Lecture 12.12.2022

dimension	**Ising**	**XY**	**Heisenberg**
1D	SRO	SRO	SRO
2D	LRO	q-LRO	SRO/q-LRO
3D	LRO	LRO	LRO

Para = paramagnetism, $\langle \vec{S}(\underline{r}) \cdot \vec{S}(0) \rangle = 0$
SRO = short-range order, $\langle \vec{S}(\underline{r}) \cdot \vec{S}(0) \rangle \sim \mathrm{e}^{-r/\xi}$
q-LRO = quasi-long-range order, $\langle \vec{S}(\underline{r}) \cdot \vec{S}(0) \rangle \sim r^{-\eta}$
LRO = long-range order, $\langle \vec{S}(\underline{r}) \cdot \vec{S}(0) \rangle =$ constant.

$$\hat{S}(\underline{n}) \cdot \hat{S}(\underline{n}') \longrightarrow \underline{\vec{S}(\underline{n}) \cdot \vec{S}(\underline{n}')}$$

- linear excit. : Spin Waves (SWs)
- topological excit. : vortices (2D XY)
  Domain Walls (DWs)

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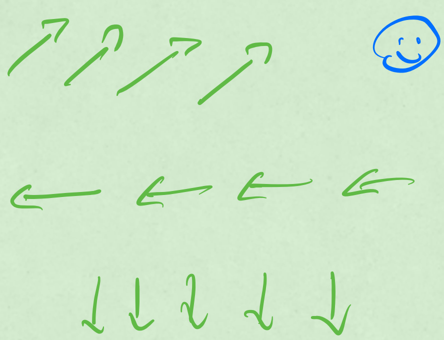
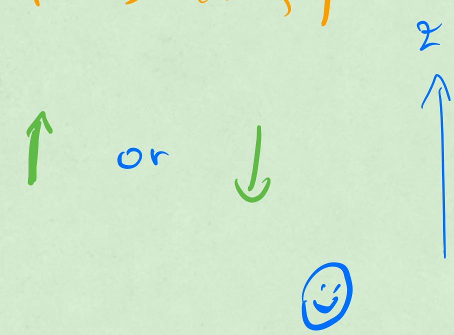
$$\mathcal{H} = -\frac{J}{2}\sum_{\langle \underline{n}\,\underline{n}'\rangle} \vec{S}(\underline{n}) \cdot \vec{S}(\underline{n}') - D\sum_{\underline{n}} \left(S^z(\underline{n})\right)^2$$

cl. Heisenberg model with uniax. anisotropy

Exchange

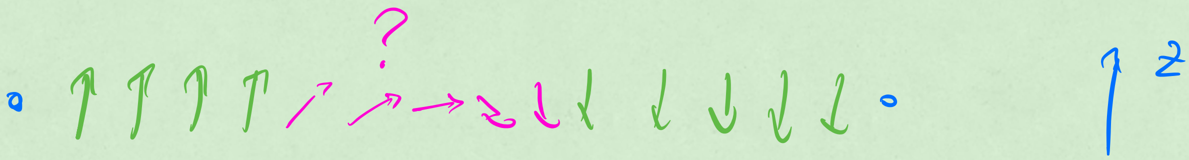


Anisotropy



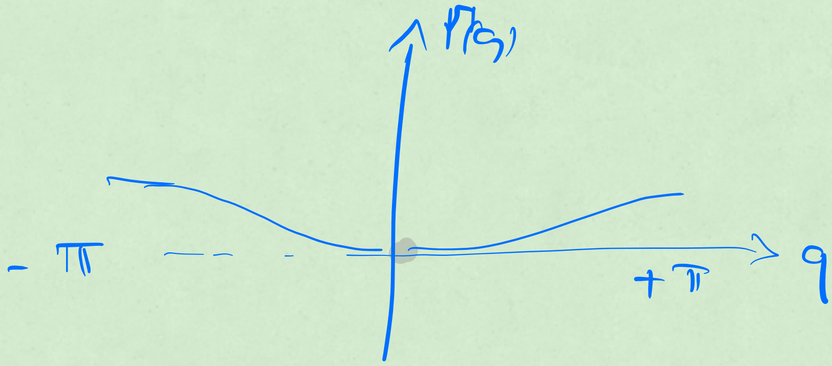
$\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow$

sharp DW
(Ising like)



Spin waves when $D=0$

$$\Gamma(q) = \hbar\omega(q) = 2J(1-\cos q)$$



NUMERICALLY

Domain walls (DWs) can be defined as the boundaries between regions with opposite magnetization and, besides the Ising model, they play a crucial role for many theoretical and applicative aspects of magnetism. In particular, their internal structure and the energy associated with the creation of a DW in a uniformly magnetized configuration are relevant (think of, e.g., the Landau's argument that rules out ferromagnetism in the 1D Ising model). Even if DWs may be characterized by a complicated internal structure dependent on several spatial variables, here we consider the case in which the spin direction depends only on one spatial coordinate. Let us identify that coordinate with the lattice index i:

$$\mathcal{H}_{\mathrm{dw}} = -\sum_{i=1}^{N_x}\left[J\vec{S}_i\cdot\vec{S}_{i+1} + D\left(S_i^z\right)^2\right] , \tag{8.2}$$

where $\vec{S}_i$ are classical spins and the constants J and D have to be thought of per unit length or per unit surface if the dimensionality of the original lattice was D=2 or D=3, respectively. With the Hamiltonian (8.2), the DW can be

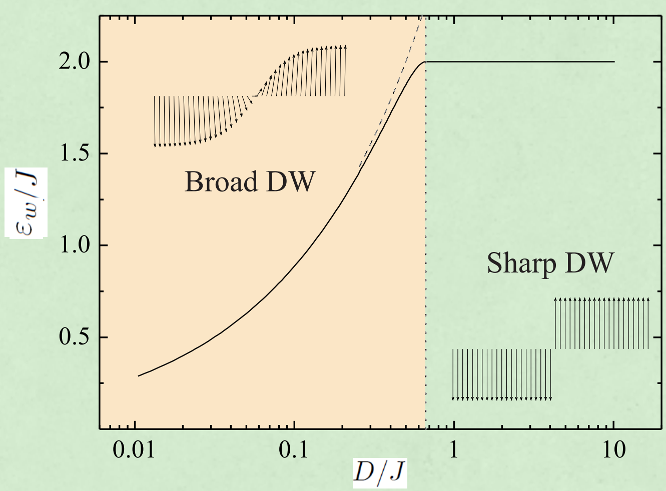


Figure 8.1: Domain-wall energy in J units *vs* D/J: minimum energy solution of the non-linear equation (8.5) computed numerically (solid line); continuum limit solution (dashed line). Inset: spin profile *vs* lattice distance: sharp wall (low-right) and broad wall for $D/J = 10^{-2}$ (up-left).

larger than one lattice spacing. In fact, spreading the wall over more than one lattice unit reduces the global exchange-energy cost. On the other hand, the anisotropy term would favor configurations with as less spins misaligned to the easy axis, z, as possible. The DW profile results from the **competition** between these two energies (two opposite limits are reported in the insets of Fig. 8.1). The lowest-energy deviations from the uniform state can be parameterized through the angle that each spin forms with the z axis, θ, as

$$\mathcal{H}_{\rm dw} = \sum_{i=1}^{N_x} \left[J - J\cos\left(\theta_{i+1} - \theta_i\right) + D\sin^2\theta_i \right] \,. \tag{8.3}$$

The energy cost for creating a DW in a uniformly magnetized configuration is given by the spin profile which fulfills the boundary conditions

$$\begin{cases} \theta_1 & = \pi \\ \theta_{N_x} & = 0 \end{cases} \tag{8.4}$$

and minimizes the energy (8.3) with respect to θ_i:

$$\frac{\partial \mathcal{H}_{\rm dw}}{\partial \theta_i} = \sin\left(\theta_i - \theta_{i-1}\right) - \sin\left(\theta_{i+1} - \theta_i\right) + \frac{D}{J}\sin\left(2\theta_i\right) = 0 \,. \tag{8.5}$$

Equation (8.5) can be solved numerically and the solution provides the spin profile with respect to which the energy (8.3) is stationary. The true lowest-energy profile can be obtained comparing different solutions, among which the sharp-wall profile (see lower-right inset of Fig. 8.1):

$$\begin{cases} \theta_i = \pi & \text{for} \quad 1 \le i < \frac{N_x}{2} \\ \theta_i = 0 & \text{for} \quad \frac{N_x}{2} \le i \le N_x \end{cases} \tag{8.6}$$

which is also a solution of Eq. (8.5). In Fig. 8.1 the resulting energy (solid line) is compared with that obtained from a continuum limit calculation (dashed line) – that we are going to present in the next paragraph – as a function of the ratio D/J.

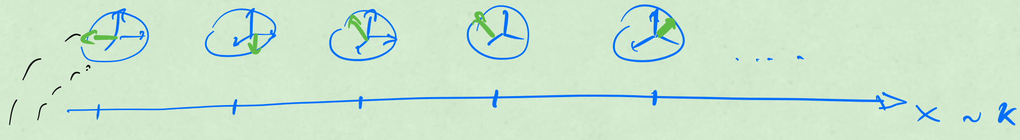
8.2 Broad domain walls: continuum limit

An analytic expression for the energy of a broad DW can be derived using the continuum formalism, in which the lattice index i becomes a continuum variable and finite summations are replaced by integrals. For simplicitly, we will assume spatial coordinates to be dimensionless or expressed in lattice

1D xy model $\quad \varphi_{k+1} - \varphi_k \simeq \partial_x \varphi \quad$ CONTINUUM LIMIT

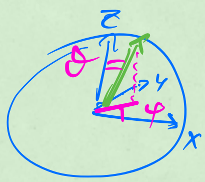
1D Heisenberg

$\vec{S}_k \sim \vec{S}(x)$



$$-\vec{S}_{k+1} \cdot \vec{S}_k \rightarrow \frac{1}{2}(\partial_x \vec{S})^2 = \frac{1}{2}\left[(\partial_x S^x)^2 + (\partial_x S^y)^2 + (\partial_x S^z)^2\right]$$

POLAR COORDINATES



$$\vec{S} = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta)$$

$$-J\vec{S}_{k+1}\cdot\vec{S}_k = \frac{J}{2}\left[(\partial_x\vartheta)^2 + \sin^2\vartheta(\partial_x\varphi)^2\right]$$

where $(\vartheta(x), \varphi(x))$ are continuous fields

$$\mathcal{H}_{dw} = \int \Big\{ \underbrace{\frac{J}{2}\left[(\partial_x\vartheta)^2 + \sin^2\vartheta(\partial_x\varphi)^2\right]}_{\text{Exchange}} - \underbrace{D\cos^2\vartheta}_{\text{Anisotropy}} \Big\} dx$$

$$\mathcal{H}_{dw} = \int \mathcal{A}[\vartheta, \varphi, \partial_x\vartheta, \partial_x\varphi]\, dx$$

Euler Langrange

1) $$\frac{\partial}{\partial x}\frac{\partial \mathcal{A}}{\partial(\partial_x\varphi)} - \frac{\partial\mathcal{A}}{\partial\varphi} = 0$$

2) $$\frac{\partial}{\partial x}\frac{\partial \mathcal{A}}{\partial(\partial_x\vartheta)} - \frac{\partial\mathcal{A}}{\partial\vartheta} = 0$$

1) $\frac{\partial}{\partial x}\left(J \sin^2\vartheta\, \partial_x \varphi\right) = 0$ $\qquad \varphi = \varphi_0$

$J\left(\partial_x\vartheta \sin\vartheta\cos\vartheta\, \partial_x\varphi + \sin^2\vartheta\, \partial_x^2\varphi\right) = 0$

2) $\frac{\partial}{\partial x}\left(J\, \partial_x\vartheta\right) - 2D\cos\vartheta\sin\vartheta = 0$

$J\,\partial_x^2\vartheta - 2D\cos\vartheta\sin\vartheta = 0$

2^{nd} E.L. $\boxed{\partial_x^2\vartheta = \frac{2D}{J}\cos\vartheta\sin\vartheta}$

$1/\delta^2$

bc $\begin{cases} \cos\vartheta = -1 & \vartheta = \pi & x \to -\infty \\ \cos\vartheta = 1 & \vartheta = 0 & x \to +\infty \end{cases}$

trial Solution $\cos\vartheta = th\left(\frac{x}{\delta}\right)$

$\frac{\partial}{\partial x}$ $\qquad -\partial_x\vartheta\sin\vartheta = \frac{1}{\delta}\left[1 - th^2(\dots)\right]$

$-\partial_x\vartheta\sin\vartheta = \frac{1}{\delta}\left(1-\cos^2\vartheta\right) = \frac{1}{\delta}\sin^2\vartheta$

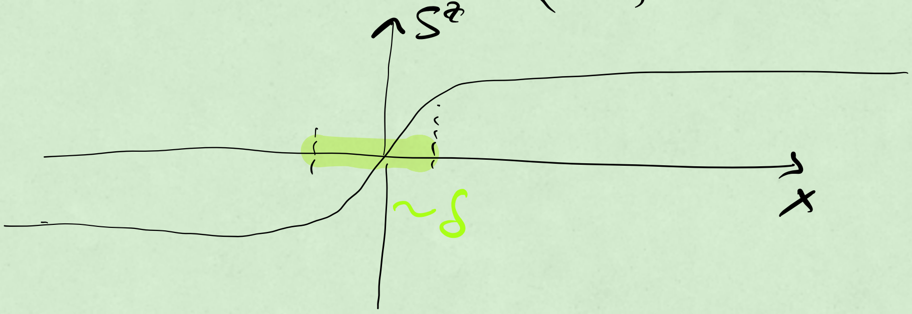
$\vartheta \neq 0, \pi$ $\qquad \partial_x\vartheta = -\frac{1}{\delta}\sin\vartheta$

$\frac{\partial^2}{\partial x^2}$ $\qquad \partial_x^2\vartheta = -\frac{1}{\delta}\partial_x\vartheta\cos\vartheta = \frac{1}{\delta^2}\cos\vartheta\sin\vartheta$

The trial solution fulfills the 2nd E.L. eq

if $\delta^2 = \frac{J}{2D} \Rightarrow \delta = \sqrt{\frac{J}{2D}}$

$$S^z(x) = \cos\vartheta = \text{th}\left(\frac{x}{\delta}\right)$$



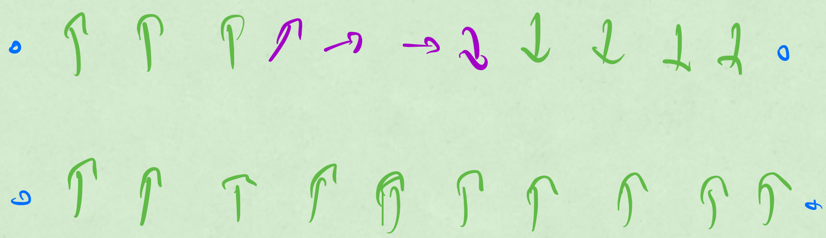
$$\mathcal{E}_{dw} = 2\sqrt{2JD}$$

$\frac{D}{J} \ll 1$ (continuum formalism meanfull)

Length scales

- 1D Ising model $\xi \sim e^{2J/kT}$
- 1D XY / Heis. model $\xi \sim \frac{J}{kT}$
- Heisenb. + Anisotr. $\delta = \sqrt{\frac{J}{2D}}$

Landau's Argument 1D Heisenberg + Anisotropy



$$\Delta F = \mathcal{E}_{dw} - kT \ln\left(\frac{N}{\delta}\right) \xrightarrow[N\to\infty]{} -\infty \qquad (A)$$

$$\Delta F = 0 : \quad \tilde{N} = \delta \, e^{\mathcal{E}_{dw}/kT}$$

$$\xi \sim \delta \, e^{\gamma_{dw}\mathcal{E}_{dw}/kT}$$

$\gamma_{dw} \sim 0.5$ because of the interplay with SWs

What is the role of spin waves?

$$\langle (S^{\perp})^2 \rangle \approx kT \int_{q_{min}}^{q_{max}} \frac{d q^D}{J q^2 + 2D} < \infty \quad (N \to \infty) \qquad (B)$$

in this model spin waves do not manage to destroy FM.!

$\Downarrow$

BUT Domain walls are also present ....

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units (formally $a = 1$). We will express the exchange coupling by a term containing spatial derivatives, as done in a previous chapter for the XY model. The continuum equivalent of the energy (8.3) reads

$$\mathcal{H}_{\mathrm{dw}} = \frac{1}{2} J \int \left|\partial_x \vec{S}(\underline{r})\right|^2 d^{\mathrm{d}}x - D \int \left[S^z(\underline{r})\right]^2 d^{\mathrm{d}}x + \quad \text{const.} \tag{8.7}$$

The exchange-energy term has to be understood as[1]

$$\left|\partial_x \vec{S}(\underline{r})\right|^2 = \left(\partial_x S^x(\underline{r})\right)^2 + \left(\partial_x S^y(\underline{r})\right)^2 + \left(\partial_x S^z(\underline{r})\right)^2 . \tag{8.8}$$

Using spherical coordinates

$$\begin{aligned} \left|\partial_x \vec{S}(\underline{r})\right|^2 \quad &\Rightarrow \quad (\partial_x \theta)^2 + \sin^2(\theta)\,(\partial_x \varphi)^2 \\ |S^z(\underline{r})|^2 \quad &\Rightarrow \quad \cos^2\theta \end{aligned} \tag{8.9}$$

the Hamiltonian (8.7) can then be written as

$$\begin{aligned} \mathcal{H}_{\mathrm{dw}} = &\frac{1}{2} J N_y N_z \int \left[\left(\frac{d\theta}{dx}\right)^2 + \sin^2(\theta(x))\left(\frac{d\varphi}{dx}\right)^2\right] dx \\ &- D N_y N_z \int \cos^2(\theta(x)) dx + \text{ const} \end{aligned} \tag{8.10}$$

where we have implicitly assumed the integration domain to be a parallelepiped $N_x\, N_y\, N_z$. The functions $\theta(x)$ and $\varphi(x)$ that minimize the functional Eq. (8.10) are obtained as solutions of the Euler-Lagrange equation

$$\left\{ \begin{array}{l} J \sin^2(\theta(x)) \frac{d^2\varphi}{dx^2} + 2J \sin(\theta(x)) \cos(\theta(x)) \left(\frac{d\theta}{dx}\right)\left(\frac{d\varphi}{dx}\right) = 0 \\ J \frac{d^2\theta}{dx^2} - J \sin(\theta(x)) \cos(\theta(x)) \left(\frac{d\varphi}{dx}\right)^2 - 2D \sin(\theta(x)) \cos(\theta(x)) = 0 \,. \end{array} \right. \tag{8.11}$$

The solution compatible with boundary conditions

$$\left\{ \begin{array}{l} \lim_{x\to-\infty} \theta(x) = \pi \\ \lim_{x\to+\infty} \theta(x) = 0 \end{array} \right. \tag{8.12}$$

[1] For the general case in which the spin profile is modulated along the three spatial directions x, y, z, the exchange-energy term reads

$$\begin{aligned} \left|\nabla \vec{S}(\underline{r})\right|^2 = &\left(\partial_x S^x(\underline{r})\right)^2 + \left(\partial_y S^x(\underline{r})\right)^2 + \left(\partial_z S^x(\underline{r})\right)^2 \\ &+ \left(\partial_x S^y(\underline{r})\right)^2 + \left(\partial_y S^y(\underline{r})\right)^2 + \left(\partial_z S^y(\underline{r})\right)^2 \\ &+ \left(\partial_x S^z(\underline{r})\right)^2 + \left(\partial_y S^z(\underline{r})\right)^2 + \left(\partial_z S^z(\underline{r})\right)^2 . \end{aligned}$$

is given by

$$\begin{cases} \cos(\theta(x)) & = \tanh\left(\frac{x}{\delta}\right) \\ \varphi(x) & = \text{const.} \end{cases} \tag{8.13}$$

with $\delta = \sqrt{J/(2D)}$ representing the DW width[2]. Such a solution was proposed by Landau and Lifshitz in 1935.

The energy density associated with the spin profile (8.13) is $\mathcal{E}_{\text{dw}} = 2\sqrt{2DJ}$ (per unit length for D=2 and per unit surface for D=3). In Fig. 8.1 the DW energy obtained numerically for the discrete-lattice calculation (solid line) is compared with that obtained in the continuum limit (dashed line) as a function of the ratio D/J. The agreement is already good for ratios $D/J < 0.3$. In the opposite limit, the discrete lattice calculation recovers the DW energy of the Ising model $\mathcal{E}_{\text{dw}} = 2J$ (sharp DW defined by Eqs. (8.6)).

In those relevant limits one has

$$\begin{cases} J \ll D \Rightarrow \delta = 1 & \text{and} \quad \mathcal{E}_{\text{dw}} = 2J \\ J \gg D \Rightarrow \delta = \sqrt{\frac{J}{2D}} > 1 & \text{and} \quad \mathcal{E}_{\text{dw}} = 2\sqrt{2DJ}\,. \end{cases} \tag{8.14}$$

For $J \ll D$, the DW cost equals the Ising case. Concerning $J \gg D$, $\mathcal{E}_{\text{dw}}$ is one-soliton energy. As one can appreciate in Fig. 8.1, the two regimes are very well recovered and the transition region, where none of the two limits (8.14) is expected to hold, is surprisingly narrow. The crossover between the sharp-wall ($\delta = 1$) and the broad-wall ($\delta > 1$) regime[3] occurs at $D/J = 2/3$.

In summary, according to Eqs. (8.14), DWs in the classical Heisenberg model behave like

$$\begin{cases} \text{Ising model} & \text{for} \ \ D/J \geq 2/3 \\ \text{continuum limit} & \text{for} \ \ D/J \leq 0.3\,. \end{cases} \tag{8.15}$$

Typically, metallic nanowires of technological relevance fall in the broad-wall regime. In fact, materials like Co, Ni or Fe are characterized by $D \simeq 1-10$ K ($\sim 0.1-1$ meV) and $J \simeq 100-500$ K ($\sim 10-50$ meV) corresponding to a DW width of the order $10-100$ nm.

[2]Sometimes the DW width is defined with some numerical factors of difference with respect to δ: $\pi\sqrt{J/(2D)}$ or $\sqrt{2J/D}$ for instance.

[3]The crossover ratio $D/J = 2/3$ can be obtained analytically by analyzing the stability of the sharp-wall profile, Eqs. (8.6), against small deviations between successive angles θ_i (B. Barbara, *Journal de Physique* **34**, p. 139 (1973)).

8.3 Loss of magnetic order

We now ask ourselves how the Mermin-Wagner argument for the absence of spontaneous magnetization at finite temperature in the 1D and the 2D Heisenberg models is affected by the introduction of a uniaxial anisotropy $D > 0$. In this case, the spin-wave dispersion relation acquire a constant term proportional to the anisotropy D

$$\Gamma(\underline{q}) \simeq Jq^2 + 2D + g\mu_{\mathrm{B}}B \,. \tag{8.16}$$

Therefore, at the same level of approximation as Eq. (7.27), the thermal average of transverse spin components scales like

$$\langle (S^\alpha)^2 \rangle \sim k_{\mathrm{B}}T \int_{q_{min}} \frac{q^{\mathrm{D}-1}\, dq}{Jq^2 + 2D} \,. \tag{8.17}$$

As this integral is never divergent for D=1, 2, or 3, we conclude that linear excitations do not manage to destroy ferromagnetism at every $T \neq 0$. In other words, as long as only spin waves are considered, this model could be compatible with ferromagnetism at finite temperature. However, domain walls are another type of excitations to be taken into account. Qualitatively, their role in this model is similar to the role they play in the Ising model. With this simple argument, we conclude that the Heisenberg model with uniaxial anisotropy behaves as the Ising model from the perspective of the "truth table" of magnetic order discussed in Section 7.3 (and falls in the same universality class).

For the 1D case, the Landau's argument put forward for the Ising model can be adapted replacing the energy of a sharp (Ising) DW with the more general expression $\mathcal{E}_{\mathrm{dw}}$. As a result, one would expect the correlation length to diverge at low temperature as

$$\xi \sim \exp\left[\mathcal{E}_{\mathrm{dw}}/(k_{\mathrm{B}}T)\right] \,. \tag{8.18}$$

In reality, thermally-excited spin waves interplay with DW excitations, suppressing the energy barrier $\mathcal{E}_{\mathrm{dw}}$. The Arrhenius dependence of Eq. (8.18) is, however, retained and we interpret this fact as an indication that right DWs are responsible for the loss of magnetic order at finite temperature.