

Magnetostatics#3

Refinement to Magnetic Energy Density

In Notes#2 we predicted a very large energy density, up to 0.1 J/cm^3 (or 100 kJ/m^3) for the energy density in a “garden variety” ferromagnetic material – AlNiCo. In reality, the energy density is less than this as shown in Table I. The reason for this is that the hysteresis curve “sags” as the magnitude of H is reduced toward zero because of the magnetic domains in all ferromagnetics (more on this later). So the figures-of-merit for ferromagnets become the coercive field, H_C , and the remanent magnetic induction B_R as shown in the more realistic hysteresis curve of Fig. 7.12

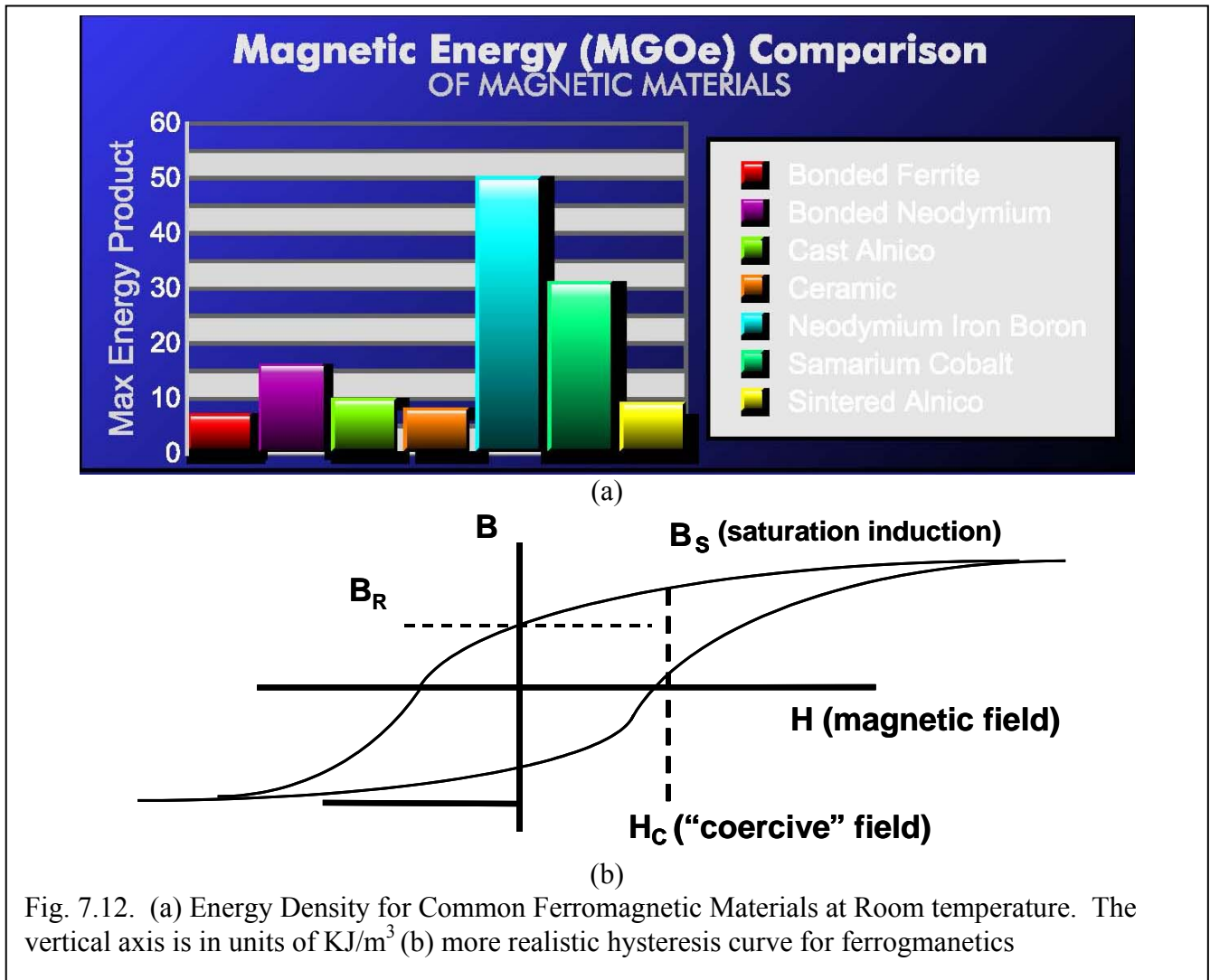


Fig. 7.12. (a) Energy Density for Common Ferromagnetic Materials at Room temperature. The vertical axis is in units of kJ/m^3 (b) more realistic hysteresis curve for ferromagnetics

Spin-Spin Interaction

To explain ferromagnetism we needed to make the term $b\mathbf{M}$ roughly 10^4 larger than a classical magnetic dipole having the same angular momentum as \mathbf{S} . Heisenberg explained this in terms of the exchange phenomenon,

$$U_m = -\mathbf{m}_i \cdot \mathbf{B}_{local} \rightarrow 2 \cdot I_E \cdot \mathbf{S}_i \cdot \mathbf{S}_j \quad (7.63)$$

where I_E is the exchange integral ($\approx 12 \text{ meV}$ in iron, for example). Exchange is strictly a quantum mechanical effect. The Pauli exclusion principle prevents particles in the same spin state from being in the same location in space. Therefore, the spins must approach counter-alignment as d decreases, as shown in Fig. 7.13. If the particles are charged, the decrease in d is equivalent to an increase in energy because electro-static potential increases as d decreases (recall $V = q^2/d$ for Coulomb potential, like charges). Again, we have an example of how important the Pauli exclusion principle is in the microscopic behavior of solids.

In a nearest neighbor approximation:

$$U = -2 \cdot I_E \cdot \mathbf{S}_p \cdot (\mathbf{S}_{p-1} + \mathbf{S}_{p+1}), \quad p \rightarrow \text{atomic index} \quad (7.64)$$

For spins:

$$\mathbf{m}_p = -g \mu_B \mathbf{S}_p \quad (7.65)$$

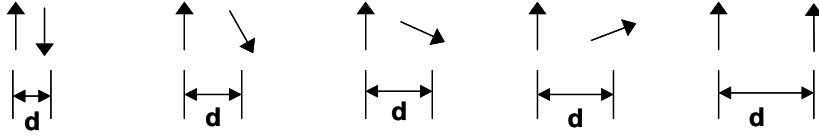


Fig. 7.13. The physical behavior of neighboring spins as a function of their spatial separation d , called the exchange interaction. At close separation, the spin vectors must be opposite in direction to comply with the Pauli exclusion principle. At greater separation, they can be parallel.

So we can rewrite the energy expression as:

$$\begin{aligned}
 U &= 2 \cdot I_E \mathbf{S}_p \cdot (-\mathbf{S}_{p-1} - \mathbf{S}_{p+1}) \\
 U &= -\mathbf{m}_p \left(\frac{-2 \cdot I_E}{g \mu_B} \right) (\mathbf{S}_{p-1} + \mathbf{S}_{p+1}) \\
 U &\equiv -\mathbf{m}_p \cdot \mathbf{B}_{E,P}
 \end{aligned}$$

(7.66)

where $\mathbf{B}_{E,P}$ is the “exchange” magnetic induction. We can now derive the dynamic equation of motion. From classical mechanics,

$$d\mathbf{L} / dt = \boldsymbol{\tau} \quad (\text{torque}) \quad (7.67)$$

In magnetic materials: $\boldsymbol{\tau} = \mathbf{m} \cdot \mathbf{B}_e$. We make the correspondence $\mathbf{L} \rightarrow \hbar \cdot \mathbf{S}$ to get:

$$\begin{aligned}
 \hbar \frac{d\mathbf{S}_p}{dt} &= -g \mu_B \mathbf{S}_p \times (\mathbf{S}_{p-1} + \mathbf{S}_{p+1}) \left(\frac{-2I_E}{g \mu_B} \right) \\
 \frac{d\mathbf{S}_p}{dt} &= \frac{2I_E}{\hbar} \mathbf{S}_p \times (\mathbf{S}_{p-1} + \mathbf{S}_{p+1})
 \end{aligned}$$

(7.68)

To proceed further, we decompose this equation into Cartesian coordinates making the z axis the nominal alignment axis of each spin. We get:

$$\frac{dS_p^x}{dt} = \frac{2I_E}{\hbar} \left[S_p^y (S_{p-1}^z + S_{p+1}^z) - S_p^z (S_{p-1}^y + S_{p+1}^y) \right] \quad (7.69)$$

$$\frac{dS_p^y}{dt} = \frac{2I_E}{\hbar} \left[S_p^z (S_{p-1}^x + S_{p+1}^x) - S_p^x (S_{p-1}^z + S_{p+1}^z) \right] \quad (7.70)$$

$$\frac{dS_p^z}{dt} = \frac{2I_E}{\hbar} \left[S_p^x (S_{p-1}^y + S_{p+1}^y) - S_p^y (S_{p-1}^x + S_{p+1}^x) \right] \quad (7.71)$$

Now in classical sense, we can assume that S_p^y and S_p^x are much less in magnitude than S_p^z and that $S_p^z \approx S_{p-1}^z \approx S_{p+1}^z \equiv S_p$ (to first order). Thus we can ignore terms where S_p^x and S_p^y occur together. We find

$$\frac{dS_p^x}{dt} = \frac{2I_E}{\hbar} \left[2S_p^y S_p - S_p^z (S_{p-1}^y + S_{p+1}^y) \right] \quad (7.72)$$

$$\frac{dS_p^y}{dt} = \frac{2I_E}{\hbar} \left[S_p (S_{p-1}^x + S_{p+1}^x) - S_p^x (2S_p) \right] \quad (7.73)$$

$$\frac{dS_p^z}{dt} = \frac{dS_p}{dt} = 0 \quad (7.74)$$

Spin Wave Equation (Optional for 2008)

As equation (7.74) is a cross-coupled set of linear difference equations; we seek lattice-wave like traveling waves for the solution:

$$S_p^z = S_p; S_p^x = V \exp[jpka] \exp[-j\omega t]; S_p^y = W \exp[jpka] \exp[-j\omega t] \quad (7.75)$$

Substituting the trial solutions of (7.75) into (7.72) above, we get

$$-j\omega V \exp[j(pka - \omega t)] = \frac{2I}{\hbar} \left[2S_p W e^{j(pka - \omega t)} - S_p W \left[e^{j[(p+1)ka - \omega t]} + e^{j[(p-1)ka - \omega t]} \right] \right] \quad (7.76)$$

or

$$-j\omega V = \frac{2I_E}{\hbar} \left[2S_p W - S_p W (e^{jka} + e^{-jka}) \right] \quad (7.77)$$

or

$$-j\omega V = \frac{4I_E}{\hbar} \left[S_p W (1 - \cos ka) \right] \quad (7.78)$$

Similar substitution of (7.75) into (7.73) yields (after simple algebra)

$$-j\omega W = \frac{4I_E}{\hbar} \left[S_p V (\cos ka - 1) \right] \quad (7.79)$$

The preceding two equations can be written in matrix form

$$\begin{bmatrix} +j\omega & \frac{4I_E S_p}{\hbar}(1-\cos ka) \\ \frac{-4I_E S_p}{\hbar}(1-\cos ka) & +j\omega \end{bmatrix} \begin{bmatrix} V \\ W \end{bmatrix} = 0 \quad (7.80)$$

From linear algebra, we know that a non-trivial solutions exist only if the matrix is “singular”, i.e., does not have an inverse. But a lack of inverse also means that the determinant must vanish:

$$\begin{aligned} \Rightarrow -\omega^2 + \left[\frac{4I_E S_p}{\hbar}(1-\cos ka) \right]^2 &= 0 \\ \omega &= \frac{4I_E S_p}{\hbar}(1-\cos ka) \end{aligned} \quad (7.81)$$

Also note that by substituting (7.79) into (7.78)

$$-j\omega V = \left[\frac{4I_E S_p}{\hbar}(1-\cos ka) \right] \cdot [W] = j\omega W^2 / V \quad (7.82)$$

which implies

$$V = jW, \text{ or } W = -jV. \quad (7.83)$$

So that S_p^x and S_p^y are 90° out of phase \rightarrow circular motion in x - y plane \rightarrow precession

The “spin-wave” dispersion relation,

$$\omega = \frac{4I_E S_p}{\hbar}(1-\cos ka) , \quad (7.84)$$

is very similar to that derived for lattice waves:

$$\omega^2 = \frac{2C}{m}(1 - \cos ka) . \quad (7.85)$$

But note the different exponent on the ω term in each. The ω^2 term for spin waves makes the dependence on k near $k = 0$ stronger (and nonlinear) for spin waves. We can see this analytically by Taylor expansion for small k :

$$\omega = \frac{4I_E S_p}{\hbar}(1 - \cos ka) \approx \frac{4I_E S_p}{\hbar} \left[1 - \left[1 + \frac{(ka)^2}{2} + \dots \right] \right] \approx \frac{2I_E S_p k^2 a^2}{\hbar} (k \ll a) . \quad (7.86)$$

Similarly, as ka approaches π (Nyquist wave vector) $d\omega/dk \rightarrow 0$ for the spin waves, just as for the lattice waves. But there is faster dependence on k . Right at the Nyquist wave

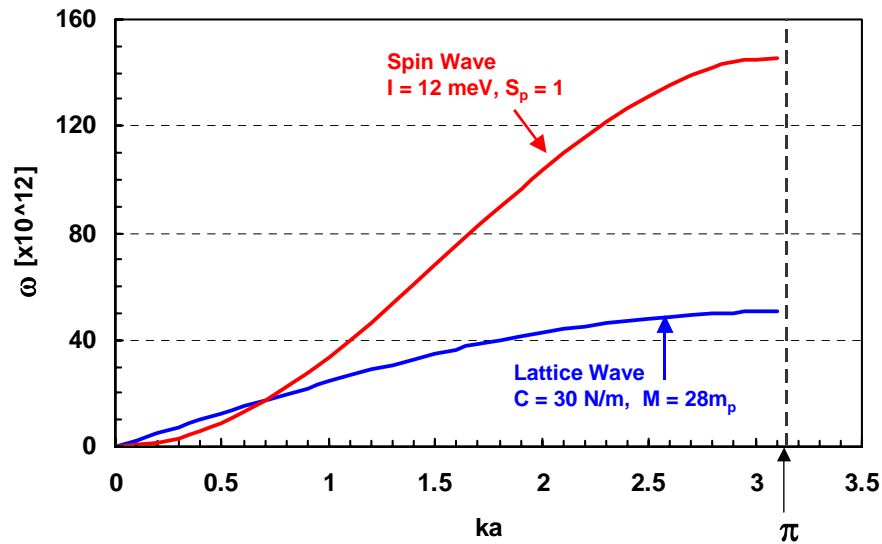


Fig. 7.14. Representative lattice-wave and spin-wave dispersion curves for the following parameters: Lattice wave: $C = 30 \text{ N/m}$, $M = 28 m_p$, where m_p is the proton rest mass; Spin wave: $I_E = 12 \text{ meV}$ (iron), $S_p = 1$.

vector $k = \pi/a$, we get $\omega = 8I_E S_p / \hbar$ - a convenient fact for doing statistical mechanics with the dispersion curve, as we will see below.

These points are illustrated in Fig. 7.14 that shows representative lattice-wave and spin-wave dispersion curves for the following parameters [lattice wave: $C = 30 \text{ N/m}$, $M = 28 m_p$, where m_p is the proton rest mass; spin wave: $I_E = 12 \text{ meV}$ (iron), $S_p = 1$].

Spin-Wave Energy and Quantization: Magnons (Optional for 2008)

As in the analysis of lattice waves, it becomes very useful to analyze the total energy of spin waves (kinetic plus potential) with a thought towards their quantization and statistical mechanics. To do this we continue our classical thinking by applying an expression from classical rotational dynamics:

$$\text{Kinetic Energy} = \frac{L^2}{2I_m} \tag{7.87}$$

Where L is the orbital angular momentum and I_m is the moment of inertia. Also we have,

$$KE = \frac{1}{2} I_m \omega^2 \quad (7.88)$$

$$\Rightarrow I_m = \frac{|\mathbf{L}|}{\omega} \Rightarrow KE = \frac{1}{2} |\mathbf{L}| \omega$$

If we make correspondence $|\mathbf{L}| \leftrightarrow |\mathbf{m}_p| = g \mu_B \mathbf{S}_p$, then

$$KE = \frac{+1}{2} g \mu_B S_p \omega = +2 g \mu_B S_p^2 \frac{I_E}{\hbar} (1 - \cos ka) \quad (7.89)$$

$$\text{Potential energy} \equiv PE = -2 I_E \mathbf{S}_p \cdot (\mathbf{S}_{p-1} + \mathbf{S}_{p+1}) \quad (7.90)$$

$$U_{total} = KE + PE = 2 g \mu_B \frac{I_E}{\hbar} (1 - \cos ka) S_p^2 - 2 I_E \mathbf{S}_p \cdot (\mathbf{S}_{p-1} + \mathbf{S}_{p+1}) \quad (7.91)$$

This looks very much like total energy for lattice waves in Chapter 4:4

$$\frac{1}{2} m \omega^2 u_s = C (1 - \cos ka) u_s = KE \quad (7.92)$$

$$\frac{1}{2} C (u_{s-1} - u_s)^2 + \frac{1}{2} C (u_{s+1} - u_s)^2 = PE \quad (7.93)$$

Following a derivation similar to that for phonons, we can now show that the spin total energy has the form of a harmonic oscillator in Fourier transform (k) space. This is yet another example in solid-state of a “collective excitation” – a wave in real space that takes on

the form of a collection of independent harmonic oscillators in k space after Fourier transformation. As before, we can associate a fictitious massless particle with each independent mode. In the case of spin waves, we call this particle a magnon. The energy of each k-space mode, or magnon, is then given by

$$\Rightarrow U_k = \left(n_k + \frac{1}{2} \right) \cdot \hbar \omega_k \quad (7.94)$$

where n_k is the number of magnons excited, or equivalently, the excitation amplitude of the associated spin wave.

Statistical Mechanics of Magnons (Optional for 2008)

Since I_E can be so large in ferromagnets, the energy stored in magnon modes is significant. As in phonons, magnons are indistinguishable and have zero mass. Therefore, they abide to photon and phonon statistics, i.e., *the Planck function*. The mean number of magnons in each mode at a bath temperature T is therefore given by

$$\langle n_k \rangle = \frac{1}{\exp[\hbar \omega_k / kT] - 1} \quad (7.95)$$

And the total number of magnons in the solid is

$$N_{total} = \sum_K \langle n_k \rangle = \int_0^{\omega_{max}} D(\omega) \langle n_k \rangle d\omega \quad (7.96)$$

where $D(\omega)$ is the magnon density of states and $\omega_{max} = 8I_E S_p / \hbar$. As usual, $D(\omega)$ is needed to convert the summation over k to an integral over ω . So it is best defined by a chain rule expansion:

$$D(\omega)d\omega = \frac{dN(k)}{dk} \frac{dk}{d\omega} d\omega \quad (7.97)$$

where

$$N(k) = \frac{V}{(2\pi)^3} \frac{4}{3} \pi k^3 \Rightarrow \frac{dN}{dk} = \frac{V}{2\pi^2} k^2. \quad (7.98)$$

In the long-wavelength approximation:

$$\omega_K = 2I_E S_p k^2 a^2 / \hbar \quad (7.99)$$

or

$$k = \sqrt{\frac{\hbar}{2I_E S_p a^2}} \sqrt{\omega_K} \quad (7.100)$$

$$\frac{dk}{d\omega} = \frac{1}{2} \sqrt{\frac{\hbar}{2I_E S_p a^2}} \omega_K^{-1/2} \quad (7.101)$$

$$D(\omega) = \frac{V}{4\pi^2} \left(\frac{\hbar \omega_k}{2I_E S_p a^2} \right)^{3/2} \omega_k^{1/2} d\omega \quad (7.102)$$

In the low temperature limit $\hbar\omega_K > k_B T$, the Planck function has significant weight only at low k where the dispersion is quadratic. Hence we can extend $\omega_{max} \rightarrow \infty$

$$N_{total} \cong \int_0^\infty \frac{V}{4\pi^2} \left(\frac{\hbar}{2I_E S_p a^2} \right)^{3/2} \frac{\omega_k^{1/2} d\omega}{\exp[\hbar\omega_k/k_B T] - 1} \quad (7.103)$$

let $x = \hbar\omega_K/k_B T$,

$$N' \equiv N_{total}/V = \frac{1}{4\pi^2} \left(\frac{k_B T}{2I_E S_p a^2} \right)^{3/2} \int_0^\infty dx \left(\frac{x^{1/2}}{e^x - 1} \right) \quad (7.104)$$

$$\text{Total energy} = \int_0^\infty D(\omega_k) \langle n_k \rangle + 1/2 \hbar \omega_k d\omega \quad (7.105)$$

$$U_{total} \approx \int_0^\infty \frac{V}{4\pi^2} \left(\frac{\hbar}{2I_E S_p a^2} \right)^{3/2} \frac{\hbar \omega_k^{3/2} d\omega}{\exp[\hbar \omega_k / k_B T] - 1} \quad (7.106)$$

Again let $x = \hbar \omega_k / k_B T$, $dx = \hbar \omega_k / k_B T$, so that

$$U' = \frac{k_B T}{4\pi^2} \left(\frac{k_B T}{2I_E S_p a^2} \right)^{3/2} \int_0^\infty dx \frac{x^{3/2}}{e^x - 1} \quad (7.107)$$

To simplify this we define a quantity A through $\omega_k = Ak^2 \equiv \frac{2I_E S_p a^2}{\hbar} k^2$. This leads to

$$U' = \frac{(k_B T)^{5/2}}{(\hbar A)^{3/2}} \left\{ \frac{1}{4\pi^2} \int_0^\infty dx \frac{x^{3/2}}{e^x - 1} \right\}, \quad (7.108)$$

where

$$\int_0^\infty \frac{dx \cdot x^{3/2}}{e^x - 1} \approx 1.80 \quad \text{from integral tables.} \quad (7.109)$$

So in the end, we get a rather simple expression for the heat capacity

$$\begin{aligned} C_V &\cong \frac{dU'}{dT} = \frac{k_B (k_B T)^{3/2}}{(\hbar A)^{3/2}} \left\{ \frac{5}{8\pi^2} (1.80) \right\} \\ &= \frac{k_B (k_B T)^{3/2}}{(\hbar A)^{3/2}} (0.114) \text{ per unit volume.} \end{aligned} \quad (7.110)$$

It is informative to do a numerical example for iron at room temperature.

$I_E = 11.9 \text{ meV}$ (Kittel p. 446); $a = 2.87 \text{ \AA}$ (Kittel p. 23); and $S_p = 1$ (Kittel p. 446), so that

$$A \equiv \frac{2IS_p a^2}{\hbar} \approx 2.97 \times 10^{-6} \quad (7.111)$$

and

$$C_v \approx 5.5 \times 10^{27} \text{ k}_B / \text{m}^3 \quad (7.112)$$

This is to be compared to the Dulong-Petit law as we did several times for phonons:

$$C_v \approx 3Nk_B . \quad (7.113)$$

Iron crystallizes in a bcc structure with $n = \frac{N}{V} = \frac{2}{[(2.87) \times 10^{-10}]^3} \rightarrow n = 8.46 \times 10^{28} / \text{m}^3$.

Therefore, the law of Dulong-Petit predicts:

$$C_v \approx 2.54 \times 10^{29} \text{ k}_B / \text{m}^3 \quad (7.114)$$

So the contribution to the total C_v of the spins is about 2% - small but not insignificant.