two spins is illustrated in Figure 2. In particular, the clockwise and counter clockwise rotations can be distinguished.

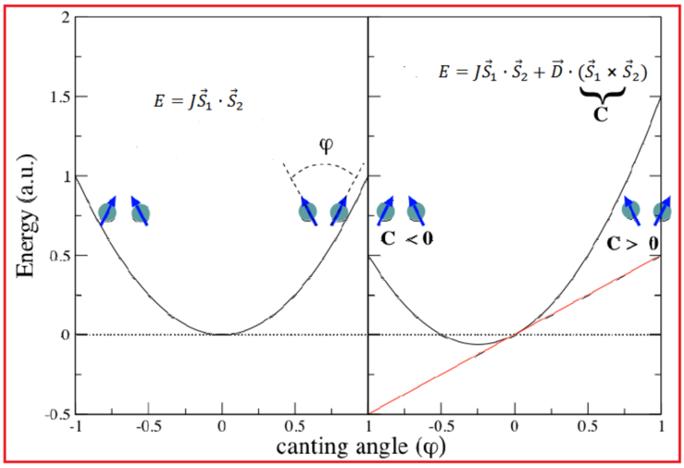

Figure 2 Comparison of Energies of Heisenberg and DM interaction as a function of canted angle.

The typical Hamiltonian for N particle system associated with this spin-spin interaction is given by

$$H_{DM} = -\sum_{ij} \overrightarrow{D_{ij}} . \left(\overrightarrow{S_i} \times \overrightarrow{S_i}\right) \qquad (3)$$

The vector $\overrightarrow{D_{ij}}$ in general depending upon the symmetry[1] lies either parallel or perpendicular to the line connecting the two spins. The antisymmetric exchange interactions (AEI) present close to magnetic surfaces or interfaces films or multilayers contributes to surface anisotropy energy[6] and the symmetry rules determine the direction of $\overrightarrow{D_{ij}}$. DM vector $\overrightarrow{D_{ij}}$ is proportional to SOC constant $\lambda(r)$, and depends critically on the position of the oxygen ion between the two relevant magnetic transition metal ions. It is interesting to note that if the crystal possesses an inversion center between two spins, then the DM vector for these two spins has to vanish identically. This is depicted in Figure 3.

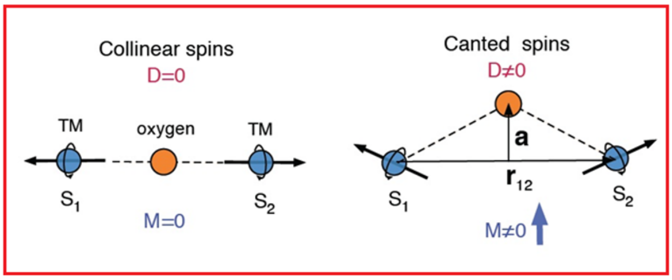

Figure 3 Effect of DMI on collinear spins and canted spins.

In fact, this canting of magnetic moments shown in Figure 3 results a net non-zero magnetization in an otherwise collinear antiferromagnetism (weak ferromagnetism) observed in α-Fe_2O_3, $MnCO_3$, $CoCO_3$ and other important multiferroics such as α-$Cu_2V_2O_7$.[10] Note that DM interaction is indeed chiral in nature because it favors one chirality of spin pair in favor of the other. In particular,

$$E_1 = -\vec{D} . \left(\overrightarrow{S_1} \times \overrightarrow{S_2}\right) \neq -\vec{D} . \left(\overrightarrow{S_1} \times (-\overrightarrow{S_2})\right) = E_2 \qquad (4)$$

Citation: Jana D.Thermodynamics of the Dzyaloshinskii-Moriya (DM) interaction. *Phys Astron Int J.* 2025;9(2):52–57. DOI: 10.15406/paij.2025.09.00363

In other words, the two configurations with equal angle between the interacting spins have different energies. This happens due to the fact that the configuration of the surrounding atoms is different. Chiral interactions emerge in non-centro symmetric systems. To summarize, the DMI arises in a magnetic atomic spin system when the spin information between the indirectly connected systems is perturbed asymmetrically by SOC. In this situation, the itinerant electrons act as intermediate factor. It is interesting to note that the magnitude of DM interaction is typically small (roughly 1% of the Heisenberg exchange) in a typical bulk magnetic materials. Besides, as mentioned, its direction essentially is dependent on the relevant crystal symmetry.

Microscopically, it is known that the DMI between two spins manifests itself as a mediated interaction provided by an impurity with strong SOC. Including SOC, inversion symmetry must be broken in order for the emergence of DMI. In other words, the crystals either have a right- or left-handed chirality. It is to be noted that Mn/W, Fe/W and Fe/Ir showcase strong interfacial DMI. Thus, ultrathin ferromagnets having perpendicular anisotropy turn out to be suitable candidates for exhibiting this phenomenon. Multilayers such as Pt/Co(0.4-1 nm)/AlO_x,Ta/CoFeB(1nm)/MgO, Pt/[Co(0.4 nm)/Ni(0.6 nm)$]_n$ are fascinating ones for applications because they inherently own a significantly large anisotropy perpendicular to their film plane. A typical multilayered system is depicted in Figure 4.

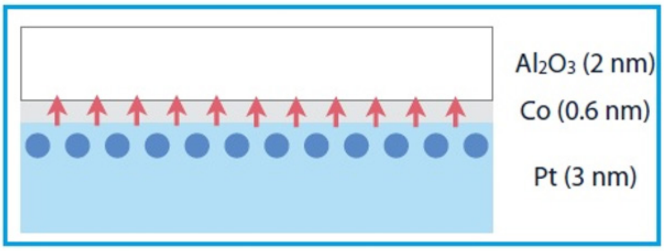

Figure 4 A schematic picture of multilayered systems with spin alignments.

The anisotropic magnetization can emerge[11-13] in a system when there is an interplay of Heisenberg spin system with DM interaction. Recently, a study[14] based on on-site mixings of the relevant 3d orbitals of binuclear transition metal complexes has revealed the significant enhancement of the orientation and magnitude of this interaction. It is expected that this study will be very helpful to researchers working on strongly correlated materials, skyrmions, multiferroics, and molecular magnets. Mermin-Wagner theorem[15] discusses the possibility phase transition with continuous symmetry in lower dimensional system.[16] Mermin and Wagner theorem[15] states that no spontaneous ferro- or antiferromagnetic long-range order is possible at $T > 0$ for one or two-dimensional Heisenberg systems with isotropic short ranged interactions. A connected study[17] on the ordering in low dimensional system taking into account both Hesisenberg and DM interaction has indicated that quantum fluctuations are diminished by DMI, however short-range correlations are enhanced.

In this paper, we would like to discuss the origin of DM interaction and the thermodynamics of Heisenberg spin Hamiltonian modified by DM interaction of spin-1/2 (S = ½) of two particles. The emergence of DM interaction can be approached from two different angles, first by perturbation theory[2] and second from symmetry point of view. The second one however uses the simple matrix algebra which is relatively easier to understand. After that, we present the interplay between Heisenberg interaction and DM between two spins to compute the thermodynamic properties from the partition function.

Emergence of DM interaction from perturbation theory

In transition-metal salts, the magnetization is mainly due to the electron spins and is not carried by the orbital angular momentum. Using this concept of quenching of $\vec{L}\left(\langle\psi|\vec{L}|\psi\rangle = 0\right)$, it is obvious from first order perturbation theory that the spin-orbit perturbation $\lambda(r)\vec{L}.\vec{S}$, has no effect, since there is no remaining degeneracy to break. But, this SOC term may trigger significant non-zero in second order perturbation theory yielding the relevant correction to the energy[2] a

$$E^{(2)} = -\vec{D}\,.\left(\vec{S_1} \times \vec{S_2}\right) \tag{5}$$

It is to be noted that the existence of this term is restricted to different species of ion in different chemical environments. Thus, this DM interaction supports the alignment of adjacent atoms neither parallel nor antiparallel. In fact, in an antiferromagnetic spin environment, the situation forces the spins to cant away from their relevant antiferromagnetic configurations so as to yield a non-zero value of net magnetisation. This spin arrangement in the background of antiferromagnetism is nothing but a form of ferrimagnetism. The emergence of DM interaction in a multilayered system is illustrated in Figure 5.

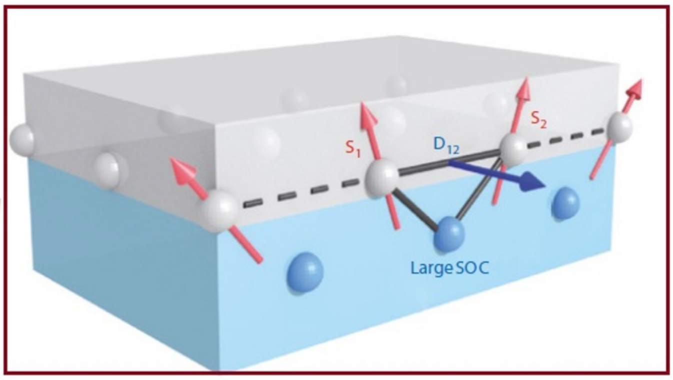

Figure 5 Emergence of DM interaction via large SOC.

To show the occurrence of the magnetization, we have to include the effect of external magnetic field in the system. Treating SOC as a weak perturbation, we have the simple model Hamiltonian

$$H = \lambda\vec{L}.\vec{S} + \mu_B\vec{B}.\left(\vec{L} + 2\vec{S}\right) \tag{6}$$

Due to quenching of orbital angular momentum $\vec{L}$, the first order correction to energy will yield $\Delta E^{(1)} = 2\mu_B\vec{B}.\vec{S}$. However, the second order effect is quite different and is given by

$$\Delta E^{(2)} = \sum_{ij}(\lambda^2 G_{ij}S_iS_j + 2\lambda\mu_B G_{ij}B_iS_j + \mu_B^2 G_{ij}B_iB_j) \tag{7}$$

where G_{ij} is defined as

$$G_{ij} = \sum_{n\neq 0}\frac{\langle n|L_i|0\rangle\langle 0|L_j|n\rangle}{E_n - E_0} \tag{8}$$

To obtain the magnetisation, we construct the effective spin Hamiltonian,

$$H_{spin} = \sum_{ij}\left[2\mu_B B_i\left(\delta_{ij} - \lambda G_{ij}\right)S_j - \lambda^2 S_iG_{ij}S_j - \mu_B^2 B_iG_{ij}B_j\right] \tag{9}$$

Citation: Jana D.Thermodynamics of the Dzyaloshinskii-Moriya (DM) interaction. *Phys Astron Int J.* 2025;9(2):52–57. DOI: 10.15406/paij.2025.09.00363

The magnetisation in this model can be calculated as

$$M_i = -\frac{\partial H_{spin}}{\partial B_i} = -\sum_j \left[2\mu_B \left(\delta_{ij} - \lambda G_{ij} \right) S_j - 2\mu_B^2 G_{ij} B_j \right]$$

$$= -2\mu_B S_i + 2\mu_B \sum_j G_{ij} \left(\lambda S_j + \mu_B B_j \right) \qquad (10)$$

Emergence of DM interaction from matrix construction

One can also construct DM interaction from a simple matrix formalism. We could write a most general bilinear form,[18] with terms $\sum_{ij}\sum_{\alpha\beta} K_{ij}^{\alpha\beta}$ where, β label cartesian components of the coupling matrix $\left\{ K_{\alpha\beta} \right\}$. It is well-known that any 3×3 matrix can be written as a sum of three types of matrices namely (i) a multiple of the identity matrix, (ii) an antisymmetric part (3 different coefficients), and (iii) a traceless symmetric part (6-1 = 5 different coefficients).

In most of the situation however it is enough to use only two spin terms that are bilinear and hence, can be written as

$$E = -\sum_{ij}\sum_{\alpha\beta} K_{ij}^{\alpha\beta} S_{i\alpha} S_{j\beta} = -\sum_{ij} \left[K_{ij}^{xx} S_{ix} S_{jx} + K_{ij}^{yy} S_{iy} S_{jy} \right] - K_{ij}^{zz} S_{iz} S_{jz} \quad (11)$$

where the anisotropy in $K(\mathrm{r}_{12})$ has been introduced. However, if the dimension of the coupling matrix K is 3×3, then the above equation for two spins at two sites should be read in the matrix format as $S_1[K]S_2$. As mentioned earlier, we try to decompose this interaction matrix, like any 3×3 matrix, into a multiple of the identity matrix, an antisymmetric part (three different coefficients), and traceless symmetric part as

$$\left[K^{\alpha\beta} \right] = \begin{pmatrix} K^{xx} & K^{xy} & K^{xz} \\ K^{yx} & K^{yy} & K^{yz} \\ K^{zx} & K^{zy} & K^{zz} \end{pmatrix} =$$

$$J \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & D^{xy} & D^{xz} \\ -D^{yx} & 0 & D^{yz} \\ -D^{zx} & -D^{zy} & 0 \end{pmatrix} + \begin{pmatrix} A_1 & A_4 & A_5 \\ A_4 & A_2 & A_6 \\ A_5 & A_6 & A_3 \end{pmatrix} \qquad (12)$$

The first decomposition can be easily identified as Heisenberg Spin Hamiltonian

$$-JS_1 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} S_2 = -J \left(S_{1x} S_{2x} + S_{1y} S_{2y} + S_{1z} S_{2z} \right) = -J \vec{S_1} . \vec{S_2} \quad (13)$$

In the same vein, one can write down the second term as

$$-S_1 \begin{pmatrix} 0 & D^{xy} & D^{xz} \\ -D^{yx} & 0 & D^{yz} \\ -D^{zx} & -D^{zy} & 0 \end{pmatrix} S_2 \qquad (14)$$

which after simplifications reads as the famous DM interaction (assuming $D^{xy} = D^{yx} = D^1, D^{xz} = D^{zx} = D^2 . D^{yz} = D^{zy} = D^3$)

$$-\left[-D^1 S_{1y} S_{2x} - D^2 S_{1z} S_{2x} + D^1 S_{1x} S_{2y} - D^3 S_{1z} S_{2y} + D^2 S_{1x} S_{2z} + D^3 S_{1y} S_{2z} \right]$$

$$= -\left(\vec{i}\, D^1, -\vec{j}\, D^2, \vec{k}\, D^3 \right) . \left(\vec{S_1} \times \vec{S_2} \right) = -\vec{D} . \left(\vec{S_1} \times \vec{S_2} \right) \qquad (15)$$

Finally, the last term can be forecast as the dipole-dipole interaction with following symmetric traceless matrix notation

$$-\frac{\mu_0}{4\pi r^3} \begin{pmatrix} 3r_x^2 - 1 & 3r_x r_y & 3r_x r_z \\ 3r_x r_y & 3r_y^2 - 1 & 3r_y r_z \\ 3r_x r_z & 3r_y r_z & 3r_z^2 - 1 \end{pmatrix} \qquad (16)$$

with $r_x^2 + r_y^2 + r_z^2 = 1$. Defining $\hat{r}$ as the unit vector joining the two spins, we can identify the popular form of dipole-dipole interaction as

$$H_{dipole-dipole} = -\frac{\mu_0}{4\pi r^3} \left(3 \left(\hat{r} . \vec{S_1} \right) \left(\hat{r} . \vec{S_2} \right) - \left(\vec{S_1} . \vec{S_2} \right) \right) \quad (17)$$

In contrast to first two interactions, this dipolar interaction is however long-range in nature and responsible for the demagnetizing field, ferromagnetic domains, etc. In fact, these dipolar interactions are important when exchange is small, and also in nuclear magnets.

Thermodynamics of two spin-1/2 system

It has already been mentioned that the DM term does not contribute anything for parallel spin configuration. In the ferromagnetic state, the parallel spin configuration (either all up or all down) is also quantum mechanical eigenstate of the Heisenberg spin Hamiltonian. We follow ħ=1 in our discussion. To see it more clearly, it is essential to write the full Hamiltonian in terms of spin raising $(S_1^+ = S_{1x} + iS_{1y})$ and lowering operator $(S_1^- = S_{1x} - iS_{1y})$ as

$$H = -J \vec{S_1} . \vec{S_2} + \vec{D} . \left(\vec{S_1} \times \vec{S_2} \right)$$

$$= -\frac{J}{2} \left(S_1^+ S_2^- + S_2^+ S_1^- + 2S_{1z} S_{2z} \right) + \frac{D}{2i} \left(S_1^+ S_2^- - S_2^+ S_1^- \right) \qquad (18)$$

Here, we have assumed $\vec{D} = (0,0,D)$. It is clearly seen that

$$\langle \uparrow\uparrow | \, H | \uparrow\uparrow \rangle = -\frac{J}{4}, \langle \downarrow\downarrow | H | \downarrow\downarrow \rangle = -\frac{J}{4} \qquad (19)$$

and are indeed degenerate states but other triplet state under the action of the Hamiltonian turns to

$$H \left\{ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \right\} = -\frac{J}{4} \left(\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \right) - \frac{D}{2i} \left(\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \right) \qquad (20)$$

Thus, it is observed that the triplet state under DM interaction changes to singlet one. If we look into the singlet state, then it is seen that

$$H \left\{ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \right\} = +\frac{3J}{4} \left(\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\uparrow\downarrow\rangle) \right) + \frac{D}{2i} \left(\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \right) \qquad (21)$$

Therefore, the singlet as well as triplet states are not the eigenstates of the Hamiltonian. In the limit of $D \to 0$, however, the energy levels are triply degenerate with eigenvalues $-\frac{J}{4}$. This is also consistent with the fact that $\vec{S_1} . \vec{S_2} = \frac{1}{2} \left[S_{tot}^2 - S_1^2 - S_2^2 \right] = \frac{1}{2} \left[2 - \frac{3}{2} \right] = \frac{1}{4}$

(in units of ħ=1) with $S_{tot} = 1$ for triplet states.

Thus, the triplet and singlet state with $S_z = 0$ are mixed up under the action of DMI. Then, with the help of

$$|\Psi\pm\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle \pm e^{-i\alpha}|\downarrow\uparrow\rangle\right] \qquad (22)$$

and mixing phase angle defined by $\tan\alpha = \frac{D}{J}$, we can easily diagonalize the Hamiltonian to find out the eigenvalues as

$$E_\pm = \frac{J}{4} \pm \frac{1}{2}\sqrt{J^2 + D^2} \qquad (23)$$

The energy levels are non-degenerate and separated by a gap of magnitude $\sqrt{J^2 + D^2}$. In the limiting case of $D \to 0$, we obtain the consistent picture of singlet and triplet states of the spins. Therefore, DM interaction effectively mixes the singlet and triplet states to remove the degeneracy and finally opens a gap. We would like to investigate the thermodynamics of these levels in a canonical ensemble. The partition function of this two-level system at a temperature T (in terms of $\beta = (k_B T)^{-1}$ is simply

$$Z(J,D,\beta) = e^{-\frac{\beta J}{4}} \times 2cosh\left(\frac{\beta\sqrt{J^2 + D^2}}{2}\right) \qquad (24)$$

and consequently, the free energy at any temperature T can be written as

$$F(J,D,\beta) = -k_B T \;\ln Z(J,D,\beta) = \frac{J}{4} - k_B T \ln\left[2cosh\left(\frac{\beta\sqrt{J^2 + D^2}}{2}\right)\right] \qquad (25)$$

The average energy $\left(\bar{E} = -\frac{\partial lnZ}{\partial\beta}\right)$ of the system as a function of T can be obtained as

$$\bar{E} = \frac{J}{4} - \frac{\sqrt{J^2 + D^2}}{2} tanh\left(\frac{\beta\sqrt{J^2 + D^2}}{2}\right) \qquad (26)$$

At high enough temperature $(\beta \to 0)$, we obtain the consistemt value of the average energy of the system as J/4. In the same tune, the entropy can be calculated as

$$S(J,D,T) = k_B \ln\left[2cosh\left(\frac{\beta\sqrt{J^2 + D^2}}{2}\right)\right] - \frac{\sqrt{J^2 + D^2}}{2T} tanh\left(\frac{\sqrt{J^2 + D^2}}{2k_B T}\right) \qquad (27)$$

As limiting cases, we observe (i) as $T \to 0$, $S \to 0$ consistent with the third law of thermodynamics while in the opposite limit (ii) $T \to \infty$, $S \to k_B \ln 2$. Besides, the specific heat of the system can be computed as

$$C_v = \frac{\partial\bar{E}}{\partial T} = \left(\frac{J^2 + D^2}{4k_B T^2}\right) sech^2\left(\frac{\sqrt{J^2 + D^2}}{2k_B T}\right) \qquad (28)$$

It is evident that the specific heat is always positive and as $T \to 0$ as well as $T \to \infty$, $C_v \to 0$. Being a continuous function of temperature T, thus it displays a peak at a characteristic temperature $T_0 = \frac{\sqrt{J^2 + D^2}}{k_B}$ well-known feature for any two level system.

Consider now a generalized DM anistropic spin Hamiltonian

$$H = D^1\left(S_{1y}S_{2z} - S_{1z}S_{2y}\right) + D^2\left(S_{1z}S_{2x} - S_{1x}S_{2z}\right) + D^3\left(S_{1x}S_{2y} - S_{1y}S_{2x}\right) \qquad (29)$$

The first three terms of the above Hamiltonian using spin raising and lowering operators is recast as

$$\begin{aligned} D^1\left(S_{1y}S_{2z} - S_{2y}S_{1z}\right) &= D^1\left[\frac{1}{2i}\left(S_1^+ - S_1^-\right)S_{2z} - \frac{1}{2i}\left(S_2^+ - S_2^-\right)S_{1z}\right] \\ D^2\left(S_{1z}S_{2x} - S_{2z}S_{1x}\right) &= D^2\left[\frac{1}{2}\left(S_2^+ + S_2^-\right)S_{1z} - \frac{1}{2}\left(S_1^+ + S_1^-\right)S_{2z}\right] \\ D^3\left(S_{1x}S_{2y} - S_{2x}S_{1y}\right) &= \frac{D^3}{2i}\left[S_1^- S_2^+ - S_1^+ S_2^-\right] \end{aligned} \qquad (30)$$

As a simple illustration, noting the spin-flip nature of the raising and lowering operators, we proceed to find

$$H|\uparrow\uparrow\rangle = \left(\frac{D^2 + iD^1}{4}\right)|\uparrow\downarrow\rangle - \left(\frac{D^2 + iD^1}{4}\right)|\downarrow\uparrow\rangle \qquad (31)$$

Note that the third term does not contribute in this state as the states are in the highest spin states so that any of the spin-raising operators will make it zero. Repeating this way, the spin Hamiltonian matrix in the basis

$|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$

looks like

$$H = \begin{pmatrix} 0 & \frac{D^1 + iD^2}{4} & -\frac{D^2 + iD^1}{4} & 0 \\ \frac{D^2 + iD^1}{4} & 0 & -\frac{iD^3}{2} & \frac{D^2 - iD^1}{4} \\ -\frac{D^2 + iD^1}{4} & \frac{iD^3}{4} & 0 & \frac{iD^1 - D^2}{4} \\ 0 & \frac{D^1 + iD^2}{4} & -\frac{iD^1 + D^2}{4} & 0 \end{pmatrix} \qquad (32)$$

It is interesting to note that Tr H = 0 and det H = 0. This indicates that at least one of the eigenvalues will be zero. Further a careful look into rows and columns reveals that the rank of H is less than equal to two. Therefore, out of four eigenvalues two are zero and others non-zero values occur such a way that the trace i.e. sum of the eigen values is zero. Thus, the two non-zero eigenvalues must be equal and opposite to each other. In fact, the diagonalization of H gives us the eigenvalues as 0,0, $\pm\frac{1}{2}\sqrt{(D^3)^2 + \frac{(D^1)^2 + (D^2)^2}{2}}$.

In the limit $D^1 = D^2 = 0; D^3 = D$, it matches with equation (23). In the most general case of the anisotropic situation, the Hamiltonian in an external magnetic field for two spin states is given by

$$H = D^1\left(S_{1y}S_{2z} - S_{1z}S_{2y}\right) + D^2\left(S_{1z}S_{2x} - S_{1x}S_{2z}\right) + D^3\left(S_{1x}S_{2y} - S_{1y}S_{2x}\right) - J\left(\overrightarrow{S_1}.\overrightarrow{S_2}\right) - B\left(S_1^z + S_1^z\right) \quad (33)$$

In such a situation, the above Hamiltonian (32) is modified as

$$H = \begin{pmatrix} -J/4 - B & \frac{D^1 + iD^2}{4} & -\frac{D^2 + iD^1}{4} & 0 \\ \frac{D^2 + iD^1}{4} & J/4 & -\frac{iD^3}{2} - \frac{J}{2} & \frac{D^2 - iD^1}{4} \\ -\frac{D^2 + iD^1}{4} & \frac{iD^3}{4} - \frac{J}{2} & J/4 & \frac{iD^1 - D^2}{4} \\ 0 & \frac{D^1 + iD^2}{4} & -\frac{iD^1 + D^2}{4} & -J/4 + B \end{pmatrix} \quad (34)$$

It will be interesting to explore the interplay of J and anisotropic D in the thermodynamics and spin response of the above Hamiltonian. This formalism can be further generalized to another simple three-particle spin-1/2 system with relevant intriguing Hamiltonian

$$H = -J(\overrightarrow{S_1}.\overrightarrow{S_2} + \overrightarrow{S_2}.\overrightarrow{S_3} + \overrightarrow{S_3}.\overrightarrow{S_1}) + \vec{D}.\left[\left(\overrightarrow{S_1} \times \overrightarrow{S_2}\right) + \left(\overrightarrow{S_2} \times \overrightarrow{S_3}\right)\right] - B\left(S_1^z + S_2^z + S_3^z\right) \quad (35)$$

The relevant (8×8) Hamiltonian matrix needs to be diagonalized to obtain the eigenvalues for further analysis of thermodynamic properties.

Conclusion

In this pedagogical article, we have explored the origin of DM interaction from the second order perturbation theory under the quenching of orbital angular momentum of the atoms. Besides, we have also highlighted the emergence of this term from anisotropic matrix formulation. Finally, we have demonstrated the exact eigen values and its related thermodynamics of two spin states and indicated the occurrence of gap in the system, leading to the peak in the specific heat of the system as a function of temperature.

Acknowledgements

I would like to thank my undergraduate and post-graduate students for motivating me to write this article.

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