A. Annex

A.1. Magnetic Moment

A.1.1. Introduction

The magnetic moment plays a fundamental role in magnetism. Classically if an electrical current I forms a loop around an area $|\mathbf{dS}|$ it will create a magnetic moment

$$\mathbf{d}\boldsymbol{\mu} = I\mathbf{dS} \ , \tag{A.1}$$

with units $\mathrm{A} \cdot \mathrm{m}^2$. The length of $\mathbf{dS}$ is as usual equal to the area of the loop and the vector is normal to the loop and pointing to the direction defined by the current considering the right-hand rule. This object can be considered as a "magnetic dipole" in analogy to the elctrical one where two electric charges (positive and negative) are separated by a small distance along $\mathbf{dS}$. Here, of course, we do not have magnetic monopoles (magnetic charges) but the analogy is very good for long distances.

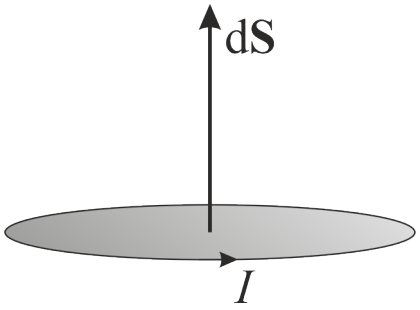

Figure A.1.: *A current forming a loop around an area will create a magnetic moment* $\mathbf{d}\boldsymbol{\mu}$*. The magnetic moment vector will point in the same direction as* $\mathbf{dS}$.

For a finite area, we can calculate the magnetic moment $\boldsymbol{\mu}$ by

$$\boldsymbol{\mu} = \int \mathbf{d}\boldsymbol{\mu} = \int I\mathbf{dS} \ . \tag{A.2}$$

A.1.2. Relation to the angular momentum

Broadly speaking, a classical extended object (e.g., the Earth) can possess two types of angular momentum. The first type is due to the rotation of the object's center of mass about some fixed external point (e.g., the Sun)-this is generally known as orbital angular momentum. The second type is due to the object's internal motion-this is generally known as spin angular momentum (since, for a rigid object, the internal motion consists of spinning about an axis passing through the center of mass). By analogy, quantum particles can possess both orbital angular momentum due to their motion through space, and spin angular momentum due to their internal motion. Actually, the analogy with classical extended objects is not entirely accurate, since electrons, for instance, are structureless point particles. In fact, in quantum mechanics, it is best to think of spin angular momentum as a kind of intrinsic angular momentum possessed by particles. It turns out that each type of elementary particle has a characteristic spin angular momentum, just as each type has a characteristic charge and mass.

A.1.2.1. Orbital angular momentum

Let first concentrate on a particle possessing no spin angular momentum. As the charges have a mass (even though very small), the orbital motion of the charges will also be associated to an angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$. The "gyromagnetic ratio" γ of a system is the ratio of its magnetic moment to its angular momentum, *i.e.*

$$\boldsymbol{\mu} = \gamma \mathbf{L} \ . \tag{A.3}$$

If we consider a charged body (charge q) rotating about an axis of symmetry, then (it its charge and mass are both distributed), its gyromagnetic ratio is

$$\gamma = \frac{q}{2m} \ . \tag{A.4}$$

This relation is obtained as follows. Suppose the ring has radius r, area $A = \pi r^2$, mass m, charge q, and angular momentum $L = mvr$ ($\mathbf{r}$ always perpendicular to the velocity). Then the value of the magnetic dipole moment is (remember that $I = dq/dt$ and we can write $I = q/T$, where T is the rotation period)

$$\mu = IA = \frac{qv}{2\pi r} \cdot \pi r^2 = \frac{q}{2m} \cdot mvr = \frac{q}{2m} L \ . \tag{A.5}$$

The Bohr atom model tells us that the angular momentum is quantified in units of $\hbar$ and therefore, if we write for the following equation that $\mathbf{L}$ is given in units of $[1/\hbar]$ and that the charge orbiting is an electron, it is natural to write

$$\boldsymbol{\mu} = -\frac{e\hbar}{2m} \mathbf{L} = -\mu_{\mathrm{B}} \mathbf{L} \ , \tag{A.6}$$

where we have defined the Bohr magneton as

$$\begin{aligned}\mu_{\mathrm{B}} &= \frac{e}{2m_{\mathrm{e}}}\hbar \\ &= 5{,}788\,381\,8012(26)\cdot 10^{-5}\,\mathrm{eV/T} \\ &= 9{,}274\,009\,994(57)\cdot 10^{-24}\,\mathrm{J/T\ or\ Am^2}\end{aligned} \tag{A.7}$$

We see that due to the negative charge of the electron its magnetic moment is always antiparallel to its angular momentum.

An electron with an angular quantum number $\ell = 1$, oriented parallel along the z-axis (magnetic quantum number $m_\ell = +1$), has a magnetic moment of $\mu_{\text{electron, }\ell=1} = -\mu_{\mathrm{B}}$.

A.1.2.2. Spin angular momentum

Above, we have omitted the spin angular momentum. Let see now its effect on the moment. The Eq. A.6 suggests that there may be a similar relationship between magnetic moment and spin angular momentum. We can write

$$\boldsymbol{\mu} = -\frac{g_e\, e\,\hbar}{2m_e}\mathbf{S}\,, \tag{A.8}$$

where g_e is called the *electron g-factor*. Classically, we would expect $g_e = 1$. In fact,

$$g_e = 2\left(1 + \frac{\alpha}{2\pi} + ...\right) = 2.0023192\,, \tag{A.9}$$

where $\alpha = e^2/(2\epsilon_0 hc) \simeq 1/137$ is the so-called *fine-structure constant*. The fact that the electron g_e-factor is (almost) twice that expected from classical physics is only explicable using relativistic quantum mechanics. Furthermore, the small corrections to the relativistic result $g_e = 2$ come from quantum field theory.

The eigenvalue of the z-component of the spin angular momentum are $S_z = \pm 1/2$. Therefore we have a value of the magnetic moment along the quantization axis

$$\mu_z = \mp\frac{g_e\, e\,\hbar}{2m}\cdot\frac{1}{2} = \mp\mu_{\mathrm{B}}\quad. \tag{A.10}$$

and here also the vector $\boldsymbol{\mu}$ is always antiparallel to the spin angular momentum.

A.2. Spin Angular Momentum

A.2.1. Spin Operators

Since spin is a type of angular momentum, it is reasonable to suppose that it possesses similar properties to orbital angular momentum. Thus, we would expect to be able to define three

operators-S_x, S_y, and S_z-which represent the three Cartesian components of spin angular momentum. Moreover, it is plausible that these operators possess analogous commutation relations to the three corresponding orbital angular momentum operators, L_x, L_y, and L_z. In other words,

$$[S_x, S_y] = i\hbar S_z \,, \tag{A.11}$$
$$[S_y, S_z] = i\hbar S_x \,, \tag{A.12}$$
$$[S_z, S_x] = i\hbar S_y \,. \tag{A.13}$$

We can represent the magnitude squared of the spin angular momentum vector by the operator

$$S^2 = S_x^2 + S_y^2 + S_z^2 \,. \tag{A.14}$$

One can demonstrate that:

$$[S^2, S_x] = [S^2, S_y] = [S^2, S_z] = 0 \,. \tag{A.15}$$

One thus conclude that one can simultaneously measure the magnitude squared of the spin angular momentum vector, together with, at most, one Cartesian component. By convention, we shall always choose to measure the z-component, S_z.

We can define raising and lowering operators for spin angular momentum:

$$S\pm = S_x \pm i S_y \,. \tag{A.16}$$

If S_x, S_y, and S_z are Hermitian operators, as must be the case if they are to represent physical quantities, then $S\pm$ are the Hermitian conjugates of one another: *i.e.*,

$$(S\pm)^\dagger = S\mp \,. \tag{A.17}$$

Finally, on can demonstrate that

$$S_+ S_- = S^2 - S_z^2 + \hbar S_z \,, \tag{A.18}$$
$$S_- S_+ = S^2 - S_z^2 - \hbar S_z \,, \tag{A.19}$$
$$[S_+, S_z] = -\hbar S_+ \,, \tag{A.20}$$
$$[S_-, S_z] = +\hbar S_- \,. \tag{A.21}$$

A.2.2. Spin Space

We now have to discuss the wavefunctions upon which the previously introduced spin operators act. Unlike regular wavefunctions, spin wavefunctions do not exist in real space. Likewise, the spin angular momentum operators cannot be represented as differential operators in real space. Instead, we need to think of spin wavefunctions as existing in an abstract (complex) vector space. The different members of this space correspond to the different internal configurations of the particle under investigation. Note that only the directions of our vectors have any physical significance (just as only the shape of a regular wavefunction has any physical significance). Thus, if the vector χ corresponds to a particular internal state

then $c\,\chi$ corresponds to the same state, where c is a complex number. Now, we expect the internal states of our particle to be superposable, since the superposability of states is one of the fundamental assumptions of quantum mechanics. It follows that the vectors making up our vector space must also be superposable. Thus, if χ_1 and χ_2 are two vectors corresponding to two different internal states then $c_1\,\chi_1 + c_2\,\chi_2$ is another vector corresponding to the state obtained by superposing c_1 times state 1 with c_2 times state 2 (where c_1 and c_2 are complex numbers). Finally, the dimensionality of our vector space is simply the number of linearly independent vectors required to span it (*i.e.*, the number of linearly independent internal states of the particle under investigation).

We now need to define the length of our vectors. We can do this by introducing a second, or *dual*, vector space whose elements are in one to one correspondence with the elements of our first space. Let the element of the second space which corresponds to the element χ of the first space be called $\chi^\dagger$. Moreover, the element of the second space which corresponds to $c\,\chi$ is $c^*\,\chi^\dagger$. We shall assume that it is possible to combine χ and $\chi^\dagger$ in a multiplicative fashion to generate a real positive-definite number which we interpret as the length, or *norm*, of χ. Let us denote this number $\chi^\dagger\chi$. Thus, we have

$$\chi^\dagger\chi \geq 0 \tag{A.22}$$

for all χ. We shall also assume that it is possible to combine unlike states in an analogous multiplicative fashion to produce complex numbers. The product of two unlike states χ and χ' is denoted $\chi^\dagger\chi'$. Two states χ and χ' are said to be mutually orthogonal, or independent, if $\chi^\dagger\chi' = 0$.

Now, when a general spin operator, A, operates on a general spin-state, χ, it converts it into a different spin-state which we shall denote $A\,\chi$. The dual of this state is $(A\,\chi)^\dagger \equiv \chi^\dagger A^\dagger$, where $A^\dagger$ is the Hermitian conjugate of A (this is the definition of an Hermitian conjugate in spin space). An eigenstate of A corresponding to the eigenvalue a satisfies

$$A\,\chi_a = a\,\chi_a\,. \tag{A.23}$$

If A corresponds to a physical variable then a measurement of A will result in one of its eigenvalues. In order to ensure that these eigenvalues are all real, A must be Hermitian: *i.e.*, $A^\dagger = A$. We expect the χ_a to be mutually orthogonal. We can also normalize them such that they all have unit length. In other words,

$$\chi_a^\dagger\,\chi_{a'} = \delta_{aa'}. \tag{A.24}$$

Finally, a general spin state can be written as a superposition of the normalized eigenstates of A: *i.e.*,

$$\chi = \sum_a c_a\,\chi_a\,. \tag{A.25}$$

A measurement of χ will then yield the result a with probability $|c_a|^2$.

A.2.3. Eigenstates of S_z and S^2

Since the operators S_z and S^2 commute, they must possess simultaneous eigenstate. Let these eigenstates take the form:

$$S_z \chi_{s,m_s} = m_s \hbar \chi_{s,m_s} , \tag{A.26}$$

$$S^2 \chi_{s,m_s} = s(s+1)\hbar^2 \chi_{s,m_s} . \tag{A.27}$$

Now, it is easily demonstrated, from the commutation relations A.20 and A.21, that

$$S_z (S_+ \chi_{s,m_s}) = (m_s + 1)\hbar (S_+ \chi_{s,m_s}) , \tag{A.28}$$

and

$$S_z (S_- \chi_{s,m_s}) = (m_s - 1)\hbar (S_- \chi_{s,m_s}) , \tag{A.29}$$

Thus, $S_+$and $S_-$are indeed the raising and lowering operators, respectively, for spin angular momentum. The eigenstates of S_z and S^2 are assumed to be orthonormal: *i.e.*,

$$\chi^\dagger_{s,m_s} \chi_{s',m_{s'}} = \delta_{ss'} \delta_{m_s m_{s'}} \tag{A.30}$$

Consider the wavefunction $\chi = S_+ \chi_{s,m_s}$. Since we know, from Eq. A.22, that $\chi^\dagger \chi \geq 0$, it follows that

$$(S_+ \chi_{s,m_s})^\dagger (S_+ \chi_{s,m_s}) = \chi^\dagger_{s,m_s} S^\dagger_+ S_+ \chi_{s,m_s} = \chi^\dagger_{s,m_s} S_- S_+ \chi_{s,m_s} = 0 , \tag{A.31}$$

where use has been made of Eq. A.17. Equations A.19, A.26, A.27, and A.30 yield

$$s(s+1) \geq m_s (m_s + 1) . \tag{A.32}$$

Likewise, if $\chi = S_- \chi_{s,m_s}$ then we obtain

$$s(s+1) \geq m_s (m_s - 1) . \tag{A.33}$$

Assuming that $s = 0$, the above two inequalities imply that

$$-s \leq m_s \leq s . \tag{A.34}$$

Hence, at fixed s, there is both a maximum and a minimum possible value that m_s can take. Let $m_{s,min}$ be the minimum possible value of m_s. It follows that

$$S_- \chi_{s,m_{s,min}} = 0 . \tag{A.35}$$

Now, from Eq. A.18,

$$S^2 = S_+ S_- + S_z^2 - \hbar S_z . \tag{A.36}$$

Hence,

$$S^2 \chi_{s,m_{s,min}} = (S_+ S_- + S_z^2 - \hbar S_z) \chi_{s,m_{s,min}} , \tag{A.37}$$

giving

$$s(s+1) = m_{s,min} (m_{s,min} - 1) . \tag{A.38}$$

Assuming that $m_{s,min} < 0$, this equation yields

$$m_{s,min} = -s \,. \tag{A.39}$$

Likewise, it is easily demonstrated that

$$m_{s,max} = +s \,. \tag{A.40}$$

Moreover,

$$S_-\chi_{s,-s} = S_+\chi_{s,s} = 0 \,. \tag{A.41}$$

Now, the raising operator S_+, acting upon $\chi_{s,-s}$, converts it into some multiple of $\chi_{s,-s+1}$. Employing the raising operator a second time, we obtain a multiple of $\chi_{s,-s+2}$. However, this process cannot continue indefinitely, since there is a maximum possible value of m_s. Indeed, after acting upon $\chi_{s,-s}$ a sufficient number of times with the raising operator S_+, we must obtain a multiple of $\chi_{s,s}$, so that employing the raising operator one more time leads to the null state (see Eq. A.41). If this is not the case then we will inevitably obtain eigenstates of S_z corresponding to $m_s > s$, which we have already demonstrated is impossible.

It follows, from the above argument, that

$$m_{s,max} - m_{s,min} = 2s = k \,, \tag{A.42}$$

where k is a positive integer. Hence, the quantum number s can either take positive integer or positive half-integer values. Up to now, our analysis has been very similar to that of the orbital angular momentum. Recall, that for orbital angular momentum the quantum number m, which is analogous to m_s, is restricted to take integer values. This implies that the quantum number l, which is analogous to s, is also restricted to take integer values. However, the origin of these restrictions is the representation of the orbital angular momentum operators as differential operators in real space. There is no equivalent representation of the corresponding spin angular momentum operators. Hence, we conclude that there is no reason why the quantum number s cannot take half-integer, as well as integer, values.

In 1940, Wolfgang Pauli proved the so-called *spin-statistics* theorem using relativistic quantum mechanics. According to this theorem, all *fermions* possess *half-integer spin* (*i.e.*, a half-integer value of s), whereas all *bosons* possess *integer spin* (*i.e.*, an integer value of s). In fact, all presently known fermions, including electrons and protons, possess spin *one-half*. In other words, electrons and protons are characterized by$s = 1/2$ and $m_s = \pm 1/2$.

A.2.4. Pauli Representation

Let us denote the two independent spin eigenstates of an electron as

$$\chi_\pm \equiv \chi_{1/2,\pm 1/2} \,. \tag{A.43}$$

It thus follows, from Eqs. A.26 and A.27, that

$$S_z\chi_\pm = \pm\frac{1}{2}\hbar\chi_\pm \,, \tag{A.44}$$

$$S^2\chi_\pm = \frac{3}{4}\hbar^2\chi_\pm \,. \tag{A.45}$$

Note that χ_+ corresponds to an electron whose spin angular momentum vector has a positive component along the z-axis. Loosely speaking, we could say that the spin vector points in the $+z$-direction (or its spin is "up"). Likewise, χ_- corresponds to an electron whose spin points in the $-z$-direction (or whose spin is "down"). These two eigenstates satisfy the orthonormality requirements

$$\chi_+^\dagger \chi_+ = \chi_-^\dagger \chi_- = 1 \,, \tag{A.46}$$

and

$$\chi_+^\dagger \chi_- = 0 \,. \tag{A.47}$$

A general spin state can be represented as a linear combination of χ_+ and χ_-: *i.e.*,

$$\chi = c_+ \chi_+ + c_- \chi_- . \tag{A.48}$$

It is thus evident that electron spin space is two-dimensional.

Up to now, we have discussed spin space in rather abstract terms. In the following, we shall describe a particular representation of electron spin space due to Pauli. This so-called *Pauli representation* allows us to visualize spin space, and also facilitates calculations involving spin. Let us attempt to represent a general spin state as a complex *column vector* in some two-dimensional space: *i.e.*,

$$\chi \equiv \begin{pmatrix} c_+ \\ c_- \end{pmatrix} . \tag{A.49}$$

The corresponding dual vector is represented as a *row vector*: *i.e.*,

$$\chi^\dagger \equiv \begin{pmatrix} c_+^* , c_-^* \end{pmatrix} . \tag{A.50}$$

Furthermore, the product $\chi^\dagger \chi$ is obtained according to the ordinary rules of matrix multiplication: *i.e.*,

$$\chi^\dagger \chi = \begin{pmatrix} c_+^* , c_-^* \end{pmatrix} \begin{pmatrix} c_+ \\ c_- \end{pmatrix} = c_+^* c_+ + c_-^* c_- = |c_+|^2 + |c_-|^2 \geq 0 \,. \tag{A.51}$$

Likewise, the product $\chi^\dagger \chi'$ of two different spin states is also obtained from the rules of matrix multiplication: *i.e.*,

$$\chi^\dagger \chi' = \begin{pmatrix} c_+^* , c_-^* \end{pmatrix} \begin{pmatrix} c'_+ \\ c'_- \end{pmatrix} = c_+^* c'_+ + c_-^* c'_- \,. \tag{A.52}$$

Note that this particular representation of spin space is in complete accordance with the discussion in Section A.2.2. For obvious reasons, a vector used to represent a spin state is generally known as *spinor*.

A general spin operator A is represented as a 2×2 matrix which operates on a spinor: *i.e.*,

$$A \chi = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} c_+ \\ c_- \end{pmatrix} . \tag{A.53}$$

As is easily demonstrated, the Hermitian conjugate of A is represented by the transposed complex conjugate of the matrix used to represent A: *i.e.*,

$$A^\dagger = \begin{pmatrix} A_{11}^* & A_{21}^* \\ A_{12}^* & A_{22}^* \end{pmatrix} . \tag{A.54}$$

Let us represent the spin eigenstates χ_+ and χ_- as

$$\chi_+ \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \tag{A.55}$$

and

$$\chi_- \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} , \tag{A.56}$$

respectively. Note that these forms automatically satisfy the orthonormality constraints A.46 and A.47. It is convenient to write the spin operators S_i (where $i = 1, 2, 3$ corresponds to x, y, z) as

$$S_i = \frac{\hbar}{2}\sigma_i . \tag{A.57}$$

Here, the σ_i are dimensionless 2×2 matrices. According to Eqs. A.11A.13, the σ_i satisfy the commutation relations

$$[\sigma_x, \sigma_y] = 2i\sigma_z , \tag{A.58}$$
$$[\sigma_y, \sigma_z] = 2i\sigma_x , \tag{A.59}$$
$$[\sigma_z, \sigma_x] = 2i\sigma_y . \tag{A.60}$$

Furthermore, Eq. A.44 yields

$$\sigma_z \chi_\pm = \pm\chi_\pm . \tag{A.61}$$

It is easily demonstrated, from the above expressions, that the σ_i are represented by the following matrices:

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \tag{A.62}$$

$$\sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \tag{A.63}$$

$$\sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{A.64}$$

Incidentally, these matrices are generally known as the *Pauli matrices*.

Finally, a general spinor takes the form

$$\chi = c_+\chi_+ + c_-\chi_- = \begin{pmatrix} c_+ \\ c_- \end{pmatrix} . \tag{A.65}$$

If the spinor is properly normalized then

$$\chi^\dagger \chi = |c_+|^2 + |c_-|^2 = 1 . \tag{A.66}$$

In this case, we can interpret $|c_+|^2$ as the probability that an observation of S_z will yield the result $+\hbar/2$, and $|c_-|^2$ as the probability that an observation of S_z will yield the result $-\hbar/2$.

A.2.5. Relating Spinor to Spin Direction

For a general spinor state

$$\chi = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}, \tag{A.67}$$

how do c_+ and c_- relate to the orientation of the spin?

Let us assume that spin is pointing along the unit vector

$$\hat{\mathbf{n}} = (n_x, n_y, n_z) = (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta) \tag{A.68}$$

i.e. in direction $(\theta,\ \phi)$ (θ is the angle with the z-axis and ϕ is the angle with the x-axis).

The spinor must be eigenstate of $\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}$ with eigenvalue unity (actually of $\hat{\mathbf{n}}\cdot\mathbf{S} = \frac{\hbar}{2}\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}$; the axis z is taken as the quantization axis and by doing $\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}$ we write the Pauli matrices along the direction of the spin).

$$\begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix}\begin{pmatrix} c_+ \\ c_- \end{pmatrix} = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}. \tag{A.69}$$

Therefore, we find that $c_+/c_- = (n_x - in_y)/(1 - n_z) = e^{-i\phi}\cot(\theta/2)$. Then, making use of the normalisation, $|c_+|^2 + |c_-|^2 = 1$, we obtain (up to an arbitrary phase)

$$\boxed{\begin{pmatrix} c_+ \\ c_- \end{pmatrix} = \begin{pmatrix} e^{-i\phi/2}\cos(\theta/2) \\ e^{+i\phi/2}\sin(\theta/2) \end{pmatrix}}. \tag{A.70}$$

A.3. The canonical momentum (or generalized momentum)

In an electromagnetic field, a charged particle will feel the Lorentz force

$$\mathbf{F} = q\left[\mathbf{E} + \mathbf{v}\times\mathbf{B}\right] \quad , \tag{A.71}$$

that we can write as (Exercises)

$$m\,\ddot{\mathbf{r}} = q\left[\mathbf{E}(\mathbf{r},t) + \mathbf{v}\times\mathbf{B}(\mathbf{r},t)\right] \quad , \tag{A.72}$$

and for the x coordinate (Exercises)

$$\begin{aligned} m\,\ddot{x} &= q\left[\mathbf{E}_x + \dot{y}B_z - \dot{z}B_y\right] \\ &= q\left[-\frac{\partial U}{\partial x} - \frac{\partial A_x}{\partial t} + \dot{y}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) - \dot{z}\left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right)\right] \quad . \end{aligned} \tag{A.73}$$

We can show (Exercises) that with the Lagrangian, given in terms of the generalized coordinates $\mathbf{r}$ and generalized velocities $\dot{\mathbf{r}}$ and time,

$$\mathcal{L}(\mathbf{r},\dot{\mathbf{r}},t) = \frac{1}{2}m\,\dot{\mathbf{r}}^2 + q\,\dot{\mathbf{r}}\cdot\mathbf{A}(\mathbf{r},t) - qU(\mathbf{r},t) \tag{A.74}$$

and using the Lagrange's equations of the second kind, *i.e.*

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{r}_j}\right) - \frac{\partial L}{\partial r_j} = 0 \tag{A.75}$$

we finally obtain the Eq. A.73.

As $\mathcal{L} = T - U$ and as the potential energy is independent or $\dot{\mathbf{r}}$, then we have that

$$\mathbf{p} = \frac{\partial T}{\partial \dot{\mathbf{r}}} = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}} \quad , \tag{A.76}$$

and for example

$$p_x = \frac{\partial \mathcal{L}}{\partial \dot{x}} = m\dot{x} + qA_x(\mathbf{r},t) \quad . \tag{A.77}$$

Therefore

$$\mathbf{p} = m\dot{\mathbf{r}} + q\mathbf{A}(\mathbf{r},t) \quad , \tag{A.78}$$

which is called the generalized (or canonical) momentum.

The question is to write now the Hamiltonian, and for this we use the Legendre transformation.

A.3.1. Legendre transformation

Consider a function of two independent variables, call it $f(x,y)$. Its differential is

$$df = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy \tag{A.79}$$

and defining $u \equiv (\partial f/\partial x)_y$ and $w \equiv (\partial f/\partial y)_x$ we can write

$$df = u\,dx + w\,dy \tag{A.80}$$

We call u and x a conjugate pair of variables, and likewise w and y.

We use now the differential

$$d(wy) = y\,dw + w\,dy \tag{A.81}$$

and we subtract Eq. A.80 from this equation and get

$$dg = y\,dw - u\,dx \tag{A.82}$$

where we have introduced the Legendre-transformed function $g \equiv wy - f$. Since we are taking differentials of x and w, we can take those two quantities as the independent variables of the new function $g(x,w)$. Therefore, we have done a Legendre transformation from an original function $f(x,y)$ to a new function $g(x,w)$ by switching from variable y to its conjugate variable w. Of course, one could instead switch x to u or one could switch both independent variables. We see therefore that for two variables, there are 4 possible variants on the function. To make contact with thermodynamics, we might call these various functions the potentials. If instead we have 3 independent variables, there are 8 different potentials, or in general there are 2^n potentials for a function of n independent variables, since each variable can be represented by either member of a conjugate pair.

Let come back to our Lagrangian $\mathcal{L}(\mathbf{r},\dot{\mathbf{r}},t)$. We want to transform to a new function (the Hamiltonian) $\mathcal{H}(\mathbf{r},\mathbf{p},t)$, where $\mathbf{p}$ is the momentum. Therefore

$$\begin{aligned} f &\equiv \mathcal{L} \\ x &\equiv \mathbf{r} \\ y &\equiv \dot{\mathbf{r}} \\ w &\equiv \left(\frac{\partial f}{\partial y}\right)_x = \left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}}\right)_{\mathbf{r}} \equiv \mathbf{p} \quad . \end{aligned}$$

So, we finally have

$$g \equiv wy - f = \mathbf{p}\cdot\dot{\mathbf{r}} - \mathcal{L} = \mathcal{H} \tag{A.83}$$

A.3.2. Rewriting the Hamiltonian

We can now write the Hamiltonian So, using Eqs. A.74, A.78 and A.83, we finally have

$$\begin{aligned}\mathcal{H}(\mathbf{r},\mathbf{p};t) &= \mathbf{p}\cdot\dot{\mathbf{r}} - \mathcal{L} \\ &= \mathbf{p}\cdot\frac{1}{m}(\mathbf{p}-q\mathbf{A}) - \frac{1}{2m}(\mathbf{p}-q\mathbf{A})^2 - \frac{q}{m}(\mathbf{p}-q\mathbf{A})\cdot\mathbf{A} + qU \\ &= \frac{1}{2m}\left[\mathbf{p}-q\mathbf{A}(\mathbf{r},t)\right]^2 - qU(\mathbf{r},t) \end{aligned} \tag{A.84}$$

A.4. The demagnetizing field

Assume a ferromagnetic system with a magnetization $\mathbf{M}$. As the second Maxwell equation (Gauss law) tells us that

$$\nabla \cdot \mathbf{B} = 0 \ , \tag{A.85}$$

and we have

$$\mathbf{B} = \mu_0 \left(\mathbf{M} + \mathbf{H} \right) \ . \tag{A.86}$$

When the magnetization meets the surface of the sample, we will have[1]

$$\nabla \cdot \mathbf{H} = -\nabla \cdot \mathbf{M} \ . \tag{A.87}$$

Therefore (and at the opposite of $\mathbf{B}$) $\mathbf{H}$ is not divergence free and behaves as if magnetic monopoles exist.

Coming back to our ferromagnetic system, the situation shown on Fig. A.2 is as if magnetic monopoles exist at the surface of the sample. The "monopoles" are the caused of the divergence of $\mathbf{H}$.

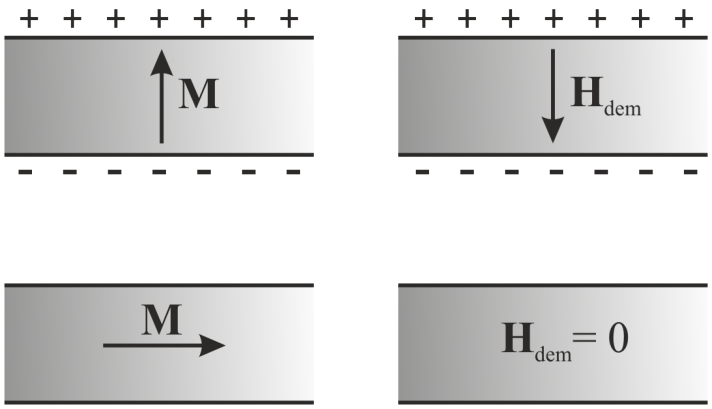

Figure A.2.: *Ferromagnetic infinite flat plate (cross section). The upper row shows the situation when the magnetization perpendicular to the plane of the plate. There is a positive (negative) divergence of the magnetization on the top (bottom) surface. The field* $\mathbf{H}_{\text{dem}}$ *will have opposite divergence. This can be seen as positive and negative poles on the surfaces as shown. If the magnetization is along the plane of the plate (bottom row), the only divergence is at the ends (supposed at an infinite distance). No divergence occurs for the magnetization and no demagnetization field is observed.*

The resulting field is called the "demagnetizing field" and we will write it as $\mathbf{H}_{\text{dem}}$, which is strongly dependendent on the shape of the sample and the position inside the sample. Taking an ellipsoid sample one can write that

$$\mathbf{H}_{\text{dem}} = -\tilde{N}\, \mathbf{M} \ , \tag{A.88}$$

[1] Outside the sample we will have $\nabla \cdot \mathbf{H} = 0$.

where $\tilde{N}$ is the demagnetizing tensor. In general, we can write

$$H_{\mathrm{dem},i} = -\sum_j N_{ij} M_j \quad . \tag{A.89}$$

If **M** is defined along the principal direction of the ellipsoid, then on can diagonalize and obtain

$$\tilde{N} = \begin{pmatrix} N_x & 0 & 0 \\ 0 & N_y & 0 \\ 0 & 0 & N_z \end{pmatrix} \tag{A.90}$$

and the trace is

$$\mathrm{Tr}(\tilde{N}) = N_x + N_y + N_z = 1 \quad . \tag{A.91}$$

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