Notes for Condensed Matter Physics 2

(Textbook: Michael P. Marder, *Condensed Matter Physics*, Wiley, 2000)

Contents page

The dipole moment

A displacement of a point charge q from the point charge $-q$ by a vector $\mathbf{x}$ gives rise to an electric dipole moment $\mathbf{p} = q\,\mathbf{x}$ (where $|\mathbf{x}|$ has to be small compared with any other distances considered). A certain dipole at $\mathbf{r}$, within the volume Ω, contributes to the polarization $\mathbf{P}(\mathbf{r})$ as determined by

$$\mathbf{P}(\mathbf{r})\Omega = \int^t \mathbf{J}(t')dt' = \int^t q\,\dot{\mathbf{x}}(t')dt' = q\,\mathbf{x} = \mathbf{p}(\mathbf{r}) \qquad (1.1)$$

and the (averaged) polarization in the volume V is

$$\mathbf{P} = \frac{1}{V}\sum_i \mathbf{p}(\mathbf{r}_i) = \frac{N}{V}\mathbf{p} = n\mathbf{p} \qquad (1.2)$$

if all dipole moments are equal $\mathbf{p}(\mathbf{r}_i) = \mathbf{p}$. The scalar potential at $\mathbf{r}$ due to a dipole at origo is

$$\phi(\mathbf{r}) = \frac{q}{r_+} - \frac{q}{r_-} = \frac{\mathbf{p}\cdot\mathbf{r}}{r^3} \quad \Rightarrow \quad \mathbf{E}(\mathbf{r}) = -\nabla\phi(\mathbf{r}) = 3\frac{(\mathbf{p}\cdot\mathbf{r})\mathbf{r}}{r^5} - \frac{\mathbf{p}}{r^3} \qquad (1.3)$$

as obtained, when $x \ll r$, from $r_\pm = r \mp (x/2)\cos\theta$ and $pr\cos\theta = \mathbf{p}\cdot\mathbf{r}$. In the presence of an electric field $\mathbf{E}$, the energy of a dipole moment at the position $\mathbf{r}$ is

$$\begin{aligned}
U &= q\phi\left(\mathbf{r} + \tfrac{1}{2}\mathbf{x}\right) - q\phi\left(\mathbf{r} - \tfrac{1}{2}\mathbf{x}\right) \\
&= q\left(\phi(\mathbf{r}) + \tfrac{1}{2}\mathbf{x}\cdot\nabla\phi(\mathbf{r})\right) - q\left(\phi(\mathbf{r}) - \tfrac{1}{2}\mathbf{x}\cdot\nabla\phi(\mathbf{r})\right) \\
&= q\mathbf{x}\cdot\nabla\phi(\mathbf{r}) = -\mathbf{p}(\mathbf{r})\cdot\mathbf{E}(\mathbf{r})
\end{aligned} \qquad (1.4)$$

The combination of (1.3) and (1.4) determines the field energy of two dipoles $\mathbf{p}_1(\mathbf{r}_1)$ and $\mathbf{p}_2(\mathbf{r}_2)$ to be

$$U_{12} = -3\frac{(\mathbf{p}_1\cdot\mathbf{r}_{12})(\mathbf{p}_2\cdot\mathbf{r}_{12})}{r_{12}^5} + \frac{\mathbf{p}_1\cdot\mathbf{p}_2}{r_{12}^3}, \qquad \mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2 \qquad (1.5)$$

We shall consider an ellipsoidal sample of a homogeneous dielectric material. Classical electrostatics shows that the polarization $\mathbf{P}$, and thus also the electric field $\mathbf{E}$ inside the ellipsoid, is uniform in the presence of an applied uniform electric field $\mathbf{E}_0$. We shall assume this to be the situation, in which case the total field $\mathbf{E}_{\text{cell}}$ acting on a certain dipole in the system is the same for all sites and equal to the field $\mathbf{E}_{\text{cell}}(\mathbf{0})$ acting on the dipole placed in the center of the sample. The dipole–dipole interaction (1.5) is of long range. It declines proportional to r^{-3}, but the number of dipoles at the distance r increases as r^2 and, as a consequence, the distribution of dipoles near the surface affects the dipole in the center no matter how far the distance is to the surface. In order to handle this enormous span of length scales, we make a cut between the microscopic world of a discrete lattice of dipoles and the macroscopic continuous material with its uniform polarization. The cut to be used is the surface of a sphere centered at the dipole considered. The radius of this sphere R_C should be large compared with the lattice spacing, but smaller than the shortest distance to the surface (or smaller than the size of crystallites in a polycrystalline sample

or the size of the domains in the case of an ordered material). The total field is the sum of the applied field and the field due to all other dipoles in the sample, i.e. the energy of the dipole at $\mathbf{r} = \mathbf{0}$ is

$$U(\mathbf{0}) = -\mathbf{p} \cdot \mathbf{E}_{\text{cell}}(\mathbf{0}) = -\mathbf{p} \cdot \mathbf{E}_0 - \sum_{r_i \neq 0} \left[3\frac{(\mathbf{p} \cdot \mathbf{r}_i)^2}{r_i^5} - \frac{p^2}{r_i^3} \right] \tag{1.6}$$

Introducing the cut and applying a continuous approximation for the macroscopic contribution of the dipoles outside the sphere, we get

$$U(\mathbf{0}) = -\mathbf{p} \cdot \mathbf{E}_0 - \sum_{r_i < R_C} \left[3\frac{(\mathbf{p} \cdot \mathbf{r}_i)^2}{r_i^5} - \frac{p^2}{r_i^3} \right] - \int_{\text{sphere}}^{\text{sample}} \left[3\frac{(\mathbf{p} \cdot \mathbf{r})^2}{r^5} - \frac{p^2}{r^3} \right] \frac{d\mathbf{r}}{\Omega} \tag{1.7}$$

Ω is the volume per dipole moment, and defining z to be along the direction of the dipole moments of length $p = P\Omega$, the lattice sum may be written

$$\sum_{r_i < R_C} \left[3\frac{(\mathbf{p} \cdot \mathbf{r}_i)^2}{r_i^5} - \frac{p^2}{r_i^3} \right] = pP\Omega \sum_{r_i < R_C} \frac{3z_i^2 - x_i^2 - y_i^2 - z_i^2}{(x_i^2 + y_i^2 + z_i^2)^{5/2}} = pP\xi \tag{1.8}$$

The field $P\xi$ due to the lattice sum vanishes by symmetry in the case of a cubic system. This is true no matter the direction of the z axis compared to the lattice vectors, but it is only true when the cutting surface is that of a sphere (the reason for making the cut of this shape). If the system is not cubic, the lattice sum may be calculated straightforwardly by numerical methods as it converges quite rapidly. The macroscopic contribution is

$$\begin{aligned} \int_{\text{sphere}}^{\text{sample}} \left[3\frac{(\mathbf{p} \cdot \mathbf{r})^2}{r^5} - \frac{p^2}{r^3} \right] \frac{d\mathbf{r}}{\Omega} &= -pP \int_{\text{sphere}}^{\text{sample}} \nabla \cdot \left(\frac{\mathbf{z}}{r^3} \right) d\mathbf{r} \\ &= pP \int_{\text{sphere}} \frac{\mathbf{z} \cdot d\mathbf{S}}{r^3} - pP \int_{\text{sample}} \frac{\mathbf{z} \cdot d\mathbf{S}}{r^3} = pP \left(\frac{4\pi}{3} - \mathcal{N}_{zz} \right) \end{aligned} \tag{1.9}$$

The first surface integral (over the sphere) is calculated straightforwardly using $\mathbf{z} \cdot d\mathbf{S} = r\cos\theta(2\pi r^2 \sin\theta d\theta)\cos\theta$ in spherical coordinates. The last integral over the surface of the sample depends on the shape of the ellipsoid. It is $4\pi/3$ in case it is a sphere, but, in general, it is a number between 0 (long thin cigar along the z axis) and 4π (flat pancake). Combining the results above, the total field is found to be

$$\mathbf{E}_{\text{cell}} = \mathbf{E}_0 + \left(\bar{\bar{\xi}} + \frac{4\pi}{3} - \bar{\bar{\mathcal{N}}} \right) \mathbf{P} = \mathbf{E} + \left(\bar{\bar{\xi}} + \frac{4\pi}{3} \right) \mathbf{P} \tag{1.10}$$

The second expression derives from that the internal electric field is $\mathbf{E} = \mathbf{E}_0 - \bar{\bar{\mathcal{N}}}\mathbf{P}$, and this way of writing the result is of more general applicability, since it also applies when the surface charges are not determined alone by the homogeneous polarization of the bulk material. Introducing $\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P} = \bar{\bar{\epsilon}}\mathbf{E}$, then the permittivity $\bar{\bar{\epsilon}}$ is a material parameter, which is independent of the shape of the system. Introducing the polarization coefficient α by $\mathbf{p} = \bar{\bar{\alpha}}\mathbf{E}_{\text{cell}}$ and assuming all tensors $\bar{\bar{\epsilon}}$, $\bar{\bar{\xi}}$, and $\bar{\bar{\alpha}}$ to be diagonal, we get the Clausius–Mossotti relation (valid for each of the three diagonal components)

$$\epsilon = \frac{3 + (8\pi - 3\xi)n\alpha}{3 - (4\pi + 3\xi)n\alpha} \tag{1.11}$$

Magnetic energy and domains

In order to derive the magnetic energy of a macroscopic sample of microscopic dipoles or of supercurrent loops in a superconductor, we start out with the classical description of the fields. Introducing the magnetic $\mathbf{H}$ field, the Maxwell equations to be considered are

$$\nabla \times \mathbf{H} = \frac{4\pi}{c}\mathbf{j}_{\text{ext}} + \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t}\,, \qquad \nabla \cdot \mathbf{B} = 0 \tag{2.1}$$

where

$$\mathbf{B} = \mathbf{H} + 4\pi\mathbf{M}\,, \qquad \nabla \cdot \mathbf{H} = -4\pi\nabla \cdot \mathbf{M} \tag{2.2}$$

The sample is assumed to be placed in a uniform applied field $\mathbf{B}_0 = \mathbf{H}_0$, and the sources of the fields (the external currents) are assumed to lie outside the reach of the fields $\mathbf{B}_d$ and $\mathbf{H}_d$ produced by the sample. The total fields are

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_d, \quad \mathbf{B} = \mathbf{B}_0 + \mathbf{B}_d, \quad \mathbf{B}_d = \mathbf{H}_d + 4\pi\mathbf{M} \tag{2.3}$$

The magnetic energy of the sample is the total magnetic energy minus the magnetic energy of the space without the sample:

$$U = \frac{1}{4\pi}\int_{\text{all space}}\left[\int \mathbf{H}\cdot\delta\mathbf{B} - \tfrac{1}{2}H_0^2\right]d\mathbf{r} \tag{2.4}$$

As shown in the appendix, $\int_{\text{all space}}\mathbf{H}_0\cdot\mathbf{B}_d\,d\mathbf{r} = \int_{\text{all space}}\mathbf{H}_d\cdot\mathbf{B}_d\,d\mathbf{r} = 0$, and the magnetic energy reduces to

$$U = \int_{\text{sample}}\left[-\mathbf{M}\cdot\mathbf{H}_0 - \tfrac{1}{2}\mathbf{M}\cdot\mathbf{H}_d + \int\mathbf{H}\cdot\delta\mathbf{M}\right]d\mathbf{r} = -\int_{\text{sample}}\left[\int\mathbf{M}\cdot\delta\mathbf{H}_0\right]d\mathbf{r} \tag{2.5}$$

Two things are worth to be noticed. The energy only involves an integration over the space occupied by the sample (where $\mathbf{M}$ is non-zero), and the applied field $\mathbf{H}_0$ is the independent variable in the final expression. This is in accordance with the experimental situation and is in contrast with the original expression (2.4), which involves $\mathbf{B}$ as the independent variable. The magnetic energy U is equal the magnetic contribution F_M to the free energy of the sample, and

$$f_M(\mathbf{r}) = -\int_0^{\mathbf{H}_0}\mathbf{M}(\mathbf{r},\mathbf{H}_0')\cdot d\mathbf{H}_0'\,, \qquad F_M = \int_{\text{sample}}f_M(\mathbf{r})d\mathbf{r} \tag{2.6}$$

is of general applicability.

If a homogeneous sample in the shape of an ellipsoid is placed in a uniform field, then the magnetization $\mathbf{M}$ is constant throughout the sample. The Maxwell equations imply that the magnetic field within the sample, i.e. the internal field, is reduced from the applied field by the "demagnetization field" $\overline{\overline{\mathcal{N}}}\mathbf{M}$, or that $\mathbf{H}_d = -\overline{\overline{\mathcal{N}}}\mathbf{M}$, or

$$\mathbf{H} = \mathbf{H}_i = \mathbf{H}_0 - \overline{\overline{\mathcal{N}}}\mathbf{M}\,, \qquad \mathbf{B} = \mathbf{B}_i = \mathbf{H}_0 - \overline{\overline{\mathcal{N}}}\mathbf{M} + 4\pi\mathbf{M} \tag{2.7}$$

inside the sample. The demagnetization tensor $\overline{\overline{\mathcal{N}}}$ is the same one as introduced in the case of an electric polarization, and it is diagonal with respect to the

main axes of an ellipsoid. Assuming the field and thus also the magnetization along a main axis z, then the demagnetization field is determined by $\mathcal{N}_{zz}$, which is a number lying between 0 (long thin needle along z) and 4π (thin disk perpendicular to z). In the latter case the internal magnetic induction is the same as the applied one $\mathbf{B} = \mathbf{B}_0$ reflecting that all the magnetic field lines of each individual magnetic moment are looping back through the sample.

Returning to the first expression in (2.5) for the magnetic energy, then the integration of $\mathbf{H}$ with respect to $\mathbf{M}$ requires a knowledge of the relation between the magnetization of the sample and the internal magnetic field. Introducing the characteristic material parameter, the magnetic susceptibility tensor (at zero field)

$$\chi_{\alpha\beta} \equiv \frac{\partial M_\alpha}{\partial H_\beta}\bigg|_{\mathbf{H}=\mathbf{0}} \tag{2.8}$$

we get in the uniform case

$$u = \frac{1}{V}U = -MH_0 + \tfrac{1}{2}\mathcal{N}_{zz}M^2 + \tfrac{1}{2}\chi_{zz}H^2 = -\tfrac{1}{2}MH_0 \tag{2.9}$$

when assuming the field and magnetization along z (as long as $M = \chi_{zz}H$).

The magnetization of a uniform sample of microscopic dipoles is

$$\mathbf{M} = \frac{1}{V}\sum_i \vec{\mu}_i \tag{2.10}$$

If these magnetic dipoles are only coupled mutually by the classical dipole field, then we may calculate the energy directly in the same way as in the case of electric dipoles (the $\mathbf{P}$ and $\mathbf{M}$ fields are equivalent and $\mathbf{E}$ corresponds to $\mathbf{H}$ not to $\mathbf{B}$). The energy of a dipole moment $\vec{\mu}$ placed in the middle of the sample is:

$$U(\mathbf{r} = \mathbf{0}) = -\vec{\mu} \cdot \mathbf{H}_{\text{cell}} = -\vec{\mu} \cdot \left(\mathbf{H}_0 + \sum_i \frac{3\mathbf{r}_i(\vec{\mu}_i \cdot \mathbf{r}_i) - \vec{\mu}_i r_i^2}{r_i^5} \right) \tag{2.11}$$

and using the procedure explained in the previous section on "the dipole moment", we get

$$\mathbf{H}_{\text{cell}} = \mathbf{H}_0 + \left(\bar{\bar{\xi}} + \frac{4\pi}{3} \right)\mathbf{M} - \overline{\overline{\mathcal{N}}}\langle\mathbf{M}\rangle = \mathbf{H} + \left(\bar{\bar{\xi}} + \frac{4\pi}{3} \right)\mathbf{M} \tag{2.12}$$

In the paramagnetic phase there is only one domain, and defining a "non-interacting" susceptibility χ_0 (the susceptibility when the dipole field is neglected) by $M = \chi_0 H_{\text{cell}}$, we get

$$\chi = \frac{M}{H} = \frac{\chi_0}{1 - (\frac{4\pi}{3} + \xi)\chi_0}, \qquad H = \frac{H_0}{1 + \mathcal{N}\chi} \tag{2.13}$$

Systems exist where this susceptibility diverges at a sufficiently low temperature T_C, i.e. where $[(4\pi/3) + \xi]\chi_0 \to 1$, in which case the system is a ferromagnet below T_C, an ordering produced exclusively by the classical dipole–dipole interaction (one example is LiHoF$_4$ where $T_C = 1.5$ K).

In the other extreme case of a ferromagnet, $|\vec{\mu}|$ and hence $|\mathbf{M}| = M$ is a constant. Introducing this in (2.11) and (2.12) and summing over all sites, the average energy density is found to be

$$u = -\langle M_z \rangle H_0 + \tfrac{1}{2}\mathcal{N}_{zz}\langle M_z \rangle^2 - \tfrac{1}{2}\left(\frac{4\pi}{3} + \xi\right)M^2 \qquad (2.14)$$

Here $\langle M_z \rangle$ is the magnetization, along the direction of the applied field, averaged over the sample, which average is equal to M if there is only one domain. In terms of this average, the expression is of general validity, since it is the dipolar energy density of the sample also in the presence of many different domains (the cutting sphere is assumed to lie within one domain with the magnetization $|\mathbf{M}| = M$). The minimization of (2.14) with respect to $\langle M_z \rangle$ leads to

$$\langle M_z \rangle = \frac{H_0}{\mathcal{N}_{zz}} \quad \text{and} \quad H = 0\,, \quad \text{when} \quad H_0 < \mathcal{N}_{zz}M \qquad (2.15)$$

and

$$\langle M_z \rangle = M \quad \text{and} \quad H = H_0 - \mathcal{N}_{zz}M\,, \quad \text{when} \quad H_0 > \mathcal{N}_{zz}M \qquad (2.16)$$

The magnetization rises linearly with H_0 and attains the saturation value M when $H_0 = H_d = \mathcal{N}_{zz}M$. The internal field is the most natural choice for the field variable when investigating the material parameters of the sample, as used in the definition of χ in (2.8). In terms of H the magnetization is a step function, $\langle M_z \rangle = M$ as soon as H is non-zero.

In this account we have neglected the energy cost due to the domain walls between the different domains. This energy cost should be included in a realistic model together with a more direct evaluation of the demagnetization field, which would change from one domain to the next. However, if the domain walls are easily created as is the case if the magnetic anisotropy is weak, the simple averaging of the domain effects is acceptable. In the case of hard magnetic systems (large magnetic anisotropy) the situation is complicated and irreversible hysteresis phenomena become important (permanent magnets).

In most magnetic material the classical dipole–dipole interaction is weak compared to other "two-ion interactions" (exchange interactions), and the difference between χ_0 and χ in (2.13) may safely be neglected. However, the long range nature of the coupling implies that it is important, in most cases, to account for the demagnetization field, i.e. to realize that the internal field is $H = H_0 - \mathcal{N}_{zz}\langle M_z \rangle$, and that the system may possibly be divided into different domains. The approximative inclusion of the dipole–dipole interaction, where $\chi \simeq \chi_0$, corresponds to the use of $\mathbf{H}_{\text{cell}} \simeq \mathbf{H}$ in (2.11), and thus that the energy of the dipole moment $\vec{\mu}$ is $U(\mathbf{r} = \mathbf{0}) \simeq -\vec{\mu} \cdot \mathbf{H}$. – Hence, when focussing on the material parameters or the principal behaviour of a certain system, we normally assume that we are left with only one magnetic domain and that the magnetic field variable is the internal field $\mathbf{H}$. The thermodynamic quantities are then derived from the partition function Z according to

$$F = -k_B T \ln Z\,, \quad S = -\frac{\partial F}{\partial T}\,, \quad U = F + TS \qquad (2.17)$$

and

$$\mathbf{M} = -\frac{1}{V}\frac{\partial F}{\partial \mathbf{H}}\,, \quad \chi_{\alpha\beta} = -\frac{1}{V}\frac{\partial^2 F}{\partial H_\alpha H_\beta}\,, \quad C = \frac{\partial U}{\partial T} = T\frac{\partial S}{\partial T} \qquad (2.18)$$

where the expressions for $\mathbf{M}$ and χ are the results derived from (2.7) and (2.8), when approximating $\mathbf{H}_0$ by $\mathbf{H}$ in (2.7). The thermodynamic magnetization derived from the free energy is actually the one, which determines what are the microscopic dipoles in (2.10).

In the mean-field approximation the interactions between the magnetic moments are replaced by effective fields acting on the single moments and $\mathcal{H} = \sum_l \mathcal{H}_l$ as for non-interacting moments. In this case, the partition function $\mathcal{Z} = \prod Z_l$ ($= Z^N$ for a uniform system) and all thermodynamic quantities are derived from the partition functions of the single moments. Determining the n eigenstates and eigenvalues of the Hamiltonian for the lth site we may introduce the population factor p_i of the ith level

$$\mathcal{H}_l|i\rangle = \varepsilon_i|i\rangle\,, \qquad p_i = \frac{e^{-\beta\varepsilon_i}}{Z_l}\,, \qquad \sum_{i=1}^{n} p_i = 1 \qquad (k_B T = 1/\beta) \qquad (2.19)$$

where the last identity follows from $Z_l = \sum_i e^{-\beta\varepsilon_i}$. The ith population factor is the probability that the ith level is occupied. Immediate consequences of this interpretation of p_i are

$$U = N\langle\mathcal{H}_l\rangle = N\sum_{i=1}^{n}\varepsilon_i p_i \qquad (2.20)$$

and

$$M_\alpha = \frac{N}{V}\langle\mu_\alpha\rangle = \frac{N}{V}\sum_{i=1}^{n}\langle i|\hat{\mu}_\alpha|i\rangle\, p_i \qquad (2.21)$$

which results agree with those obtained from the thermodynamic definitions and relations (see the solution to HS's problem 4).

Appendix

The Maxwell equations are

$$\nabla \cdot \mathbf{D} = 4\pi\rho_{\text{ext}} \qquad , \qquad \nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} \qquad , \qquad \nabla \times \mathbf{H} = \frac{4\pi}{c}\mathbf{j}_{\text{ext}} + \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} \qquad (a.1)$$

where

$$\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P} \qquad , \qquad \mathbf{B} = \mathbf{H} + 4\pi\mathbf{M}$$

$$\nabla \cdot \mathbf{P} = -\rho_{\text{int}} \qquad , \qquad c\,\nabla \times \mathbf{M} + \frac{\partial \mathbf{P}}{\partial t} = \mathbf{j}_{\text{int}} \qquad (a.2)$$

The work done by the "surroundings" on the system (a certain volume in space) derives exclusively from the current density $\mathbf{j}_{\text{ext}}$ applied in the outside world, and the energy gain of the system is

$$\delta U = -\int d\mathbf{r}\,(\mathbf{j}_{\text{ext}} \cdot \mathbf{E})\,\delta t = -\int d\mathbf{r}\left(\frac{c}{4\pi}\nabla \times \mathbf{H} - \frac{1}{4\pi}\frac{\partial \mathbf{D}}{\partial t}\right) \cdot \mathbf{E}\,\delta t \qquad (a.3)$$

The second term is the electric part of the energy (when $\rho_{\text{ext}} = 0$):

$$\delta U_E = \frac{1}{4\pi} \int d\mathbf{r} \, \frac{\partial \mathbf{D}}{\partial t} \cdot \mathbf{E} \, \delta t = \frac{1}{4\pi} \int d\mathbf{r} \, \mathbf{E} \cdot \delta \mathbf{D} \qquad (a.4)$$

whereas the first term in $(a.3)$ is the magnetic energy part δU_M. Using the identity $\nabla \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot \nabla \times \mathbf{a} - \mathbf{a} \cdot \nabla \times \mathbf{b}$, we get

$$\delta U_M = -\int d\mathbf{r} \frac{c}{4\pi} \Big[\mathbf{H} \cdot \nabla \times \mathbf{E} + \nabla \cdot (\mathbf{H} \times \mathbf{E}) \Big] \delta t \qquad (a.5)$$

Due to the divergence theorem of Gauss, the second volume integral over "all space" may be written as an integral of $\mathbf{H} \times \mathbf{E}$ over a closed surface lying infinitely far away from the system and its surroundings. Here all fields vanish and the second integral is zero, which implies that

$$\delta U_M = -\int d\mathbf{r} \, \mathbf{H} \cdot \nabla \times \mathbf{E} \, \delta t = \frac{1}{4\pi} \int d\mathbf{r} \, \mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} \, \delta t = \frac{1}{4\pi} \int d\mathbf{r} \, \mathbf{H} \cdot \delta \mathbf{B} \qquad (a.6)$$

According to equation (2.3), the magnetic fields $\mathbf{H}_d$ and $\mathbf{B}_d = \mathbf{H}_d + 4\pi \mathbf{M}$, are the fields produced by a magnetic sample. The fields within the sample are given by (2.7) (in the homogeneous case). Outside the sample $\mathbf{M} = \mathbf{0}$ and $\mathbf{B}_d = \mathbf{H}_d$, but this field is not easy to calculate. It is clear from Maxwell equations that $\nabla \cdot \mathbf{B}_d = 0$ and also $\nabla \times \mathbf{H}_d = \mathbf{0}$, since $\nabla \times \mathbf{H}_0$ accounts for all the external currents. Because $\nabla \times \mathbf{H}_d = \mathbf{0}$ it is possible to determine a potential field ψ so that $\mathbf{H}_d = -\nabla \psi$. Hence

$$\int_{\text{all space}} \mathbf{H}_d \cdot \mathbf{B}_d \, d\mathbf{r} = -\int \nabla \psi \cdot \mathbf{B}_d \, d\mathbf{r} = -\int \big[\nabla \cdot (\psi \mathbf{B}_d) - \psi \nabla \cdot \mathbf{B}_d \big] \, d\mathbf{r}$$
$$= -\int \nabla \cdot (\psi \mathbf{B}_d) \, d\mathbf{r} = -\lim_{r \to \infty} \int_{\text{surface}} \psi \, \mathbf{B}_d \cdot d\mathbf{S} = 0 \qquad (a.7)$$

because $\psi \mathbf{B}_d$ must become vanishing small sufficiently far away from the sample ($\psi \, B_d \propto r^{-5}$ for a dipole field). By the same arguments, the integral where $\mathbf{H}_d$ is replaced by $\mathbf{H}_0$ is also found to be vanishing small. Now $\nabla \times \mathbf{H}_0$ is not zero, but it is sensible to assume that the applied field is generated by currents $\mathbf{j}_{\text{ext}}$ "outside" the space where $\mathbf{B}_d$ is of any importance, or that the surface integral has vanished before $\nabla \times \mathbf{H}_0 = \mathbf{0}$ is violated.

Introducing $\delta \mathbf{B} = \delta (\mathbf{H} + 4\pi \mathbf{M})$ in $(a.6)$, then

$$U_M = \frac{1}{4\pi} \int d\mathbf{r} \int \mathbf{H} \cdot \delta \left(\mathbf{H} + 4\pi \mathbf{M} \right) = \frac{1}{8\pi} \int d\mathbf{r} \, H^2 + \int d\mathbf{r} \int \mathbf{H} \cdot \delta \mathbf{M} \qquad (a.8)$$

where

$$\frac{1}{8\pi} \int d\mathbf{r} \, H^2 = \frac{1}{8\pi} \int d\mathbf{r} \left[H_0^2 + 2\mathbf{H}_0 \cdot \mathbf{H}_d + H_d^2 \right]$$
$$= \frac{1}{8\pi} \int d\mathbf{r} \left[H_0^2 + 2\mathbf{H}_0 \cdot (\mathbf{B}_d - 4\pi \mathbf{M}) + \mathbf{H}_d \cdot (\mathbf{B}_d - 4\pi \mathbf{M}) \right] \qquad (a.9)$$
$$= \frac{1}{8\pi} \int d\mathbf{r} \, H_0^2 - \int d\mathbf{r} \left(\mathbf{M} \cdot \mathbf{H}_0 + \tfrac{1}{2} \mathbf{M} \cdot \mathbf{H}_d \right)$$

introducing this result in $(a.8)$, we get the expression for the magnetic energy of the sample given by (2.5), when subtracting the background energy.

Pauli paramagnetism

Figure 25.3 in Marder (p. 718 or p. 770) may easily be misunderstood (he has just changed the numbers of spin-up and spin-down electrons without moving the electronic bands up or down). Replace it by the following figure:
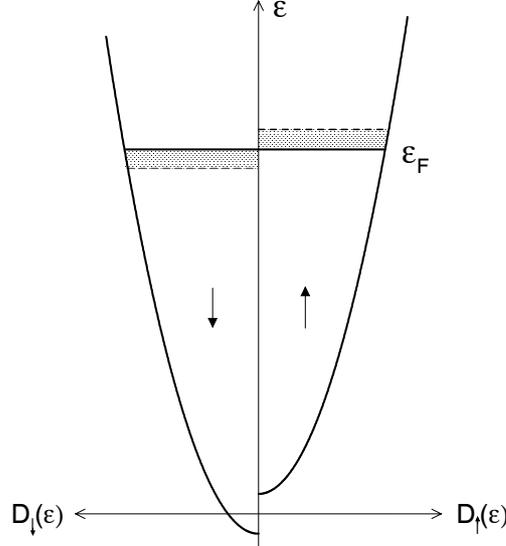
The Hamiltonian for the band electrons are changed, when applying a field along the z axis, $\mathbf{H} = (0, 0, H)$:

$$\Delta \mathcal{H} = \sum_i 2\mu_{\mathrm{B}} \mathbf{H} \cdot \mathbf{s}_i = \sum_i \mu_{\mathrm{B}} H \sigma_z(i) \tag{3.1}$$

implying that the spin-up and spin-down bands are shifted rigidly up and down by an equal amount:

$$\varepsilon_\uparrow(\mathbf{q}) = \varepsilon(\mathbf{q}) + \Delta \,, \qquad \varepsilon_\downarrow(\mathbf{q}) = \varepsilon(\mathbf{q}) - \Delta \,, \qquad \Delta = \mu_{\mathrm{B}} H \tag{3.2}$$

The Fermi energy is common for the spin-up and spin-down electrons, and the spin-up electrons in the cross-hatched area on the figure are removed and appear instead as spin-down electrons in the corresponding cross-hatched spin-down area. To a first approximation the small changes of the total density of states between ε_{F} and $\varepsilon_{\mathrm{F}} \pm \Delta$ may be neglected (at least in the limit of $H \to 0$), and the two spin-components of the density of states:

$$D_\uparrow(\varepsilon) = \tfrac{1}{2} D(\varepsilon - \Delta) \,, \qquad D_\downarrow(\varepsilon) = \tfrac{1}{2} D(\varepsilon + \Delta) \tag{3.3}$$

may both be approximated with $\frac{1}{2} D(\varepsilon_{\mathrm{F}})$ at $\varepsilon = \varepsilon_{\mathrm{F}}$. This means that, at zero temperature, the field-induced magnetization of the band electrons is

$$M = \mu_{\mathrm{B}}(n_\downarrow - n_\uparrow) \simeq \mu_{\mathrm{B}} \left(D_\downarrow(\varepsilon_{\mathrm{F}})\Delta + D_\uparrow(\varepsilon_{\mathrm{F}})\Delta \right) \simeq \mu_{\mathrm{B}} D(\varepsilon_{\mathrm{F}})\Delta = \mu_{\mathrm{B}}^2 D(\varepsilon_{\mathrm{F}})H \tag{3.4}$$

or that the zero-temperature susceptibility is

$$\chi = \frac{M}{H} = \mu_{\mathrm{B}}^2 D(\varepsilon_{\mathrm{F}}) \tag{3.5}$$

The Hall effect

Marder has made a few mistakes in his discussion of the Hall effect: Figure 17.5 is showing the orbits in $\vec{k}$-space (reciprocal space), and assuming $\vec{B}$ to point out of the page, then the k-vector of the electron-like orbit moves the opposite way of what is shown in the figure to the left.

The derivation of the Hall effect, in section 17.4.8, does not account for that the velocities of most of the electrons are only weakly perturbed by the magnetic field. The more accurate treatment of the Boltzmann equation referred to the problem 17.9, leads to the result that

$$\overline{\overline{\rho}} = \frac{1}{\sigma_0} \begin{pmatrix} 1 & -\mathcal{R}B\sigma_0 & 0 \\ \mathcal{R}B\sigma_0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \sigma_0 = \frac{ne^2\tau}{m^*} \tag{4.1}$$

in the case of $\mathbf{B} = (0, 0, B)$. The resistivity tensor $\overline{\overline{\rho}} = (\overline{\overline{\sigma}})^{-1}$ is defined by $\mathbf{E} = \overline{\overline{\rho}}\mathbf{j}$, see Eq. (17.98). In order to get this result, the band mass tensor has to be isotropic (equals to m^* times the unit matrix).

Inverting the resistivity tensor one finds

$$\overline{\overline{\sigma}} = \frac{\sigma_0}{1 + (\mathcal{R}B\sigma_0)^2} \begin{pmatrix} 1 & \mathcal{R}B\sigma_0 & 0 \\ -\mathcal{R}B\sigma_0 & 1 & 0 \\ 0 & 0 & 1 + (\mathcal{R}B\sigma_0)^2 \end{pmatrix} \tag{4.2}$$

In the limit of $|\mathcal{R}B\sigma_0| \gg 1$ then $\overline{\overline{\sigma}}$ has the same B dependence as given by Eq. (17.99), but $\mathcal{R}$ should be placed in the denominators, rather than in the numerators, of the different matrix elements in Eq. (17.99):

$$\overline{\overline{\sigma}} = \begin{pmatrix} \dfrac{1}{\mathcal{R}^2 B^2 \sigma_0} & \dfrac{1}{\mathcal{R}B} & 0 \\ -\dfrac{1}{\mathcal{R}B} & \dfrac{1}{\mathcal{R}^2 B^2 \sigma_0} & 0 \\ 0 & 0 & \sigma_0 \end{pmatrix}, \qquad |\mathcal{R}B\sigma_0| \gg 1 \tag{4.3}$$

The Ginzburg–Landau free energy

The "Landau–Ginzburg" free energy presented by Marder in Eq. (27.27) is derived from the total magnetic contribution to the free energy density:

$$\mathcal{F}_M = \frac{1}{4\pi} \int \frac{d\vec{r}}{V} \left[\int \vec{H} \cdot \delta\vec{B} \right] = \frac{1}{8\pi} \int \frac{d\vec{r}}{V} B^2 - \int \frac{d\vec{r}}{V} \left[\int \vec{M} \cdot \delta\vec{B} \right] \qquad (5.1)$$

by the use of $\vec{B} = \vec{H} + 4\pi\vec{M}$. Introducing the vector potential, $\vec{B} = \nabla \times \vec{A}$ and applying the vector identity $\nabla \cdot (\vec{a} \times \vec{b}) = \vec{b} \cdot \nabla \times \vec{a} - \vec{a} \cdot \nabla \times \vec{b}$, the last integral may be written

$$\int \frac{d\vec{r}}{V} \left[\int \vec{M} \cdot \delta\vec{B} \right] = \int \frac{d\vec{r}}{V} \left[\int \vec{M} \cdot \nabla \times \delta\vec{A} \right] =$$
$$\int \frac{d\vec{r}}{V} \left[\int \delta\vec{A} \cdot \nabla \times \vec{M} \right] - \int \frac{d\vec{r}}{V} \nabla \cdot \left[\int (\vec{M} \times \delta\vec{A}) \right] = \int \frac{d\vec{r}}{V} \left[\int \delta\vec{A} \cdot \nabla \times \vec{M} \right]$$
$$(5.2)$$

Because of Gauss theorem, the integral of the divergence may be written as an integral over a surface outside the sample, where $\vec{M} = \vec{0}$, and this integral is zero. Introducing the internal current density $\vec{j}(\vec{r})$ of the sample, then $\nabla \times \vec{M} = \vec{j}/c$ and we finally get

$$\mathcal{F}_M = \int \frac{d\vec{r}}{V} \left[\frac{1}{8\pi} B^2 - \frac{1}{c} \int \vec{j} \cdot \delta\vec{A} \right] \qquad (5.3)$$

in agreement with the magnetic part of $\mathcal{F}$ in Eq. (27.27), when introducing the superconducting current given by Eq. (27.29a). Formally, this expression is right, but one has to be careful with the integration of B^2 as the integral should really be performed over "all space" (the field outside the sample is modified when $\vec{M}$ is non-zero). Furthermore, the independent variable in (5.3) is $\vec{B}$, whereas the actual one is the applied field, and in order to change variable one has to perform a Legendre transformation:

$$\tilde{\mathcal{G}}_M = \mathcal{F}_M - \frac{1}{4\pi} \int \frac{d\vec{r}}{V} \vec{H} \cdot \vec{B} = -\frac{1}{4\pi} \int \frac{d\vec{r}}{V} \left[\int \vec{B} \cdot \delta\vec{H} \right] \qquad (5.4)$$

Both the two complications are circumvented by applying instead the magnetic energy expression (2.6) derived in the section "Magnetic energy and domains":

$$\mathcal{G}_M = - \int \frac{d\vec{r}}{V} \left[\int \vec{M} \cdot \delta\vec{H} \right] \qquad \left(= \tilde{\mathcal{G}}_M + \frac{1}{8\pi} \int \frac{d\vec{r}}{V} H^2 \right) \qquad (5.5)$$

The integrand in (5.5) is only non-zero within the sample and $\vec{H}$ is the independent variable. [Here and in (5.4), we neglect the extra complication discussed in problem 27.1, that the internal field $\vec{H} = \vec{H}_i$ may differ from the applied one. Since the derivation of this energy does not involve a Legendre transformation, one may argue that this is the "Helmholtz" ($\mathcal{F}_M$) and not the "Gibbs" ($\mathcal{G}_M$) free energy]. Using (5.5) rather than (5.1) as the starting point then (5.3) is replaced by

$$\mathcal{G}_M = \int \frac{d\vec{r}}{V} \left[\int \vec{M} \cdot \delta(4\pi\vec{M}) - \int \vec{M} \cdot \delta\vec{B} \right] = \int \frac{d\vec{r}}{V} \left[2\pi M^2 - \frac{1}{c} \int \vec{j} \cdot \delta\vec{A} \right] \quad (5.6)$$

Hence, the only difference is that $B^2/(8\pi)$ in the Ginzburg–Landau free energy expression Eq. (27.27) is being replaced by $2\pi M^2$.

Henrik Smith's problems

HS's problem 1: Heat capacity of a two-dimensional electron gas.

We consider a two-dimensional gas of electrons in a GaAs/AlGaAs heterostructure. The areal density is $n = 10^{11}$ cm^{-2} and the dispersion relation of the electrons is given by

$$\varepsilon = \frac{\hbar^2 k^2}{2m^*}.$$

Here k is the magnitude of the two-dimensional wave vector and ε the single-particle energy. The quantity m^* is the effective mass, given by $m^* = 0.067\, m_e$, where m_e is the electron mass.

1) Calculate the heat capacity of the electron gas at the temperature $T = 1$ K, taking its area to be 1 cm^2.

2) Compare the value obtained in 1) with an estimate of the phonon contribution to the heat capacity for a GaAs crystal of volume 1 cm^3 at the same temperature – the Debye temperature of GaAs is $\theta_D = 344$ K. At what temperature are the two contributions equal to each other?

HS's problem 3: Hall effect of a two-dimensional electron gas.

In this problem we consider a two-dimensional electron gas with an anisotropic dispersion relation given by

$$\varepsilon_{\vec{k}} = \varepsilon = a(k_x^2 + k_y^2) + b(k_x^4 + k_y^4),$$

where a and b are constants that are taken to be positive.

1) Sketch a curve of constant energy and indicate the direction of the velocity $\vec{v}_{\vec{k}} = \partial \varepsilon_{\vec{k}} / \partial(\hbar\vec{k})$ at selected points on the curve.

2) We assume that the electric field points in the x direction, while the magnetic field is in the z direction, perpendicular the plane in which the electrons move. Show that the linearized Boltzmann equation in the relaxation-time approximation can be written as

$$-ev_x E \frac{\partial f}{\partial \varepsilon_{\vec{k}}} = \left[\frac{eB}{\hbar c}\left(v_y \frac{\partial}{\partial k_x} - v_x \frac{\partial}{\partial k_y} \right) - \frac{1}{\tau} \right](g - f)$$

where g is the distribution function and f its value in equilibrium.

3) When the magnetic field is sufficiently high, we may neglect the relaxation term $-(g-f)/\tau$. Show that the Boltzmann equation in this limit is satisfied by a solution of the form $g = f + k_y F(\varepsilon)$ and determine F. Find the ratio between the electric field and the current density j_y in the y direction, and show that its value can be expressed in terms of the number, n, of electrons per unit area.

HS's problem 4:   Localized atoms: heat capacity and magnetic susceptibility.

We consider N identical atoms which are localized at different sites in a lattice. The atoms are assumed to be non-interacting. The non-degenerate energy levels ε_i ($i = 1, 2, 3$) of an atom are assumed to be given by

$$\varepsilon_1 = -\Delta, \qquad \varepsilon_2 = 0, \qquad \varepsilon_3 = \Delta,$$

where Δ is a positive constant.

1) Determine the partition function Z and the internal energy U as a function of the temperature T.

2) In this and the following question we consider only the high temperature limit, $kT \gg \Delta$. Expand the partition function and calculate the internal energy, the free energy F and the entropy $\mathcal{S}$ to lowest non-trivial order in Δ. Determine the specific heat $C = \partial U / \partial T$ and show that the result agrees with the one obtained from $C = T \partial \mathcal{S} / \partial T$.

3) Determine the derivative of F with respect to Δ in the high-temperature limit. Assuming that Δ is proportional to the magnitude of an applied magnetic field, what is the physical significance of this derivative? Compare your result to (25.31) and explain the connection.

4) Find the leading contribution to C in the limit of low temperatures ($kT \ll \Delta$) and use this together with the result in 2) to sketch the specific heat as a function of temperature.

————————————