VIII. MAGNETIC PROPERTIES OF IDEAL FERMI-DIRAC SYSTEMS

VIII.1. The Landau's problem.

In order to study the magnetic properties of an ideal Fermi-Dirac gas, it is necessary to study the quantum mechanical dynamics of a charged point particle of mass m and charge $-e\,,\ e > 0$ – an electron – in the presence of a uniform (i.e. constant and homogeneous) magnetic field: the solution to this problem [Leon Davidovic Landau (1930): *Z. Phys.* **64**, 629] is provided by the celebrated Landau's levels and degeneracy, which will represent the starting point for the thermodynamical analysis of the magnetization of an ideal electron gas.

Owing to its spin, an electron is carrying an intrinsic magnetic moment. According to relativistic Dirac's theory - disregarding radiative corrections - the intrinsic magnetic moment of the electron is given by

$$\vec{\mu} = \frac{-e}{2mc}\, g\vec{s} = \frac{-e\hbar}{2mc}\,\vec{\sigma} = -\mu\vec{\sigma}\ , \tag{1.1}$$

where we have set the Landé's g–factor equal to two, according to Dirac's equation, whereas $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli's matrices and we have introduced the *Bohr's magneton* $\mu \equiv (eh/4\pi mc) = 9.273 \times 10^{-21}$ erg G^{-1}.

Let us suppose that the uniform magnetic field is along the positive Oz axis and let us choose the *asymmetric Landau's gauge*: namely

$$A_x = -By\ , \quad A_y = A_z = 0\ , \quad B = |\mathbf{B}|\ . \tag{1.2}$$

Then the Schrödinger–Pauli hamiltonian operator can be written as

$$
\begin{aligned}
\widehat{H} &= \frac{1}{2m}\left\{\widehat{\mathbf{p}} + \frac{e}{c}\mathbf{A}(\mathbf{r})\right\}^2 - \vec{\mu}\cdot\mathbf{B} \\
&= \frac{1}{2m}\left(\hat{p}_x - \frac{e}{c}By\right)^2 + \frac{1}{2m}\left(\hat{p}_y^2 + \hat{p}_z^2\right) + \mu B\sigma_3 \ ,
\end{aligned} \tag{1.3}
$$

in which $\hat{p}_x \equiv -i\hbar\partial_x$, et cetera. Since we have $\left[\hat{H}, \sigma_3\right] = 0$, we can write the 2–components Schrödinger–Pauli spinor in the form

$$
\psi(\mathbf{r}) = \begin{vmatrix} \psi_+(\mathbf{r}) \\ \psi_-(\mathbf{r}) \end{vmatrix} \ ,
$$

in such a way that

$$
\sigma_3\psi_\pm(\mathbf{r}) = \pm\psi_\pm(\mathbf{r}) \ .
$$

Then the eigenvalue equation can be written as

$$
\left\{\frac{1}{2m}\left(\hat{p}_x - \frac{e}{c}By\right)^2 + \frac{1}{2m}\left(\hat{p}_y^2 + \hat{p}_z^2\right) \pm \mu B - E\right\}\psi_{\pm,E}(\mathbf{r}) = 0 \ . \tag{1.4}
$$

Now, taking into account that $\left[\hat{H}, \hat{p}_x\right] = \left[\hat{H}, \hat{p}_z\right] = 0$, we can set

$$
\psi_{\pm,E}(\mathbf{r}) \equiv \frac{1}{2\pi}\exp\left\{\frac{i}{\hbar}\left(xp_x + zp_z\right)\right\} Y_{\pm,E}(y) \ , \tag{1.5}
$$

and in so doing the reduced eigenfunctions $Y_{\pm,E}(y)$ fulfill the differential equation

$$
\frac{\hbar^2}{2m} Y''_{\pm,E}(y) + \left\{E \mp \mu B - \frac{p_z^2}{2m} - \frac{1}{2}m\omega_c^2\left(y - y_0\right)^2\right\} Y_{\pm,E}(y) = 0 \ , \tag{1.6}
$$

in which we have set

$$
\omega_c \equiv \frac{eB}{mc} \ , \quad y_0 \equiv \frac{p_x}{m\omega_c} \ , \tag{1.7}
$$

ω_c being the classical cyclotron angular frequency. It can be immediately realized that eq. (1.6) is nothing but the eigenvalue equation for a one dimensional harmonic oscillator in the Oy direction, with equilibrium position given by y_0 and energy $\varepsilon_\pm = E \mp \mu B - (p_z^2/2m)$. It follows therefrom that the eigenvalues of the original problem are provided by

$$E_{\pm,n,p_z} = \hbar\omega_c\left(n+\frac{1}{2}\right) + \frac{p_z^2}{2m} \pm \mu B \geq 0\ , \qquad n+1 \in \mathbf{N}\ , \qquad p_z \in \mathbf{R}\ , \tag{1.8}$$

which represent the celebrated Landau's spectrum. It turns out that the spectrum is continuous and, within the present asymmetric gauge choice, the degeneracy of each eigenvalue is labelled by $p_x \in \mathbf{R}$, i.e. a continuous infinity[1]. The corresponding eigenfunctions turn out to be

$$\psi_{n,p_z,p_x}(x,y,z) = \frac{1}{2\pi\hbar}\exp\left\{\frac{i}{\hbar}\left(xp_x + zp_z\right)\right\} Y_n\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y - \frac{p_x}{m\omega_c}\right)\right]\ , \tag{1.9a}$$

$$\begin{aligned} Y_n\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y-\frac{p_x}{m\omega_c}\right)\right] &= \left(\frac{m\omega_c}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{n!2^n}} \times \\ \exp\left\{-\frac{m\omega_c}{2\hbar}\left(y-\frac{p_x}{m\omega_c}\right)^2\right\} & H_n\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y-\frac{p_x}{m\omega_c}\right)\right]\ , \end{aligned} \tag{1.9b}$$

in which H_n denotes the n-th Hermite's polynomial. The above improper degenerate eigenfunctions, which do realize a complete orthonormal set, are normalized according to

$$\begin{aligned} &\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dz\ \psi_{n,p_z,p_x}(x,y,z)\,\psi^*_{m,q_z,q_x}(x,y,z) \\ &\qquad = \delta_{n,m}\,\delta\left(p_z - q_z\right)\delta\left(p_x - q_x\right)\ . \end{aligned} \tag{1.10}$$

Although the degeneracy of each eigenvalue of the continuous Landau's spectrum results to be infinite, it turns out that the number of degenerate states *per* unit area is finite. As a matter of fact, let us suppose to consider a very large rectangular box, centered at the origin in the Oxy plane, of sides $2L_x$ and $2L_y$ respectively. The plane-wave part of

[1] Notice that, after solving the problem in the symmetric gauge $A_x = -\frac{1}{2}By,\ A_y = \frac{1}{2}Bx,\ A_z = 0$, the degeneracy turns out to be infinite although numerable: consequently, although the spectrum is gauge invariant, the eigenvalues degeneracy appears to be gauge dependent.

the eigenfunction (1.9) along the Ox direction can be seen as the continuous limit, when L_x becomes very large, of the eigenfunctions in the presence of periodic boundary conditions at $\pm L_x$: namely,

$$\psi_{\pm,n,p_z}(x=-L_x,y,z;p_x)=\psi_{\pm,n,p_z}(x=L_x,y,z;p_x)\ , \tag{1.11}$$

that means

$$p_x(N)=\frac{\pi N\hbar}{L_x}\ , \qquad N\in\mathbf{Z}\ . \tag{1.12}$$

It follows therefrom that, if we require

$$|y_0|=\frac{|p_x|}{m\omega_c}=\frac{\pi\hbar|N|}{m\omega_c L_x}\le L_y\ , \tag{1.13}$$

we eventually find

$$\frac{|N|h}{2m\omega_c}\le L_xL_y \Leftrightarrow |N|\le\frac{m\omega_c}{2h}\,4L_xL_y\ . \tag{1.14}$$

The above equation means that we can understand the quantity

$$\Delta_L\equiv\frac{m\omega_c}{h}=\frac{eB}{hc}\ , \tag{1.15}$$

as the number of degenerate states *per* unit area, as anticipated: this is the so called Landau's degeneracy. It is worthwhile to remark that the quantity $\phi_0\equiv hc/e\simeq 4.136\times 10^{-7}$ G cm^2 is the *unit of quantum flux*. Consequently, for a standard laboratory magnetic field of one Tesla, we have approximately 2.5×10^{10} energy eigenstates *per* cm^2 in each Landau's band.

To sum up, the number of the degenerate eigenstates within an infinitesimal interval of the continuous spectrum between p_z and p_z+dp_z is

$$\Delta\Gamma=\frac{2L_zdp_z}{h}\,\frac{eB}{hc}\,4L_xL_y=V dp_z\frac{eB}{h^2c}\ , \tag{1.16}$$

if we consider a symmetric parallelepiped of volume $V = 8L_xL_yL_z$.

We are ready now to compute the one-electron partition function density: actually we easily find

$$\begin{aligned} Z(\beta;B) &= \int_{-\infty}^{+\infty} dp_z\ \frac{eB}{h^2c}\sum_{\pm}\sum_{n=0}^{\infty}\exp\left\{-\beta\left[\hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{p_z^2}{2m}\pm\mu B\right]\right\} \\ &= \left(\frac{2\pi m}{h^2\beta}\right)^{3/2} 2\beta\mu B\coth\{\beta\mu B\}\ , \qquad \left(\beta\equiv\frac{1}{kT}\right) \end{aligned} \tag{1.17}$$

from which all the magnetic properties of an ideal electron gas will be extracted as we shall see below.

VIII.2. The density of the states.

According to § VII.1., from eq. (1.17) we can now compute the so called *distribution of the states* $\tau(\epsilon_F;B)$, i.e., the number of the one-electron energy eigenstates *per* unit volume up to the Fermi energy ϵ_F in the presence of the uniform magnetic field B. To this purpose, we have to evaluate the following inverse Laplace transform: namely,

$$\tau(\epsilon_F;B)=\left(\frac{2\pi m}{h^2}\right)^{3/2}\frac{\mu B}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}ds\;2\exp\{s\epsilon_F\}\,s^{-3/2}\coth\{\mu Bs\}\;. \tag{2.1}$$

The integrand can be rewritten as

$$I(s;\epsilon_F,B)\equiv\frac{4\exp\{s\,(\epsilon_F-\mu B)\}\cosh\{\mu Bs\}}{s\sqrt{s}\,(1-\exp\{-2\mu Bs\})}\;;$$

it has a branch point at $s=0$ and simple poles at $\mu Bs=\pm r\pi i,\ r\in\mathbf{N}$ and, consequently, we have to choose $\gamma>0$.

Let us now consider the contour $(ABCDEFA)\equiv\mathrm{C}$ in the complex s-plane (see Fig. VIII.1), such that it does not pass through any of the poles of the integrand. The residues at the poles $\mu Bs=\pm r\pi i$ are given by

$$\begin{aligned}&2\exp\left\{\pm\,(\epsilon_F-\mu B)\,\frac{\pi ir}{\mu B}\right\}\cosh\{\pm r\pi i\}(\mu B)^{1/2}(\pm r\pi i)^{-3/2}=\\&\mp\,2i\sqrt{\mu B}\left(\frac{1}{\pi r}\right)^{3/2}\exp\left\{\pm i\left(\frac{r\pi\epsilon_F}{\mu B}-\frac{\pi}{4}\right)\right\}\end{aligned}$$

and after summation over $\pm$ we obtain

$$4\sqrt{\mu B}\left(\frac{1}{\pi r}\right)^{3/2}\sin\left\{\pi r\frac{\epsilon_F}{\mu B}-\frac{\pi}{4}\right\}\;,$$

whence we can write

$$\begin{aligned}&\left(\frac{2\pi m}{h^2}\right)^{3/2}\mu B\oint_{\mathrm{C}}\frac{ds}{2\pi i}\;2\exp\{s\epsilon_F\}\,s^{-3/2}\coth\{\mu Bs\}\\&=\frac{3}{2\pi}\left(\frac{\mu B}{\epsilon_F}\right)^{3/2}\frac{8}{3}\pi\left(\frac{2m\epsilon_F}{h^2}\right)^{3/2}\sum_{r=1}^{\infty}r^{-3/2}\sin\left\{\pi r\frac{\epsilon_F}{\mu B}-\frac{\pi}{4}\right\}\;.\end{aligned} \tag{2.2}$$

Now, the integrals over the arcs BC and AF do vanish as the radius of the arcs goes to infinity: for instance, if $s \in BC \ \Rightarrow\ s = Re^{i\theta},\ \pi/2 < \theta \le \pi$, then we get

$$\int_{BC} ds\ I(s;\epsilon_F,B) = 2\int_{\pi/2}^{\pi} \frac{d\theta}{2\pi}\ \frac{\exp\{-i\theta/2\}}{\sqrt{R}} \times \exp\{R\epsilon_F(\cos\theta + i\sin\theta)\}\coth\left\{\mu B R e^{i\theta}\right\}\ ,$$

which goes to zero as $R \to \infty$ owing to $\cos\theta \le 0$.

Let us then consider the contour $CDEF \equiv \sigma$ in the limit when the radius r of the small circle goes to zero; from the expansion

$$\frac{\coth x}{x\sqrt{x}} = \frac{1}{x^2\sqrt{x}} + \frac{1}{3\sqrt{x}} - \frac{x\sqrt{x}}{45} + \dots\ ,$$

it follows that

$$\begin{aligned}
&\int_\sigma \frac{ds}{2\pi i}\exp\{s\epsilon_F\}(\mu B s)^{-3/2}\coth\{\mu B s\} = \\
&\int_\sigma \frac{ds}{2\pi i}\exp\{s\epsilon_F\}\left\{(\mu B s)^{-5/2} + \frac{1}{3}(\mu B s)^{-1/2}\right\} - \\
&\int_\sigma \frac{ds}{2\pi i}\exp\{s\epsilon_F\}\left\{(\mu B s)^{-5/2} + \frac{1}{3}(\mu B s)^{-1/2} - (\mu B s)^{-3/2}\coth\{\mu B s\}\right\}\ .
\end{aligned} \tag{2.3}$$

The first two terms in the RHS of the above equation just correspond to the Hankel's representation of the inverse of the Euler's gamma function: namely,

$$\frac{1}{\Gamma(z)} = -\int_\sigma \frac{ds}{2\pi i}\ e^s s^{-z}\ , \tag{2.4}$$

whilst the last contour integral in the RHS of eq. (2.3) becomes a real integral as the small circle contribution goes to zero when $r \to 0$, the argument of s being $(-\pi)$ on EF and $(+\pi)$ on CD. Collecting all together we eventually find

$$\begin{aligned}
\tau(\epsilon_F;B) &= \frac{8}{3}\pi\left(\frac{2m\epsilon_F}{h^2}\right)^{3/2} \times \\
&\times \left\{1 + \frac{1}{4}x_F^2 + \frac{3}{2\pi}x_F^{3/2}\sum_{r=1}^{\infty} r^{-3/2}\sin\left(\frac{\pi r}{x_F} - \frac{\pi}{4}\right)\right. \\
&- \left.\frac{3}{4}x_F^{3/2}\int_0^\infty \frac{dy}{\sqrt{\pi y}}\ \exp\left\{-\frac{y}{x_F}\right\}\left(\frac{1}{3} + \frac{1}{y^2} - \frac{\coth y}{y}\right)\right\}\ ,
\end{aligned} \tag{2.5}$$

where we have set $x_F \equiv (\mu B/\epsilon_F)$.

The *density of the states*, i.e., the number of the one-electron energy eigenstates *per* unit volume with energies between E and $E + dE$, can be obtained in this case from the very definition and a direct calculation – quite similar to that one outlined above – yields

$$\begin{aligned}
\varrho(E;B) &= \left(\frac{2\pi m}{h^2}\right)^{3/2} \frac{\mu B}{\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{ds}{\sqrt{s}}\ \exp\{sE\}\ \coth\{\mu B s\} \\
&= 4\pi\sqrt{E}\left(\frac{2m}{h^2}\right)^{3/2} \left\{1 + \sum_{r=1}^{\infty} \sqrt{\frac{\mu B}{r^2 E}}\ \cos\left(\frac{\pi r E}{\mu B} - \frac{\pi}{4}\right)\right. \\
&+ \left.\sqrt{\frac{\mu B}{\pi E}} \int_0^\infty \frac{dy}{\sqrt{y}}\ \exp\left\{-\frac{yE}{\mu B}\right\}\left(\frac{1}{y} - \coth y\right)\right\} \ .
\end{aligned} \tag{2.6}$$

It should be noticed that, even if we set $\epsilon_F \equiv (\mathbf{p}_F^2/2m)$, what is still consistent with the fact that the Landau's spectrum is continuous, the Fermi surface in the present case turns out to be geometrically represented by a quite complicated manifold in the three-dimensional $\mathbf{p}_F$ space.

From the expression (2.5) of the distribution of the states, i.e., the number of one-electron energy eigenstates *per* unit volume up to the energy E, from the basic eq. (VII.1.22a) and after setting $z \equiv \exp\{\beta\epsilon_F\} = \exp\{T_F/T\}$, $x \equiv (\mu B/kT)$, $x_F \equiv (\mu B/kT_F)$, we can write

$$\begin{aligned}
\beta\,\frac{\lambda_T^3}{2V}\,\Omega(z,T;B) &= f_{5/2}(z) + \frac{1}{3}\,x^2 f_{1/2}(z) \\
&+ 2\sum_{r=1}^{\infty}\left(\frac{x}{\pi r}\right)^{3/2} \int_0^\infty dt\ \frac{\sin\{\pi r\,t/x - \pi/4\}}{1 + z^{-1}e^t} \\
&+ \frac{x^{3/2}}{\pi}\int_0^\infty dy\left(y^{-3/2}\coth y - y^{-5/2} - \frac{1}{3}\,y^{-1/2}\right) \\
&\times \int_0^\infty dt\ \frac{\exp\{-t\,y/x\}}{1 + z^{-1}e^t} \ .
\end{aligned} \tag{2.7}$$

Now, the third term in the RHS of the above equation can be rewritten in the form

$$
\begin{aligned}
&2\sum_{r=1}^{\infty}\left(\frac{x}{\pi r}\right)^{3/2}\Im m\left\{\exp\left(\frac{i\pi r}{x_F}-\frac{i\pi}{4}\right)\int_{-\beta\epsilon_F}^{\infty}dt\ \frac{\exp\left(-t+i\pi r\,t/x\right)}{1+e^{-t}}\right\} \\
&= \ -2\sum_{r=1}^{\infty}\left(\frac{x}{\pi r}\right)^{3/2}\cos\left(\frac{\pi r}{x_F}-\frac{\pi}{4}\right)\mathrm{csch}\left(\frac{\pi^2 r}{x}\right)+O\left(1/z\right)\ ,
\end{aligned}
\tag{2.8}
$$

where we used the asymptotic result when $z \gg 1$: namely,

$$
\begin{aligned}
&\int_{-\beta\epsilon_F}^{\infty}dt\ \frac{\exp\left(-t+i\pi r\,t/x\right)}{1+e^{-t}}= \\
&\int_{-\infty}^{+\infty}\frac{\exp\left(-t+i\pi r\,t/x\right)}{1+e^{-t}}+O\left(\frac{1}{z}\right)=\pi\csc\pi\left(1-i\frac{\pi r}{x}\right)+O\left(1/z\right)\ .
\end{aligned}
\tag{2.9}
$$

As a consequence, we can eventually cast eq. (2.7) in the simpler form

$$
\begin{aligned}
\frac{\lambda_T^3}{2V}\ln\mathcal{Z}(z,T;B) &= f_{5/2}(z)+\frac{1}{3}\,x^2 f_{1/2}(z) \\
&-2\pi\sum_{r=1}^{\infty}\left(\frac{x}{\pi r}\right)^{3/2}\cos\left(\frac{\pi r}{x_F}-\frac{\pi}{4}\right)\mathrm{csch}\left(\frac{\pi^2 r}{x}\right) \\
&+\mathcal{R}\left(x,\frac{T_F}{T}\right)+O\left(1/z\right)\ ,
\end{aligned}
\tag{2.10}
$$

in which we have set

$$
\begin{aligned}
\mathcal{R}\left(x,\frac{T_F}{T}\right) &\equiv x^{3/2}\int_0^{\infty}\frac{dy}{\pi}\ \exp\left\{-\frac{y\,T_F}{xT}\right\}\left(y^{-3/2}\coth y-y^{-5/2}-\frac{1}{3}\,y^{-1/2}\right) \\
&\times\int_{-(T_F/T)}^{\infty}dt\ \frac{\exp\{-\,ty/x\}}{1+e^{t}}\ .
\end{aligned}
\tag{2.11}
$$

It is possible to show – see Appendix – that the above expression can be neglected in the high degeneracy case.

To sum up, in the highly degenerate regime $z \gg 1$ we can write

$$
\begin{aligned}
\beta\,\frac{\lambda_T^3}{2V}\,\Omega(z,x,x_F) &\overset{z\gg 1}{\approx} f_{5/2}(z)+\frac{1}{3}\,x^2 f_{1/2}(z) \\
&-2\pi\sum_{r=1}^{\infty}\left(\frac{x}{\pi r}\right)^{3/2}\cos\left(\frac{\pi r}{x_F}-\frac{\pi}{4}\right)\mathrm{csch}\left(\frac{\pi^2 r}{x}\right)\ ,
\end{aligned}
\tag{2.12}
$$

Starting from the above basic equation (2.12), we shall be able to discuss in details the different regimes of physical interest, i.e., the high-degeneracy case in the weak magnetic field limit and for small or large x respectively. As we shall see below, this study will beautifully unravel the diamagnetic and paramagnetic properties of the metals.

VIII.3. Magnetic properties.

We start the discussion of the magnetic properties of an ideal electrons gas from the low degenerate case. From the general form of the state equation (VII.2.5), we can immediately write the lowest order contibution as

$$\beta\Omega(z,\beta,V;B) \overset{z\ll 1}{\approx} zVZ(\beta;B) = \frac{V}{\lambda_T^3}\, 2zx\coth x\ , \qquad \left(x \equiv \frac{\mu B}{kT}\right)\ , \tag{2.13a}$$

$$n \overset{z\ll 1}{\approx} \frac{2}{\lambda_T^3}\, zx\coth x\ . \tag{2.13b}$$

On the other hand, the *mean magnetic moment per* unit volume, or *magnetization*, or even *magnetic polarizability*, of the electron gas is defined by

$$\overline{M} \equiv \frac{1}{V}\left(\frac{\partial\Omega}{\partial B}\right)_{z,T,V}\ . \tag{2.14}$$

Notice that in the C. G. S. gaussian system of units the magnetization has the same dimension of an electromagnetic field, i.e. G or dine/ues. Now, up to the same lowest order approximation we find

$$\overline{M} \overset{z\ll 1}{\approx} \mu\, n\left\{\tanh x - \left(\coth x - \frac{1}{x}\right)\right\}\ , \tag{2.15}$$

where the first term in the RHS represents the paramegnetic contribution, whereas the second one the (negative) diamagnetic amount to the total magnetization.

In the *weak field and/or high temperature limit*, i.e. $x \ll 1$, we obtain

$$\overline{M} \overset{x\ll 1}{\approx} \frac{2}{3}\, n\, \frac{\mu^2 B}{kT}\ , \tag{2.16}$$

that means the Curie's law with a magnetic susceptibility given by

$$\chi_{\mathrm{m}} \equiv \left(\frac{\partial\overline{M}}{\partial B}\right) \overset{x\ll 1}{\approx} \frac{2n\mu^2}{3kT}\ . \tag{2.17}$$

At room temperature and for ordinary Alkali metals the magnetic susceptibility, which turns out to be dimensionless in the C. G. S. gaussian system of units, turns out to be of the order $10^{-5} \div 10^{-4}$, taking into account that an effective (smaller) electron's mass is suitably involved to correctly estimate the diamagnetic contribution due to the orbital motion.

For *strong applied magnetic fields*, i.e. $x \gg 1$, eq. (2.15) yields $\overline{M} \simeq 0$, which means that the para- and dia-magnetic contributions exactly compensate for the low degenerate electrons gas in the presence of strong magnetic fields.

Let us now turn to the more interesting case of a highly degenerate electrons gas, that means $z \gg 1$ or, equivalently, $T \ll T_F$. In order to carefully treat this regime, we have to start from the corresponding expression of eq. (2.12): namely,

$$\begin{aligned}\frac{\Omega\,\lambda_T^3}{2VkT} &\overset{z\gg 1}{\approx} f_{5/2}(z) + \frac{1}{3}\,x^2 f_{1/2}(z)\\ &\quad - 2\pi\sum_{r=1}^{\infty}\left(\frac{x}{\pi r}\right)^{3/2}\cos\left(\frac{\pi r}{x_F}-\frac{\pi}{4}\right)\operatorname{csch}\left(\frac{\pi^2 r}{x}\right)\ ,\end{aligned}$$

from which, taking the definition of eq. (2.14) into account, we can easily obtain

$$\begin{aligned}\frac{\overline{M}\lambda_T^3}{2\mu} &= \frac{2}{3}\,x f_{1/2}(z) - 2\,\frac{\sqrt{\pi x}}{x_F}\sum_{r=1}^{\infty} r^{-1/2}\sin\left(\frac{\pi r}{x_F}-\frac{\pi}{4}\right)\operatorname{csch}\left(\frac{\pi^2 r}{x}\right)\\ &\quad - 2\pi\sqrt{\frac{\pi}{x}}\sum_{r=1}^{\infty} r^{-1/2}\cos\left(\frac{\pi r}{x_F}-\frac{\pi}{4}\right)\operatorname{csch}\left(\frac{\pi^2 r}{x}\right)\coth\left(\frac{\pi^2 r}{x}\right)\\ &\quad - 3\sqrt{\frac{x}{\pi}}\sum_{r=1}^{\infty} r^{-3/2}\cos\left(\frac{\pi r}{x_F}-\frac{\pi}{4}\right)\operatorname{csch}\left(\frac{\pi^2 r}{x}\right) + o\left(\frac{T}{T_F}\right)\ .\end{aligned} \tag{2.18}$$

Now, we notice that in the highly degenerate case $T \ll T_F$ and taking into account that $x_F \ll 1$ because $(\mu/\epsilon_F) \simeq 1.84 \times 10^{-9}\ \mathrm{G}^{-1}$, we can retain the leading terms within the two regimes:

(i) *weak fields* $x \ll 1$, in which only the first term in the RHS of the above equation is relevant, owing to the presence of $\operatorname{csch}(\pi^2 r/x)$;

(ii) *strong fields* $x > 1$, in which only the first two terms of the RHS of the above equation are the leading ones.

Moreover, from eq. (VII.2.10) we readily get the leading terms in the asymptotic expansion

$$f_s(z) \overset{T\ll T_F}{\approx} \frac{(T_F/T)^s}{\Gamma(s+1)} \left\{ 1 + s(s-1)\frac{\pi^2}{6}\left(\frac{T}{T_F}\right)^2 + O\left(\frac{T}{T_F}\right)^4 \right\} . \tag{2.19}$$

As a consequence, according to the previous remarks, we can rewrite eq. (2.18) keeping only the leading terms into account: namely

$$\begin{aligned} \overline{M} \overset{T\ll T_F}{\approx} & \ B\,\frac{16\pi}{3h^3}\,m^{3/2}\mu^2\sqrt{2\epsilon_F} \\ & \times \left\{ 1 - \frac{3}{2}\,\pi\,\frac{kT}{\mu B}\sqrt{\frac{\epsilon_F}{\mu B}} \sum_{r=1}^{\infty} r^{-1/2} \sin\left(\frac{\pi r}{x_F} - \frac{\pi}{4}\right) \mathrm{csch}\left(\frac{\pi^2 r}{x}\right) \right\} , \end{aligned} \tag{2.20}$$

and taking one more derivative with respect to the magnetic field strength we finally come to the *magnetic susceptibility*, whose leading terms for $x_F \ll 1$ and $x > 1$ read

$$\begin{aligned} \chi_{\mathrm{m}} \equiv \left(\partial\overline{M}/\partial B\right) \overset{T\ll T_F}{\approx} & \ \frac{16\pi}{3h^3}\,m^{3/2}\mu^2\sqrt{2\epsilon_F} \\ & \times \left\{ 1 + \frac{3\pi^2}{2\,x}\,x_F^{-3/2} \sum_{r=1}^{\infty} \sqrt{r}\cos\left(\frac{\pi r}{x_F} - \frac{\pi}{4}\right) \mathrm{csch}\left(\frac{\pi^2 r}{x}\right) \right\} . \end{aligned} \tag{2.21}$$

In order to compare the above expression for the susceptibility with the experimental data on metals, we have to notice that the effect of the weak binding of the electrons to the crystal lattice of the metal can be represented, as is done in many other branches of the theory of metals, by the introduction of an *effective mass* m_* for the electron, i.e., typically $m_* = 0.98\,m_e$. In so doing, the Bohr's magneton due to the orbital motion – which is responsible for the diamagnetism – has to be replaced by $\mu_* = (e\hbar/2m_*c)$, whilst the spin magnetic moment – which is responsible for the paramagnetism – however, is still μ whatever the effective mass of the electron may be, so that the one–electron partition function density of eq. (1.17) is replaced by

$$Z(\beta;B) = \left(\frac{2\pi m_*}{h^2\beta}\right)^{3/2} \frac{2\beta\mu_* B}{\sinh\{\beta\mu_* B\}}\cosh\{\beta\mu B\} . \tag{2.22}$$

Furthermore, to the lowest order in the high degeneracy case, from eq. (2.5) we can write

$$n \simeq \frac{8}{3}\,\pi \left(\frac{2m_*\epsilon_F}{h^2}\right)^{3/2} , \tag{2.23}$$

in such a way that it is a simple exercise to show that the magnetic susceptibility, up to the leading terms, can be cast in the form

$$\begin{aligned}\chi_{\mathrm{m}} \ \stackrel{T\ll T_F}{\approx}\ \chi_0 + \chi_{\mathrm{osc}} \ &= \ \frac{1}{2}\,n\,\frac{\mu_*^2}{\epsilon_F}\left\{3\,\frac{m_*^2}{m^2} - 1 + 3\pi^2\,\frac{kT}{\mu_* B}\left(\frac{\epsilon_F}{\mu_* B}\right)^{3/2}\right.\\ &\left.\times \sum_{r=1}^{\infty}(-1)^r\sqrt{r}\cos\left(\frac{r\pi m_*}{m}\right)\cos\left(\frac{\pi r\epsilon_F}{\mu_* B} - \frac{\pi}{4}\right)\mathrm{csch}\left(r\pi^2\,\frac{kT}{\mu_* B}\right)\right\} .\end{aligned} \tag{2.24}$$

(i) $x \ll 1$: in this case it is the first line in the RHS to be the dominant one and to give rise to the *steady susceptibility* of the metals, *viz.*

$$\chi_0 = \frac{n\mu_*^2}{2\epsilon_F}\left(3\,\frac{m_*^2}{m^2} - 1\right) , \tag{2.25}$$

which is temperature independent and of the order 10^{-7}, in a reasonable accordance with experimental data keeping in mind the crudeness of the present approximation. For instance we have, after multiplication by 10^7, the experimental (theoretical) values of the susceptibilities for the following metals in the IA group of the Mendeleev's periodic table: 5.8 (4.38) for Sodium (Na), 5.1 (3.40) for Potassium (K), 0.6 (3.26) for Rubidium (Rb), –0.5 (3.02) for Cesium (Cs). The disagreements, especially for Rb and Cs – in which also the sign is opposite – are basically due to the fact that the assumption that the valence electrons are free particles is too a rough one and corrections are mandatory. Notice that the term $(3m_*^2/m^2)$ is the *Pauli's steady paramagnetism* - the spin contribution - whereas the (-1) is the *Landau's steady diamagnetism*. It is also worthwhile to stress that the Curie's susceptibility - see eq. (2.16) - at room temperature is such that $\chi_{\mathrm{Curie}}(T = 300\ ^\circ\mathrm{K}) \simeq 1.33\times 10^2\ \chi_0$, what endorses that at room temperature the valence electrons in metals can be thought, in a first approximation, to behave like a highly degenerate ideal Fermi-Dirac gas of *quasi*–free particles.

(ii) $x > 1$: in this case, a further oscillatory contribution to the magnetism arises, which is known as the *de Haas - van Alphen effect*: namely,

$$\chi_{\rm osc} \simeq \frac{3n\mu_*}{2B^{3/2}}\sqrt{\frac{\epsilon_F}{\mu_*}}\cos\left(\frac{\pi\,\epsilon_F}{\mu_* B}-\frac{\pi}{4}\right) \ .$$

This effect, which appears at sufficiently low temperatures as $T/B < \mu_*/\pi^2 k \simeq 6.8 \times 10^{-6}$ °K G^{-1}, is quite important since it allows an experimental determination of the Fermi energy: for ordinary metals the latter turns out to be of the order $\epsilon_F \simeq 3.14$ eV$= 5.03 \times 10^{-12}$ erg, which corresponds to a Fermi temperature $T_F \simeq 3.64 \times 10^4$ °K.

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Appendix D: evaluation of integral representations.

Here we want to evaluate the double integral

$$\mathcal{R}\,(x,z) \equiv \frac{x^{3/2}}{\pi}\int_0^\infty dy\int_0^\infty dt\ \frac{e^{-ty/x}}{1+z^{-1}\,e^t}\,y^{-3/2}\left(\coth y-\frac{1}{y}-\frac{y}{3}\right)\ . \qquad (A1)$$

To this aim, let us first change the integration variable $y = wx/t$ so that

$$\mathcal{R}\,(x,z) \equiv \frac{x}{\pi}\int_0^\infty dt\int_0^\infty dw\ \frac{t^{1/2}w^{-3/2}e^{-w}}{1+z^{-1}\,e^t}\left\{\coth\left(\frac{wx}{t}\right)-\frac{t}{wx}-\frac{wx}{3t}\right\} \qquad (A2)$$

and then consider the following change of variables in the double integral: namely,

$$\xi \equiv \frac{wx}{t\pi}\ , \qquad \eta \equiv t+w\ , \qquad 0\le\xi\le 1\ , \qquad \eta\ge 0\ , \qquad (A3)$$

the inversion of which reads

$$w=\frac{x\eta}{x+\pi\xi}\ , \qquad t=\frac{\pi\xi\eta}{x+\pi\xi}\ , \qquad (A4)$$

whereas the jacobian turns out to be

$$\left|\frac{\partial(w,t)}{\partial(\xi,\eta)}\right| = \frac{\pi x\eta}{(x+\pi\xi)^2}\ . \qquad (A5)$$

Then we have

$$\begin{aligned}\mathcal{R}\,(x,z) &= \frac{x^{5/2}}{\pi\sqrt{\pi}}\int_0^\infty d\eta\int_0^1 d\xi\ \frac{\xi^{-3/2}}{x+\pi\xi}\ \exp\left\{-\frac{\pi\xi\eta}{x+\pi\xi}\right\}\\ &\times\left(\coth\pi\xi-\frac{1}{\pi\xi}-\frac{\pi\xi}{3}\right)\left(1+z^{-1}\exp\left\{\frac{x\eta}{x+\pi\xi}\right\}\right)^{-1}\ .\end{aligned} \qquad (A6)$$

Now we can expand the hyperbolic cotangent according to [I. S. Gradshteyn and I. M. Ryzhik: *Table of Integrals, Series, and Products*, Fifth Edition, Academic Press, San Diego (1994); Eq. **1.411**8. pg. 42] and integrating by series we finally obtain

$$\mathcal{R}\,(x,z) = \left(\frac{x}{\pi}\right)^{5/2}\sum_{k=2}^\infty\frac{(2\pi)^{2k}B_{2k}}{(2k)!}\int_0^1 d\xi\ \frac{\xi^{2k-5/2}}{x+\pi\xi}\int_0^\infty d\eta\ \frac{z\,e^{-\eta}}{1+z\exp\{-x\eta/(x+\pi\xi)\}}\ , \qquad (A7)$$

where B_{2k} denote *the Bernoulli's numbers*. Here we write the first values:

$$B_1 = \frac{1}{6}\ , \qquad B_2 = \frac{1}{30}\ , \qquad B_3 = \frac{1}{42}\ , \qquad B_4 = \frac{1}{30}\ . \tag{A8}$$

Let us first consider the case of weak magnetic fields, *i.e.* $x \ll 1$: then the leading term clearly reads

$$\mathcal{R}\,(x,z) \stackrel{x\ll 1}{\sim} x^{5/2}\,\frac{z}{1+z}\,\pi^{-7/2}\sum_{k=2}^{\infty}\frac{(2\pi)^{2k}B_{2k}}{(2k)!(2k-5/2)}\ . \tag{A9}$$

It follows therefrom that in the highly degenerate regime $z \to \infty$ and for weak fields we definitely find

$$\mathcal{R}\,(x,z) = O(x^{5/2})\ , \qquad \ln z \gg 1\ , \quad x \ll 1\ , \tag{A10}$$

which is manifestly negligible with respect to the second addendum in the right hand side of eq. (2.10).

On the other hand, in the case of strong magnetic fields $x \gg 1$ it is convenient to set $\eta = t(1+\pi\xi/x)$ so that the double integral of eq. (A7) can be rewritten in the form

$$\mathcal{R}\,(x,z) = \frac{x^{3/2}}{\pi^{5/2}}\sum_{k=2}^{\infty}\frac{(2\pi)^{2k}B_{2k}}{(2k)!}\int_0^1 d\xi\ \xi^{2k-5/2}\int_0^{\infty} dt\ \frac{z\,e^{-t}}{1+z\,e^{-t}}\ \exp\{-t\pi\xi/x\}\ . \tag{A11}$$

Now, in the limit of strong magnetic fields the dominant contribution reads

$$\mathcal{R}\,(x,z) \stackrel{x\gg 1}{\sim} x^{3/2}\sum_{k=2}^{\infty}\frac{(2\pi)^{2k}B_{2k}}{(2k)!(2k-3/2)}\,\pi^{-5/2}\,\ln(1+z) \tag{A12}$$

and turns out to be manifestly negligible with respect to the second addendum of the right hand side of eq. (2.10), as well as with respect to the third addendum of the right hand side of eq. (2.10), the behaviour of which is $O(x^{5/2})$ for large magnetic fields. In conclusion, the leading behaviour of eq. (2.12) does indeed hold true.

As a final remark, it is interesting to notice that the state distribution *per* unit volume can be expressed in terms of the Riemann's zeta function. As a matter of fact, according to eq.s (2.1) and (2.2), the states distribution can be written as follows

$$\begin{aligned}\tau(E;B) &= \left(\frac{2\pi m}{h^2}\right)^{3/2}\frac{\mu B}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} ds\ 2\exp\{sE\}\,s^{-3/2}\coth\{\mu Bs\}\\ &= -\left(\frac{2\pi m}{h^2}\right)^{3/2}\mu B\int_\sigma \frac{ds}{2\pi i}\ 2\exp\{sE\}\,s^{-3/2}\coth\{\mu Bs\} \qquad (A13)\\ &+\ 4\left(\frac{2m\mu B}{h^2}\right)^{3/2}\sum_{r=1}^{\infty} r^{-3/2}\sin\left\{\pi r\frac{E}{\mu B}-\frac{\pi}{4}\right\}\ ,\end{aligned}$$

where $E>0$ and for a given $\varepsilon,\ 0<\varepsilon<1$, the oriented contour σ consists of the half-line $\{\Re\mathrm{e}s \le -\varepsilon,\ \arg(s)=\pi\}$ covered from the left to the right, of the circle $\{s=\varepsilon e^{i\theta};\ -\pi\le\theta\le\pi\}$ covered clockwise, and of the half-line $\{\Re\mathrm{e}s\le-\varepsilon,\ \arg(s)=-\pi\}$ covered from the right to the left. The above integral can be expressed in terms of the Riemann's ζ-function [I. S. Gradshteyn and I. M. Ryzhik: *Table of Integrals, Series, and Products*, Fifth Edition, Academic Press, San Diego (1994); Eq. **3.551**3. pg. 403]. To this aim, let us change the integration variable $2s=-w$ to rewrite the integral in the second line of eq. (A1): namely,

$$\begin{aligned}\tau(q;B) &= \left(\frac{4\pi m\mu B}{h^2}\right)^{3/2}\int_\infty^{(0+)}\frac{dw}{2\pi i}\,(-w)^{-3/2}\,\frac{\exp\{-wq\}+\exp\{-w(1+q)\}}{1-\exp\{-w\}}\\ &+\ 4\left(\frac{2m\mu B}{h^2}\right)^{3/2}\sum_{r=1}^{\infty} r^{-3/2}\sin\left\{2\pi rq-\frac{\pi}{4}\right\}\\ &= -\,4\pi\sqrt{2}\left(\frac{2m\mu B}{h^2}\right)^{3/2}\left\{\zeta\left(-\frac{1}{2};q\right)+\zeta\left(-\frac{1}{2};q+1\right)\right\}\\ &+\ 4\left(\frac{2m\mu B}{h^2}\right)^{3/2}\sum_{r=1}^{\infty} r^{-3/2}\sin\left\{2\pi rq-\frac{\pi}{4}\right\} \qquad (A14)\\ &= 8\pi\sqrt{2}\left(\frac{2m\mu B}{h^2}\right)^{3/2}\left\{\frac{\sqrt{q}}{2}-\zeta\left(-\frac{1}{2};q\right)\right\}\\ &+\ 4\left(\frac{2m\mu B}{h^2}\right)^{3/2}\sum_{r=1}^{\infty} r^{-3/2}\sin\left\{2\pi rq-\frac{\pi}{4}\right\}\ ,\end{aligned}$$

where $q \equiv E/2\mu B$ whereas the path integration now consists of the half-line $\{\Re\mathrm{e}\, w \geq \varepsilon,\ \arg(w) = \pi\}$ covered from the right to the left, of the circle $\{w = \varepsilon e^{i\theta};\ -\pi \leq \theta \leq \pi\}$ covered counterclockwise, and of the half-line $\{\Re\mathrm{e}\, w \geq \varepsilon,\ \arg(w) = -\pi\}$ covered from the left to the right. To sum up we eventually have

$$\tau(E;B) = \frac{4}{\pi^2}\left(\frac{m\mu B}{\hbar^2}\right)^{3/2}\left\{\sqrt{\frac{E}{8\mu B}} - \zeta\left(-\frac{1}{2};\frac{E}{2\mu B}\right) + \sum_{r=1}^{\infty}\frac{\sin\left[\,(\pi r E/\mu B) - (\pi/4)\,\right]}{\pi(2r)^{3/2}}\right\}\ .$$

Ferro .... $T_f = 1808$ °K .... $T_c = 1043$ °K

Nichel .... $T_f = 1726$ °K .... $T_c = 631$ °K

Cobalto ..... $T_f = 1768$ °K .... $T_c = 1295$ °K

T_f temperatura di *fusione* T_c temperatura di *Curie*

Magnetic susceptibilities at room temperature in units of 10^{-7}

Bismuth .... –1700

Copper .... –100

Silver .... –190

Alluminium 220

Platinum 3600

PROBLEMS

Problema VIII.1. Un sistema meccanico é costituito da N elettroni identici puntiformi di massa m e carica $-e$, immersi in un campo magnetico omogeneo e indipendente dal tempo $\mathbf{B} = \nabla \times \mathbf{A}(\mathbf{r})$. Se indichiamo con $(\mathbf{r}_i, \widehat{\mathbf{p}}_i)$, $i = 1, 2, \ldots, N$, le coordinate e l'operatore momento canonico del i-esimo elettrone, l'operatore di Hamilton del sistema si scrive

$$\widehat{H} = \sum_{i=1}^{N} \left\{ \frac{1}{2m} \left[\widehat{\mathbf{p}}_i + \frac{e}{c}\,\mathbf{A}(\mathbf{r}_i) \right]^2 + \frac{g\mu}{\hbar}\,\widehat{\mathbf{S}}_i \cdot \mathbf{B} \right\} + U_{\text{Coulomb}}$$

dove $\mu = e\hbar/2mc = 0.927 \times 10^{-20}$ erg/Gauss é il magnetone di Bohr, $g = 2.0023$ é il fattore di Landé dell'elettrone, $\widehat{\mathbf{S}}_i$ rappresenta l'operatore di spin dell'i-esimo elettrone, mentre U_{Coulomb} rappresenta l'energia coulombiana tra gli elettroni stessi e gli elettroni e i nuclei. Il sistema é posto in contatto termico con un termostato a temperatura assoluta T. Si calcoli la suscettivitá diamagnetica del sistema.

Soluzione

Scegliamo la gauge simmetrica

$$\mathbf{A}(\mathbf{r}_i) = \frac{1}{2}\,\mathbf{B} \times \mathbf{r}_i\,, \qquad i = 1, 2, \ldots, N$$

in modo tale che

$$[\,\widehat{\mathbf{p}}_j\,,\,\mathbf{A}(\mathbf{r}_k)\,] = -i\hbar\,\delta_{jk}\,\nabla \cdot \mathbf{A}(\mathbf{r_j}) \equiv 0$$

Tenendo conto di questa circostanza l'hamiltoniano si puó mettere nella forma

$$\begin{aligned}
\widehat{H} &= \widehat{H}_0 + \frac{e}{mc} \sum_{i=1}^{N} \mathbf{A}(\mathbf{r}_i) \cdot \widehat{\mathbf{p}}_i + \frac{e^2}{8mc^2} \sum_{i=1}^{N} (\mathbf{B} \times \mathbf{r}_i)^2 + \frac{g\mu}{\hbar}\,\widehat{\mathbf{S}} \cdot \mathbf{B} \\
&= \widehat{H}_0 + \frac{\mu}{\hbar} \left(\widehat{\mathbf{L}} + 2\widehat{\mathbf{S}} \right) \cdot \mathbf{B} + \frac{e^2}{8mc^2} \sum_{i=1}^{N} (\mathbf{B} \times \mathbf{r}_i)^2
\end{aligned}$$

dove $\mathbf{S} := \sum_{i=1}^N \widehat{\mathbf{S}}_i$ é l'operatore dello spin totale elettronico, $\mathbf{L} := \sum_{i=1}^N \mathbf{r}_i \times \mathbf{p}_i$ é l'operatore del momento angolare totale elettronico, mentre

$$\widehat{H}_0 := \sum_{i=1}^N \frac{\widehat{\mathbf{p}}_i^2}{2m} + U_{\mathrm{Coulomb}}$$

denota l'hamiltoniano in assenza del campo magnetico.

Problem VIII.2. Calculate the Green's function of the Schrödinger-Pauli hamiltonian operator (1.3) in the asymmetric Landau's gauge $\quad A_x = -By\,,\ A_y = A_z = 0\,,\ B > 0\,.$

Solution. By definition the Green's function of the hamiltonian self-adjoint operator is the integral kernel of the resolvent operator $\widehat{R}(E) \equiv (E - \widehat{H})^{-1}$ when the complex energy variable is in the upper or lower half planes. Thus we have

$$G^+(E;\mathbf{r},\mathbf{r}') \equiv \langle\,\mathbf{r}|\left(E - \widehat{H}\right)^{-1}|\mathbf{r}'\,\rangle\ , \qquad \Im\mathrm{m}(E) > 0\ .$$

From eq.s (1.8) and (1.9) we obtain the spectral resolution $\quad [\ \omega_c = eB/mc\ ]$

$$\begin{aligned}
G^+(E;\mathbf{r},\mathbf{r}') &= \sum_{n=0}^{\infty}\int_{-\infty}^{+\infty} dp_z\ \left(E - n\hbar\omega_c - \frac{\hbar\omega_c}{2} - \frac{p_z^2}{2m} \mp \mu B\right)^{-1} \\
&\times \int_{-\infty}^{+\infty} dp_x\ \psi_{n,p_z,p_x}(x,y,z)\,\psi^*_{n,p_z,p_x}(x',y',z') \\
&= \left(\frac{m\omega_c}{\pi\hbar}\right)^{1/2}\left(4\pi^2\hbar^2 n!\,2^n\right)^{-1}\ \sum_{n=0}^{\infty}\ \int_{-\infty}^{+\infty} dp_z \\
&\times \left(E - n\hbar\omega_c - \frac{\hbar\omega_c}{2} - \frac{p_z^2}{2m} \mp \mu B\right)^{-1} \\
&\times \int_{-\infty}^{+\infty} dp_x\ \exp\left\{\frac{i}{\hbar}\left[\,p_x(x-x') + p_z(z-z')\,\right]\right\} \\
&\times \exp\left\{-\frac{m\omega_c}{2\hbar}\left(y - \frac{p_x}{m\omega_c}\right)^2 - \frac{m\omega_c}{2\hbar}\left(y' - \frac{p_x}{m\omega_c}\right)^2\right\} \\
&\times H_n\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y - \frac{p_x}{m\omega_c}\right)\right]\ H_n\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y' - \frac{p_x}{m\omega_c}\right)\right]\ .
\end{aligned}$$

Let us first consider an integral representation for the Green's function which is valid for $\Re\mathrm{e}(E) < 0$: from the identity

$$(E - E_{\pm,n,p_z})^{-1} = -\int_0^\infty dt\ \exp\left\{tE - \frac{t\hbar\omega_c}{2} - tn\hbar\omega_c - \frac{tp_z^2}{2m} \mp t\mu B\right\}$$

after a suitable rearrangement of the factorized integrals and series we easily obtain

$$\begin{aligned}
G(E;\mathbf{r},\mathbf{r}') = &-\sqrt{\frac{m\omega_c}{\pi\hbar}}\ \exp\left\{-\frac{m\omega_c}{2\hbar}\left(y^2 + y'^2\right)\right\}\\
&\times \int_0^\infty dt\ \exp\left\{t\left(E - \frac{\hbar\omega_c}{2} \mp \mu B\right)\right\}\\
&\times \int_{-\infty}^{+\infty} \frac{dp_z}{2\pi\hbar}\ \exp\left\{-\frac{tp_z^2}{2m} + \frac{ip_z}{\hbar}(z - z')\right\}\\
&\times \int_{-\infty}^{+\infty} \frac{dp_x}{2\pi\hbar}\ \exp\left\{-\frac{p_x^2}{m\hbar\omega_c} - \frac{ip_x}{\hbar}\left[\,(x - x') + i(y + y')\,\right]\right\}\\
&\times \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{\exp\{-t\hbar\omega_c\}}{2}\right)^n\\
&\times H_n\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y - \frac{p_x}{m\omega_c}\right)\right] H_n\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y' - \frac{p_x}{m\omega_c}\right)\right]\ .
\end{aligned}$$

The gaussian integral over p_z can be easily performed, whilst the series can also be summed thanks to the formula $\quad [\ |u| < 1/2\ ]$

$$\sum_{n=0}^{\infty} \frac{u^n}{n!}\, H_n(\xi)\, H_n(\xi') = (1 - 4u^2)^{-1/2} \exp\left[\frac{4u\xi\xi' - 4u^2(\xi^2 + \xi'^2)}{1 - 4u^2}\right]$$

and the result is

$$\begin{aligned}
G(E;\mathbf{r},\mathbf{r}') = &-\sqrt{\frac{m\omega_c}{\pi\hbar}}\ \exp\left\{-\frac{m\omega_c}{2\hbar}\left(y^2 + y'^2\right)\right\}\\
&\times \int_0^\infty dt\, t^{-1/2}\ \exp\left\{t\left(E - \frac{\hbar\omega_c}{2} \mp \mu B\right)\right\}\\
&\times \sqrt{\frac{m}{2\pi\hbar^2}}\ \exp\left\{-\frac{m}{2\hbar^2 t}(z - z')^2\right\}\\
&\times \int_{-\infty}^{+\infty} \frac{dp_x}{2\pi\hbar}\ \exp\left\{-\frac{p_x^2}{m\hbar\omega_c} - \frac{ip_x}{\hbar}\left[\,(x - x') + i(y + y')\,\right]\right\}\\
&\times \frac{\exp\{t\hbar\omega_c/2\}}{\sqrt{2\sinh(t\hbar\omega_c)}}\ \exp\left\{\frac{m\omega_c}{\hbar\sinh(t\hbar\omega_c)}\left(yy' - p_x\frac{y + y'}{m\omega_c} + \frac{p_x^2}{m^2\omega_c^2}\right)\right\}\\
&\times \exp\left\{-\frac{m\omega_c}{2\hbar}\left[\coth(t\hbar\omega_c) - 1\right]\left(y^2 + y'^2 - 2p_x\frac{y + y'}{m\omega_c} + \frac{2p_x^2}{m^2\omega_c^2}\right)\right\}\ .
\end{aligned}$$

The gaussian integral over p_x gives

$$
\begin{aligned}
&\int_{-\infty}^{+\infty} \frac{dp_x}{2\pi\hbar}\ \exp\left\{-\frac{p_x^2}{m\hbar\omega_c} + \frac{ip_x}{\hbar}\,[\,(x-x') + i(y+y')\,]\right\} \\
&\times \exp\left\{\frac{m\omega_c}{\hbar\sinh(t\hbar\omega_c)}\left(p_x\,\frac{y+y'}{m\omega_c} + \frac{p_x^2}{m^2\omega_c^2}\right)\right\} \\
&\times \exp\left\{-\frac{m\omega_c}{2\hbar}\,[\,\coth(t\hbar\omega_c) - 1\,]\left(2p_x\,\frac{y+y'}{m\omega_c} + \frac{2p_x^2}{m^2\omega_c^2}\right)\right\} \\
&= \sqrt{\frac{m\omega_c}{4\pi\hbar}\,\coth\left(\frac{t\hbar\omega_c}{2}\right)} \\
&\times \exp\left\{-\frac{m\omega_c}{4\hbar}\left[(x-x')^2\coth\left(\frac{t\hbar\omega_c}{2}\right) - (y+y')^2\tanh\left(\frac{t\hbar\omega_c}{2}\right) + 2i(x-x')(y+y')\right]\right\}
\end{aligned}
$$

so that we finally obtain for $\Re\mathrm{e}(E) < 0$

$$
\begin{aligned}
G(E;\mathbf{r},\mathbf{r}') =\ & -\frac{m\omega_c}{4\pi\hbar^2}\sqrt{\frac{m}{2\pi}}\ \exp\left\{-im\omega_c\,(x-x')(y+y')/2\hbar\right\} \\
&\times \int_0^\infty \frac{dt\,t^{-1/2}}{\sinh(t\hbar\omega_c/2)}\ \exp\left\{Et \mp t\mu B - \frac{m}{2\hbar^2 t}(z-z')^2\right\} \\
&\times \exp\left\{-\frac{m\omega_c}{4\hbar}\ [\,(x-x')^2 + (y-y')^2\,]\ \coth\left(\frac{t\hbar\omega_c}{2}\right)\right\}\ .
\end{aligned}
$$

Notice that the canonical dimensions [G] of the Green's function in the C.G.S. Gaussian units system are $[\mathrm{G}] = \mathrm{erg}^{-1}\ \mathrm{cm}^{-3} = \mathrm{cm}^{-5}\ \mathrm{g}^{-1}\ \mathrm{s}^2$. It is now convenient to change the integration variable and to introduce the dimensionless integration variable $\alpha \equiv t\hbar\omega_c/2$:

$$
\begin{aligned}
G(E;\mathbf{r},\mathbf{r}') =\ & -\frac{m\omega_c}{4\pi\hbar^2}\sqrt{\frac{m}{\pi\hbar\omega_c}}\ \exp\left\{-im\omega_c\,(x-x')(y+y')/2\hbar\right\} \\
&\times \int_0^\infty \frac{d\alpha}{\sqrt{\alpha}\sinh\alpha}\ \exp\left\{2\alpha\,\frac{E\mp\mu B}{\hbar\omega_c} - \frac{m\omega_c}{4\hbar\alpha}(z-z')^2\right\} \\
&\times \exp\left\{-\frac{m\omega_c}{4\hbar}\ [\,(x-x')^2 + (y-y')^2\,]\ \coth\alpha\right\}\ .
\end{aligned}
$$

Analytic continuation to the upper half-plane of the complex energy $\Im\mathrm{m}(E) > 0$ can be obtained under the change of variable $\alpha = i\theta$ that gives

$$
\begin{aligned}
G^{+}(E;\mathbf{r},\mathbf{r}') =\ & \frac{m\omega_c}{4\pi\hbar^2}\sqrt{\frac{m}{\pi\hbar\omega_c}}\ \exp\left\{-i\,\frac{m\omega_c}{2\hbar}\,(x-x')(y+y') + \frac{3\pi i}{4}\right\} \\
&\times \int_0^\infty \frac{d\theta}{\sqrt{\theta}\sin\theta}\ \exp\left\{2i\theta\,\frac{E\mp\mu B}{\hbar\omega_c} + i\,\frac{m\omega_c}{4\hbar\theta}(z-z')^2\right\} \\
&\times \exp\left\{i\,\frac{m\omega_c}{4\hbar}\ [\,(x-x')^2 + (y-y')^2\,]\ \cot\theta\right\}\ .
\end{aligned}
$$

Problem VIII.3. Calculate the gauge transformation which connects the asymmetric Landau's gauge $A_x = -By\,,\ A_y = A_z = 0$ to the symmetric gauge $A'_x = -By/2\,,\ A'_y = Bx/2\,,\ A'_z = 0\,$, with $B > 0\,$.

Solution. In classical Electrodynamics the time independent gauge transformation on the vector potentials relating two different gauge choices is given by

$$\mathbf{A}'(\mathbf{r}) = \mathbf{A}(\mathbf{r}) + \nabla f(\mathbf{r}) \ .$$

Notice that the canonical dimensions of the *gauge function* $f(t, \mathbf{r})$ are G cm^2, i.e. the gauge function is a magnetic field flux. In Quantum Mechanics the gauge transformations on the wave functions are defined as follows: under the above gauge transformation on the vector potentials, the wave function must undergo a *local phase transformation*

$$\psi'(t, \mathbf{r}) = \psi(t, \mathbf{r}) \ \exp\{-i\phi(\mathbf{r})\} \ ,$$

such that

$$\left[\,\widehat{\mathbf{p}} - \frac{e}{c}\,\mathbf{A}'(\mathbf{r})\right]\,\psi'(t, \mathbf{r}) = \exp\{-i\phi(\mathbf{r})\}\left[\,\widehat{\mathbf{p}} - \frac{e}{c}\,\mathbf{A}(\mathbf{r})\right]\,\psi(t, \mathbf{r}) \ ,$$

that means, the wave function must transform *covariantly* under the local phase transformation. It is very easy to find the phase function $\phi(\mathbf{r})$ in terms of the gauge function $f(\mathbf{r})$. As a matter of fact we have

$$\begin{aligned}
&\left[\,\widehat{\mathbf{p}} - \frac{e}{c}\,\mathbf{A}'(\mathbf{r})\right]\,\psi'(t, \mathbf{r}) = \\
&\left[\,\widehat{\mathbf{p}} - \frac{e}{c}\,\mathbf{A}(\mathbf{r}) - \frac{e}{c}\,\nabla f(\mathbf{r})\right]\,\psi(t, \mathbf{r}) \ \exp\{-i\phi(\mathbf{r})\} = \\
&\exp\{-i\phi(\mathbf{r})\}\left[\,\widehat{\mathbf{p}} - \frac{e}{c}\,\mathbf{A}(\mathbf{r})\right]\,\psi(t, \mathbf{r}) - \frac{e}{c}\,\nabla f(\mathbf{r})\psi'(t, \mathbf{r}) - \hbar\psi'(t, \mathbf{r})\nabla\phi(\mathbf{r}) \ ,
\end{aligned}$$

so that we must require

$$\phi(\mathbf{r}) = -\frac{e}{\hbar c}\,f(\mathbf{r}) \ + \ \text{constant} \ .$$

Notice that the phase function is dimensionless, as it does, owing to the presence of the so called *quantum flux* $hc/e = 4.136 \times 10^{-7}$ G cm^2. Now we have evidently

$$f(x,y) \;=\; \frac{B}{2}\,xy\ , \qquad\qquad \phi(x,y) \;=\; -\frac{ef}{\hbar c}\ ,$$

so that the gauge transformation of the Schrödinger-Pauli's spinor reads

$$\psi'(t,\mathbf{r}) = \exp\left\{ i\pi\frac{eB}{hc}\,xy \right\}\, \psi(t,\mathbf{r})\ .$$

As a consequence, taking eq. (1.9) into account, it follows that the degenerate eigenfunctions of the Landau's problem in the symmetric gauge turn out to be

$$\begin{aligned}
&\psi_{n,p_z,p_x}(x,y,z) = \frac{1}{2\pi\hbar}\exp\left\{ \frac{i}{\hbar}\,(xp_x + zp_z) + i\pi\frac{eB}{hc}\,xy \right\}\ \times \\
&\left(\frac{m\omega_c}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{n!2^n}}\exp\left\{ -\frac{m\omega_c}{2\hbar}\left(y + \frac{p_x}{m\omega_c}\right)^2 \right\} H_n\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y + \frac{p_x}{m\omega_c}\right) \right]\ ,
\end{aligned}$$

in which H_n denotes the n-th Hermite's polynomial. The above improper degenerate eigenfunctions are normalized according to

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dxdydz\ \psi_{n,p_z,p_x}(x,y,z)\,\psi^*_{m,q_z,q_x}(x,y,z) = \delta_{nm}\,\delta\left(p_z - q_z\right)\delta\left(p_x - q_x\right)\ .$$

As a matter of fact, it is not difficult to show that the stationary Schrödinger-Pauli's equation transforms covariantly under the local phase change of the spinor: actually,

$$\begin{aligned}
&\left[\widehat{\mathbf{p}} - \frac{e}{c}\,\mathbf{A}'(\mathbf{r})\right]^2 \psi'(t,\mathbf{r}) = \\
&\left[\widehat{\mathbf{p}} - \frac{e}{c}\,\mathbf{A}'(\mathbf{r})\right]\ \exp\{-i\phi(\mathbf{r})\}\left[\widehat{\mathbf{p}} - \frac{e}{c}\,\mathbf{A}(\mathbf{r})\right]\ \psi(t,\mathbf{r}) = \\
&\exp\{-i\phi(\mathbf{r})\}\ \left[\widehat{\mathbf{p}} - \frac{e}{c}\,\mathbf{A}(\mathbf{r})\right]^2 \psi(t,\mathbf{r})\ .
\end{aligned}$$

It immediately follows therefrom

$$\widehat{H}'\psi'(t,\mathbf{r}) = \left[\frac{1}{2m}\left\{\widehat{\mathbf{p}} - \frac{e}{c}\mathbf{A}'(\mathbf{r})\right\}^2 - \vec{\mu}\cdot\mathbf{B} \right]\psi'(t,\mathbf{r}) = \exp\{-i\phi(\mathbf{r})\}\,\widehat{H}\,\psi(t,\mathbf{r})$$

which manifestly implies that *the spectrum of the hamiltonian is gauge invariant, whereas the eigenfunctions are related through an overall multiplicative local phase factor.*

Problem VIII.4. Calculate the electric current density carried on by the Landau's bands.

Solution. In Quantum Mechanics the *probability current density vector* $\mathbf{j}(t,\mathbf{r})$ is defined to be [cfr. e.g. E. Merzbacher (1970): *Quantum Mechanics*, John Wiley & Sons, New York, eq. (4.5a) p. 37]

$$\mathbf{j}(t,\mathbf{r}) \;=\; \frac{\hbar}{2mi}\,[\,\psi^*\nabla\psi - (\nabla\psi^*)\psi\,] \;\; .$$

Notice that, iff the wave functions have the canonical dimension $[\;\psi\;]=\mathrm{cm}^{-3/2}$, then the canonical dimensions of the probability current density are $[\;\mathbf{j}\;] = \mathrm{cm}^{-2}\;\mathrm{s}^{-1}$ as it does. However, in the presence of the electromagnetic field, in order to keep the property of the gauge invariance of the probability current density vector, it must be generalized as follows: namely,

$$\mathbf{j}(t,\mathbf{r}) \;=\; \frac{\hbar}{2mi}\,[\,\psi^*\mathbf{D}\psi - \psi(\mathbf{D}\psi)^*\,] \;\; ,$$

where we have introduced the so called *covariant derivative*

$$D_x \;:=\; \partial_x - \frac{ie}{\hbar c}\,A_x(x,y,z)\;, \qquad \text{et cetera}\;.$$

Then we have

$$\begin{aligned} D'_x\psi'(\mathbf{r}) &= \left\{\partial_x - \frac{ie}{\hbar c}\,[\,A_x(\mathbf{r}) + \partial_x f(\mathbf{r})\,]\right\}\exp\left\{\frac{ie}{\hbar c}\,f(\mathbf{r})\right\}\psi(\mathbf{r}) \\ &= \exp\left\{\frac{ie}{\hbar c}\,f(\mathbf{r})\right\}D_x\,\psi(\mathbf{r})\;,\;\text{et cetera}\;, \end{aligned}$$

so that the probability current density vector turns out to be manifestly gauge invariant. In the asymmetric Landau's gauge, the Landau's bands are spread out by the continuous infinity of the degenerate eigenfunctions

$$\Psi_{n,p_z,p_x}(x,y,z) = (2\pi\hbar)^{-1} \exp\left\{\frac{i}{\hbar}\,(xp_x + zp_z)\right\}\, \sqrt{m\hbar\omega_c}\ \times$$
$$\left(\frac{m\omega_c}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{n!2^n}} \exp\left\{-\frac{m\omega_c}{2\hbar}\left(y + \frac{p_x}{m\omega_c}\right)^2\right\} H_n\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y + \frac{p_x}{m\omega_c}\right)\right]\ ,$$

where p_x is the degeneracy quantum number, whereas the pairs (n, p_z) uniquely identify a specific Landau's band. Notice that the above eigenfunctions differ from those ones of eq. (1.9) by an overall factor $\sqrt{m\hbar\omega_c}$ to guarantee $[\ \Psi\ ] = \mathrm{cm}^{-3/2}$. Then we readily find

$$j_x(n,p_z,p_x;\mathbf{r}) = \left(\frac{p_x}{m} + \omega_c y\right) |\Psi_{n,p_z,p_x}(x,y,z)|^2 = \frac{\omega_c}{4\pi^2\hbar}\,(p_x + m\omega_c y)\left(\frac{m\omega_c}{\pi\hbar}\right)^{1/2} \frac{2^{-n}}{n!}$$
$$\times\ \exp\left\{-\frac{m\omega_c}{\hbar}\left(y + \frac{p_x}{m\omega_c}\right)^2\right\} H_n^2\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y + \frac{p_x}{m\omega_c}\right)\right]\ .$$

For any Landau's band, it is convenient to label its continuous infinite degeneracy in terms of the dimensionless real parameter $\eta := p_x(m\hbar\omega_c)^{-1/2}$. Then the probability current density along the Ox-direction carried on by each Landau's band becomes

$$j_x^{\mathrm{b}} = \int_{-\infty}^{+\infty} \frac{dp_x}{\sqrt{m\hbar\omega_c}}\ \frac{\omega_c}{4\pi^2\hbar}\,(p_x + m\omega_c y)\left(\frac{m\omega_c}{\pi\hbar}\right)^{1/2} \frac{2^{-n}}{n!}$$
$$\times\ \exp\left\{-\frac{m\omega_c}{\hbar}\left(y + \frac{p_x}{m\omega_c}\right)^2\right\} H_n^2\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y + \frac{p_x}{m\omega_c}\right)\right]$$

and after setting $\upsilon := y\sqrt{m\omega_c/\hbar}$ we can write

$$j_x^{\mathrm{b}} = \frac{m\omega_c^2}{4\pi^2\hbar} \int_{-\infty}^{+\infty} d\eta\ \frac{\eta + \upsilon}{n!2^n\sqrt{\pi}}\ \exp\left\{-(\upsilon + \eta)^2\right\}\ H_n^2(\upsilon + \eta)\ =\ 0\ .$$

Concerning the Oy-direction we find instead

$$D_y\Psi_{n,p_z,p_x} = \partial_y\Psi_{n,p_z,p_x}(x,y,z) = -\frac{m\omega_c}{\hbar}\left(y + \frac{p_x}{m\omega_c}\right)\Psi_{n,p_z,p_x}(x,y,z)$$
$$+\sqrt{\frac{m\omega_c}{\hbar}}\,(2\pi\hbar)^{-1} \exp\left\{\frac{i}{\hbar}\,(xp_x + zp_z)\right\}\left(\frac{m\omega_c}{\pi\hbar}\right)^{1/4} \sqrt{\frac{m\hbar\omega_c}{n!2^n}}$$
$$\times\ \exp\left\{-\frac{m\omega_c}{2\hbar}\left(y + \frac{p_x}{m\omega_c}\right)^2\right\} 2nH_{n-1}\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y + \frac{p_x}{m\omega_c}\right)\right]\ .$$

From the recursion formula of the Hermite's polynomials

$$2nH_{n-1}(\xi) = 2\xi H_n(\xi) - H_{n+1}(\xi) \ ,$$

we get

$$\begin{aligned}
D_y \Psi_{n,p_z,p_x}(x,y,z) &= \frac{m\omega_c}{\hbar}\left(y + \frac{p_x}{m\omega_c}\right)\Psi_{n,p_z,p_x}(x,y,z) \\
&- \sqrt{\frac{m\omega_c}{\hbar}}\,(2\pi\hbar)^{-1}\exp\left\{\frac{i}{\hbar}\,(xp_x + zp_z)\right\}\left(\frac{m\omega_c}{\pi\hbar}\right)^{1/4}\sqrt{\frac{m\hbar\omega_c}{n!2^n}} \\
&\times\ \exp\left\{-\frac{m\omega_c}{2\hbar}\left(y + \frac{p_x}{m\omega_c}\right)^2\right\} H_{n+1}\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(y + \frac{p_x}{m\omega_c}\right)\right]
\end{aligned}$$

that means eventually

$$\begin{aligned}
&D_y \Psi_{n,p_z,p_x}(x,y,z) \ = \\
&\frac{m\omega_c}{\hbar}\left(y + \frac{p_x}{m\omega_c}\right)\Psi_{n,p_z,p_x}(x,y,z) - \sqrt{\frac{2m\omega_c}{\hbar}\,(n+1)}\ \Psi_{n+1,p_z,p_x}(x,y,z)
\end{aligned}$$

whence we finally obtain

$$j_y(n,p_z,p_x;x,y,z) \ = \ 0 \ .$$

Along the Oz-direction we have

$$j_z(n,p_z,p_x;x,y,z) = \frac{p_z}{m}\ |\Psi_{n,p_z,p_x}(x,y,z)|^2 \ ,$$

so that the resulting current intensities are

$$I_x = I_y = 0 \ , \qquad dI_z = -ev_z\,\frac{eB}{hc}\,\mathcal{A}\,\frac{dp_z}{h} \ = \ -ev_z\,\frac{N}{\nu}\,\frac{dp_z}{h} \ ,$$

where $\mathcal{A}$ is the area of a section in the $Oxy-$plane, N is the average number of electrons whereas $\nu \equiv hcN/eB\mathcal{A}$ is the so called *filling fraction* of the Landau's bands.