

5.8: The Ideal Fermi Gas

Grand potential and particle number

The grand potential of the ideal Fermi gas is, per Equation [Oqsm],

$$\begin{aligned}\Omega(T, V, \mu) &= -V k_B T \sum_{\alpha} \ln \left(1 + e^{\mu/k_B T} e^{-\varepsilon_{\alpha}/k_B T} \right) \\ &= -V k_B T \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \ln \left(1 + e^{(\mu-\varepsilon)/k_B T} \right).\end{aligned}$$

The average number of particles in a state with energy ε is

$$n(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} + 1}, \quad (5.8.1)$$

hence the total number of particles is

$$N = V \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \frac{1}{e^{(\varepsilon-\mu)/k_B T} + 1}. \quad (5.8.2)$$

The Fermi distribution

We define the function

$$f(\varepsilon) \equiv \frac{1}{e^{\varepsilon/k_B T} + 1}, \quad (5.8.3)$$

known as the *Fermi distribution*. In the $T \rightarrow \infty$ limit, $f(\varepsilon) \rightarrow \frac{1}{2}$ for all finite values of ε . As $T \rightarrow 0$, $f(\varepsilon)$ approaches a step function $\Theta(-\varepsilon)$. The average number of particles in a state of energy ε in a system at temperature T and chemical potential μ is $n(\varepsilon) = f(\varepsilon - \mu)$. In Figure [fermidist] we plot $f(\varepsilon - \mu)$ versus ε for three representative temperatures.

$T = 0$ and the Fermi surface

At $T = 0$, we therefore have $n(\varepsilon) = \Theta(\mu - \varepsilon)$, which says that all single particle energy states up to $\varepsilon = \mu$ are filled, and all energy states above $\varepsilon = \mu$ are empty. We call $\mu(T = 0)$ the *Fermi energy*: $\varepsilon_F = \mu(T = 0)$. If the single particle dispersion $\varepsilon(\mathbf{k})$ depends only on the wavevector \mathbf{k} , then the locus of points in \mathbf{k} -space for which $\varepsilon(\mathbf{k}) = \varepsilon_F$ is called the *Fermi surface*. For isotropic systems, $\varepsilon(\mathbf{k}) = \varepsilon(k)$ is a function only of the magnitude $k = |\mathbf{k}|$, and the Fermi surface is a sphere in $d = 3$ or a circle in $d = 2$. The radius of this circle is the *Fermi wavevector*, k_F . When there is internal (spin) degree of freedom, there is a Fermi surface and Fermi wavevector (for isotropic systems) for each polarization state of the internal degree of freedom.

[fermidist] The Fermi distribution, $f(\varepsilon) = \frac{1}{e^{\varepsilon/k_B T} + 1}$. Here we have set $k_B = 1$ and taken $\mu = 2$, with $T = \{1, 2, 20\}$ (blue), $T = \{3, 10, 100\}$ (green), and $T = 2$ (red). In the $T \rightarrow 0$ limit, $f(\varepsilon)$ approaches a step function $\Theta(-\varepsilon)$.

[fermidist] The Fermi distribution, $f(\varepsilon) = \frac{1}{e^{\varepsilon/k_B T} + 1}$. Here we have set $k_B = 1$ and taken $\mu = 2$, with $T = \frac{1}{20}$ (blue), $T = \frac{1}{4}$ (green), and $T = 2$ (red). In the $T \rightarrow 0$ limit, $f(\varepsilon)$ approaches a step function $\Theta(-\varepsilon)$.

Let's compute the Fermi wavevector k_F and Fermi energy ε_F for the IFG with a ballistic dispersion $\varepsilon(\mathbf{k}) = \hbar^2 \mathbf{k}^2 / 2m$. The number density is

$$n = g \int \frac{d^d k}{(2\pi)^d} \Theta(k_F - k) = \frac{g \Omega_d}{(2\pi)^d} \cdot \frac{k_F^d}{d} = \begin{cases} g k_F / \pi & (d = 1) \\ g k_F^2 / 4\pi & (d = 2) \\ g k_F^3 / 6\pi^2 & (d = 3) \end{cases}, \quad (5.8.4)$$

where $\Omega_d = 2\pi^{d/2} / \Gamma(d/2)$ is the area of the unit sphere in d space dimensions. Note that the form of $n(k_F)$ is independent of the dispersion relation, so long as it remains isotropic. Inverting the above expressions, we obtain $k_F(n)$:

$$k_F = 2\pi \left(\frac{dn}{g \Omega_d} \right)^{1/d} = \begin{cases} \pi n / g & (d = 1) \\ (4\pi n / g)^{1/2} & (d = 2) \\ (6\pi^2 n / g)^{1/3} & (d = 3) \end{cases}. \quad (5.8.5)$$

The Fermi energy in each case, for ballistic dispersion, is therefore

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{2\pi^2 \hbar^2}{m} \left(\frac{dn}{g \Omega_d} \right)^{2/d} = \begin{cases} \frac{\pi^2 \hbar^2 n^2}{2g^2 m} & (d = 1) \\ \frac{2\pi \hbar^2 n}{g m} & (d = 2) \\ \frac{\hbar^2}{2m} \left(\frac{6\pi^2 n}{g} \right)^{2/3} & (d = 3) \end{cases}. \quad (5.8.6)$$

Another useful result for the ballistic dispersion, which follows from the above, is that the density of states at the Fermi level is given by

$$g(\varepsilon_F) = \left(\frac{S_d}{(2\pi)^d} \right) \frac{\Omega_d}{k_F} \frac{dk_F}{d\varepsilon_F} = \frac{S_d \Omega_d}{(2\pi)^d} \frac{1}{k_F} \frac{1}{\hbar^2} \frac{d k_F^2}{d\varepsilon_F} = \frac{S_d \Omega_d}{(2\pi)^d} \frac{2 k_F}{\hbar^2}.$$

For the electron gas, we have $g = 2$. In a metal, one typically has $k_F \sim 0.5 \text{ \AA}^{-1}$ to 2 \AA^{-1} , and $\varepsilon_F \sim 1 \text{ eV} - 10 \text{ eV}$. Due to the effects of the crystalline lattice, electrons in a solid behave as if they had an *effective mass* m^* which is typically on the order of the electron mass but very often about an order of magnitude smaller, particularly in semiconductors.

Nonisotropic dispersions $\varepsilon(\mathbf{k})$ are more interesting in that they give rise to non-spherical Fermi surfaces. The simplest example is that of a two-dimensional 'tight-binding' model of electrons hopping on a square lattice, as may be appropriate in certain layered materials. The dispersion relation is then

$$\varepsilon(k_x, k_y) = -2t \cos(k_x a) - 2t \cos(k_y a), \quad (5.8.7)$$

where k_x and k_y are confined to the interval $[-\frac{\pi}{a}, \frac{\pi}{a}]$. The quantity t has dimensions of energy and is known as the *hopping integral*. The Fermi surface is the set of points (k_x, k_y) which satisfies $\varepsilon(k_x, k_y) = \varepsilon_F$. When ε_F achieves its minimum value of $\varepsilon_F^{\min} = -4t$, the Fermi surface collapses to a point at $(k_x, k_y) = (0, 0)$. For energies just above this minimum value, we can expand the dispersion in a power series, writing

$$\varepsilon(k_x, k_y) = -4t + ta^2 (k_x^2 + k_y^2) - \frac{1}{12} ta^4 (k_x^4 + k_y^4) + \dots \quad (5.8.8)$$

If we only work to quadratic order in k_x and k_y , the dispersion is isotropic, and the Fermi surface is a circle, with $k_F^2 = (\varepsilon_F + 4t)/ta^2$. As the energy increases further, the continuous $O(2)$ rotational invariance is broken down to the discrete group of rotations of the square, C_{4v} . The Fermi surfaces distort and eventually, at $\varepsilon_F = 0$, the Fermi surface is itself a square. As ε_F increases further, the

square turns back into a circle, but centered about the point $(\frac{\pi}{a}, \frac{\pi}{a})$. Note that everything is periodic in k_x and k_y modulo $\frac{2\pi}{a}$. The Fermi surfaces for this model are depicted in the upper right panel of Figure [fermisurfs].

[fermisurfs] Fermi surfaces for two and three-dimensional structures. Upper left: free particles in two dimensions. Upper right: 'tight binding' electrons on a square lattice. Lower left: Fermi surface for cesium, which is predominantly composed of electrons in the 6s orbital shell. Lower right: the Fermi surface of yttrium has two parts. One part (yellow) is predominantly due to 5s electrons, while the other (pink) is due to 4d electrons. (Source: www.phys.ufl.edu/fermisurface/)

[fermisurfs] Fermi surfaces for two and three-dimensional structures. Upper left: free particles in two dimensions. Upper right: 'tight binding' electrons on a square lattice. Lower left: Fermi surface for cesium, which is predominantly composed of electrons in the 6s orbital shell. Lower right: the Fermi surface of yttrium has two parts. One part (yellow) is predominantly due to 5s electrons, while the other (pink) is due to 4d electrons. (Source: www.phys.ufl.edu/fermisurface/)

Fermi surfaces in three dimensions can be very interesting indeed, and of great importance in understanding the electronic properties of solids. Two examples are shown in the bottom panels of Figure [fermisurfs]. The electronic configuration of cesium (Cs) is $[Xe] 6s^1$. The 6s electrons 'hop' from site to site on a body centered cubic (BCC) lattice, a generalization of the simple two-dimensional square lattice hopping model discussed above. The elementary unit cell in \mathbf{k} space, known as the *first Brillouin zone*, turns out to be a dodecahedron. In yttrium, the electronic structure is $[Kr] 5s^2 4d^1$, and there are two electronic energy bands at the Fermi level, meaning two Fermi surfaces. Yttrium forms a hexagonal close packed (HCP) crystal structure, and its first Brillouin zone is shaped like a hexagonal pillbox.

Spin-split Fermi surfaces

Consider an electron gas in an external magnetic field H . The single particle Hamiltonian is then

$$H = \frac{p^2}{2m} + \mu_B H \sigma$$

where μ_B is the *Bohr magneton*,

$$\mu_B = \frac{e\hbar}{2m} = 5.788 \times 10^{-9} \text{ eV} \quad \mu_B/k_B = 6.717 \times 10^{-5} \text{ K}$$

where m is the electron mass. What happens at $T = 0$ to a noninteracting electron gas in a magnetic field?

Electrons of each spin polarization form their own Fermi surfaces. That is, there is an up spin Fermi surface, with Fermi wavevector $k_{F\uparrow}$, and a down spin Fermi surface, with Fermi wavevector $k_{F\downarrow}$. The individual Fermi energies, on the other hand, must be equal, hence

$$\frac{\hbar^2 k_{F\uparrow}^2}{2m} + \mu_B H = \frac{\hbar^2 k_{F\downarrow}^2}{2m} - \mu_B H,$$

which says

$$k_{F\downarrow}^2 - k_{F\uparrow}^2 = \frac{2eH}{\hbar c}. \quad (5.8.9)$$

The total density is

$$n = \frac{k_{F\uparrow}^3}{6\pi^2} + \frac{k_{F\downarrow}^3}{6\pi^2} \implies k_{F\uparrow}^3 + k_{F\downarrow}^3 = 6\pi^2 n. \quad (5.8.10)$$

Clearly the down spin Fermi surface grows and the up spin Fermi surface shrinks with increasing H . Eventually, the minority spin Fermi surface vanishes altogether. This happens for the up spins when $k_{F\uparrow} = 0$. Solving for the critical field, we obtain

$$H_c = \frac{\hbar c}{2e} \cdot (6\pi^2 n)^{1/3}. \quad (5.8.11)$$

In real magnetic solids, like cobalt and nickel, the spin-split Fermi surfaces are not spheres, just like the case of the (spin degenerate) Fermi surfaces for Cs and Y shown in Figure [fermisurfs].

The Sommerfeld expansion

In dealing with the ideal Fermi gas, we will repeatedly encounter integrals of the form

$$\mathcal{I}(T, \mu) \equiv \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon - \mu) \phi(\varepsilon). \quad (5.8.12)$$

The Sommerfeld expansion provides a systematic way of expanding these expressions in powers of T and is an important analytical tool in analyzing the low temperature properties of the ideal Fermi gas (IFG).

We start by defining

$$\Phi(\varepsilon) \equiv \int_{-\infty}^{\varepsilon} d\varepsilon' \phi(\varepsilon') \quad (5.8.13)$$

so that $\phi(\varepsilon) = \Phi'(\varepsilon)$. We then have

$$\begin{aligned} \mathcal{I} &= \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon - \mu) \frac{d\Phi}{d\varepsilon} \\ &= - \int_{-\infty}^{\infty} d\varepsilon f'(\varepsilon) \Phi(\mu + \varepsilon), \end{aligned}$$

where we assume $\Phi(-\infty) = 0$. Next, we invoke Taylor's theorem, to write

$$\begin{aligned} \Phi(\mu + \varepsilon) &= \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} \frac{d^n \Phi}{d\mu^n} \\ &= \exp\left(\varepsilon \frac{d}{d\mu}\right) \Phi(\mu). \end{aligned}$$

This last expression involving the exponential of a differential operator may appear overly formal but it proves extremely useful. Since

$$f'(\varepsilon) = -\frac{1}{k_B T} \frac{e^{\varepsilon/k_B T}}{(e^{\varepsilon/k_B T} + 1)^2}, \quad (5.8.14)$$

we can write

$$\mathcal{I} = \int_{-\infty}^{\infty} d\varepsilon \frac{e^{\varepsilon/k_B T}}{(e^{\varepsilon/k_B T} + 1)^2} \Phi(\mu + \varepsilon), \quad (5.8.15)$$

with $v = \varepsilon/k_B T$, where

$$D = k_B T \frac{d}{d\mu} \quad (5.8.16)$$

is a dimensionless differential operator. The integral can now be done using the methods of complex integration:¹⁴

$$\begin{aligned} \int_{-\infty}^{\infty} dv \frac{e^{vD}}{(e^v + 1)(e^{-v} + 1)} &= 2\pi i \sum_{n=1}^{\infty} \operatorname{Res} \left[\frac{e^{vD}}{(e^v + 1)(e^{-v} + 1)} \right]_{v=(2n+1)i\pi} \\ &= -2\pi i \sum_{n=0}^{\infty} D e^{(2n+1)i\pi D} \\ &= -\frac{2\pi i D e^{i\pi D}}{1 - e^{2\pi i D}} = \pi D \csc \pi D . \end{aligned}$$

 [vcontour] Deformation of the complex integration contour in Equation [vcon].

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Thus,

$$\mathcal{I}(T, \mu) = \pi D \csc(\pi D) \Phi(\mu) , \quad (5.8.17)$$

which is to be understood as the differential operator $\pi D \csc(\pi D) = \pi D / \sin(\pi D)$ acting on the function $\Phi(\mu)$. Appealing once more to Taylor's theorem, we have

$$\pi D \csc(\pi D) = 1 + \frac{\pi^2}{6} (k_B T)^2 \frac{d^2}{d\mu^2} + \frac{7\pi^4}{360} (k_B T)^4 \frac{d^4}{d\mu^4} + \dots \quad (5.8.18)$$

Thus,

$$\begin{aligned} \mathcal{I}(T, \mu) &= \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon - \mu) \phi(\varepsilon) \\ &= \int_{-\infty}^{\mu} d\varepsilon \phi(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 \phi'(\mu) + \frac{7\pi^4}{360} (k_B T)^4 \phi'''(\mu) + \dots \end{aligned}$$

If $\phi(\varepsilon)$ is a polynomial function of its argument, then each derivative effectively reduces the order of the polynomial by one degree, and the dimensionless parameter of the expansion is $(T/\mu)^2$. This procedure is known as the *Sommerfeld expansion*.

Chemical potential shift

As our first application of the Sommerfeld expansion formalism, let us compute $\mu(n, T)$ for the ideal Fermi gas. The number density $n(T, \mu)$ is

$$\begin{aligned} n &= \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) f(\varepsilon - \mu) \\ &= \int_{-\infty}^{\mu} d\varepsilon g(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 g'(\mu) + \dots \end{aligned}$$

Let us write $\mu = \varepsilon_F + \delta\mu$, where $\varepsilon_F = \mu(T = 0, n)$ is the Fermi energy, which is the chemical potential at $T = 0$. We then have

$$\begin{aligned} n &= \int_{-\infty}^{\varepsilon_F + \delta\mu} d\varepsilon g(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 g'(\varepsilon_F + \delta\mu) + \dots \\ &= \int_{-\infty}^{\varepsilon_F} d\varepsilon g(\varepsilon) + g(\varepsilon_F) \delta\mu + \frac{\pi^2}{6} (k_B T)^2 g'(\varepsilon_F) + \dots , \end{aligned}$$

from which we derive

$$\delta\mu = -\frac{\pi^2}{6} (k_B T)^2 \frac{g'(\varepsilon_F)}{g(\varepsilon_F)} + \mathcal{O}(T^4) . \quad (5.8.19)$$

Note that $g'/g = (\ln g)'$. For a ballistic dispersion, assuming $g = 2$,

$$g(\varepsilon) = 2 \int \frac{d^3k}{(2\pi)^3} \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right) = \frac{m k(\varepsilon)}{\pi^2 \hbar^2} \Big|_{k(\varepsilon) = \frac{1}{\hbar} \sqrt{2m\varepsilon}} \quad (5.8.20)$$

Thus, $g(\varepsilon) \propto \varepsilon^{1/2}$ and $(\ln g)' = \frac{1}{2} \varepsilon^{-1}$, so

$$\mu(n, T) = \varepsilon_F - \frac{\pi^2}{12} \frac{(k_B T)^2}{\varepsilon_F} + \dots , \quad (5.8.21)$$

where $\varepsilon_F(n) = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}$.

Specific heat

The energy of the electron gas is

$$\delta\mu(T, n, H) = -\left\{ \frac{\pi^2}{6} (k_B T)^2 + (\tilde{\mu} H)^2 \right\} \frac{g'(\varepsilon_F)}{g(\varepsilon_F)} + \dots \quad (5.8.26)$$

[FSmag] Fermi distributions in the presence of an external Zeeman-coupled magnetic field.

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We next compute the difference $n_{\uparrow} - n_{\downarrow}$ in the densities of up and down spin electrons:

$$\begin{aligned} n_{\uparrow} - n_{\downarrow} &= \int_{-\infty}^{\infty} d\varepsilon \left\{ g_{\uparrow}(\varepsilon) - g_{\downarrow}(\varepsilon) \right\} f(\varepsilon - \mu) \\ &= \frac{1}{2} \int_{-\infty}^{\infty} d\varepsilon \left\{ g(\varepsilon - \tilde{\mu} H) - g(\varepsilon + \tilde{\mu} H) \right\} f(\varepsilon - \mu) \\ &= -\tilde{\mu} H \cdot \pi D \csc(\pi D) g(\mu) + \mathcal{O}(H^3). \end{aligned}$$

We needn't go beyond the trivial lowest order term in the Sommerfeld expansion, because H is already assumed to be small. Thus, the magnetization density is

$$M = \mu_B (n_{\uparrow} - n_{\downarrow}) = \tilde{\mu} \pi D \csc(\pi D) g(\mu) + \mathcal{O}(H^3),$$

in which the magnetic susceptibility is

$$\chi = \frac{\partial M}{\partial H} = \pi D \csc(\pi D) g(\mu) + \mathcal{O}(H^2).$$

This is called the *Pauli paramagnetic susceptibility*.

Landau Diamagnetism

When orbital effects are included, the single particle energy levels are given by

$$\varepsilon(n, k_z, \sigma) = \left(n + \frac{1}{2}\right) \hbar \omega_c + \frac{\hbar^2 k_z^2}{2m^*} + \tilde{\mu} H \sigma. \quad (5.8.27)$$

Here n is a Landau level index, and $\omega_c = eH/m^*c$ is the *cyclotron frequency*. Note that

$$\frac{\tilde{\mu} H}{\hbar \omega_c} = \frac{ge\hbar H}{4mc} \cdot \frac{m^* c}{\hbar e H} = \frac{g}{4} \cdot \frac{m^*}{m}. \quad (5.8.28)$$

Accordingly, we define the ratio $r \equiv (g/2) \times (m^*/m)$. We can then write

$$\varepsilon(n, k_z, \sigma) = \left(n + \frac{1}{2} + \frac{1}{2} r \sigma\right) \hbar \omega_c + \frac{\hbar^2 k_z^2}{2m^*}. \quad (5.8.29)$$

The grand potential is then given by

$$\Omega = -\frac{HA}{\phi_0} \cdot L_z \cdot k_B T \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \sum_{n=0}^{\infty} \sum_{\sigma=\pm 1} \ln \left[1 + e^{\mu/k_B T} e^{-(n+\frac{1}{2}+\frac{1}{2}r\sigma)\hbar\omega_c/k_B T} e^{-\hbar^2 k_z^2/2m^*k_B T} \right]. \quad (5.8.30)$$

A few words are in order here regarding the prefactor. In the presence of a uniform magnetic field, the energy levels of a two-dimensional ballistic charged particle collapse into Landau levels. The number of states per Landau level scales with the area of the system, and is equal to the number of flux quanta through the system: $N_{\phi} = HA/\phi_0$, where $\phi_0 = hc/e$ is the Dirac flux quantum. Note that

$$\frac{HA}{\phi_0} \cdot L_z \cdot k_B T = \hbar \omega_c \cdot \frac{V}{\lambda_T^3}, \quad (5.8.31)$$

hence we can write

$$\Omega(T, V, \mu, H) = \hbar \omega_c \sum_{n=0}^{\infty} \sum_{\sigma=\pm 1} Q\left(\left(n + \frac{1}{2} + \frac{1}{2} r \sigma\right) \hbar \omega_c - \mu\right), \quad (5.8.32)$$

where

$$Q(\varepsilon) = -\frac{V}{\lambda_T^3} \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \ln \left[1 + e^{-\varepsilon/k_B T} e^{-\hbar^2 k_z^2/2m^*k_B T} \right]. \quad (5.8.33)$$

We now invoke the Euler-MacLaurin formula,

$$\sum_{n=0}^{\infty} F(n) = \int_0^{\infty} dx F(x) + \frac{1}{2} F(0) - \frac{1}{12} F'(0) + \dots, \quad (5.8.34)$$

resulting in

$$\begin{aligned} \Omega = \sum_{\sigma=\pm 1} \left\{ \int_{\frac{1}{2}(1+r\sigma)\hbar\omega_c}^{\infty} d\varepsilon Q(\varepsilon - \mu) + \frac{1}{2} \hbar \omega_c Q\left(\frac{1}{2}(1+r\sigma)\hbar\omega_c - \mu\right) \right. \\ \left. - \frac{1}{12} (\hbar \omega_c)^2 Q'\left(\frac{1}{2}(1+r\sigma)\hbar\omega_c - \mu\right) + \dots \right\} \end{aligned}$$

We next expand in powers of the magnetic field H to obtain

$$\Omega(T, V, \mu, H) = 2 \int_0^{\infty} d\varepsilon Q(\varepsilon - \mu) + \left(\frac{1}{4} r^2 - \frac{1}{12}\right) (\hbar \omega_c)^2 Q'(-\mu) + \dots \quad (5.8.35)$$

Thus, the magnetic susceptibility is

$$\chi = \frac{\partial M}{\partial H} = \frac{2}{\phi_0} \left(\frac{1}{4} r^2 - \frac{1}{12} \right) \hbar \omega_c Q'(-\mu) + \dots$$

where κ_T is the isothermal compressibility^[6]. In most metals we have $m^* \approx m$ and the term in brackets is positive (recall $g \approx 2$). In semiconductors, however, we can have $m^* \ll m$; for example in GaAs we have $m^* = 0.067 m$. Thus, semiconductors can have a *diamagnetic* response. If we take $g = 2$ and $m^* = m$, we see that the orbital currents give rise to a diamagnetic contribution to the

magnetic susceptibility which is exactly $-\frac{1}{3}$ times as large as the contribution arising from Zeeman coupling. The net result is then paramagnetic ($\chi > 0$) and $\frac{2}{3}$ as large as the Pauli susceptibility. The orbital currents can be understood within the context of *Lenz's law*.

Exercise : Show that $-\frac{2}{V} Q'(-\mu) = n^2 \kappa_T$.

Moment formation in interacting itinerant electron systems

The Hubbard model

A noninteracting electron gas exhibits paramagnetism or diamagnetism, depending on the sign of χ , but never develops a spontaneous magnetic moment: $\mathbf{M}(\mathbf{H} = 0) = 0$. What gives rise to magnetism in solids? Overwhelmingly, the answer is that Coulomb repulsion between electrons is responsible for magnetism, in those instances in which magnetism arises. At first thought this might seem odd, since the Coulomb interaction is spin-independent. How then can it lead to a spontaneous magnetic moment?

To understand how Coulomb repulsion leads to magnetism, it is useful to consider a model interacting system, described by the Hamiltonian

$$\hat{H}_H = -t \sum_{\langle ij \rangle} \sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \mu_B B \sum_i (c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow})$$

This is none other than the famous *Hubbard model*, which has served as a kind of Rosetta stone for interacting electron systems. The first term describes hopping of electrons along the links of some regular lattice (the symbol $\langle ij \rangle$ denotes a link between sites i and j). The second term describes the local (on-site) repulsion of electrons. This is a single orbital model, so the repulsion exists when one tries to put two electrons in the orbital, with opposite spin polarization. Typically the Hubbard U parameter is on the order of electron volts. The last term is the Zeeman interaction of the electron spins with an external magnetic field. Orbital effects can be modeled by associating a phase $\exp(iA_{ij})$ to the hopping matrix element t between sites i and j , where the directed sum of A_{ij} around a plaquette yields the total magnetic flux through the plaquette in units of $\phi_0 = hc/e$. We will ignore orbital effects here. Note that the interaction term is short-ranged, whereas the Coulomb interaction falls off as $1/|\mathbf{R}_i - \mathbf{R}_j|$. The Hubbard model is thus unrealistic, although screening effects in metals do effectively render the interaction to be short-ranged.

Within the Hubbard model, the interaction term is local and written as $U n_{i\uparrow} n_{i\downarrow}$ on any given site. This term favors a local moment. This is because the chemical potential will fix the mean value of the total occupancy $n_{i\uparrow} + n_{i\downarrow}$, in which case it always pays to maximize the difference $|n_{i\uparrow} - n_{i\downarrow}|$.

Stoner mean field theory

There are no general methods available to solve for even the ground state of an interacting many-body Hamiltonian. We'll solve this problem using a *mean field* theory due to Stoner. The idea is to write the occupancy $n_{i\sigma}$ as a sum of average and fluctuating terms:

$$n_{i\sigma} = \langle n_{i\sigma} \rangle + \delta n_{i\sigma} \quad (5.8.36)$$

Here, $\langle n_{i\sigma} \rangle$ is the thermodynamic average; the above equation may then be taken as a definition of the fluctuating piece, $\delta n_{i\sigma}$. We assume that the average is site-independent. This is a significant assumption, for while we understand why each site should favor developing a moment, it is not clear that all these local moments should want to line up parallel to each other. Indeed, on a bipartite lattice, it is possible that the individual local moments on neighboring sites will be antiparallel, corresponding to an *antiferromagnetic* order of the spins. Our mean field theory will be one for *ferromagnetic* states.

We now write the interaction term as

$$\begin{aligned} n_{i\uparrow} n_{i\downarrow} &= \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + \langle n_{i\uparrow} \rangle \delta n_{i\downarrow} + \langle n_{i\downarrow} \rangle \delta n_{i\uparrow} + \overbrace{\delta n_{i\uparrow} \delta n_{i\downarrow}}^{(\text{fluct})^2} \\ &= -\langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + \langle n_{i\uparrow} \rangle \delta n_{i\downarrow} + \langle n_{i\downarrow} \rangle \delta n_{i\uparrow} + \mathcal{O}((\delta n)^2) \\ &= \frac{1}{4}(m^2 - n^2) + \frac{1}{2}n(n_{i\uparrow} + n_{i\downarrow}) + \frac{1}{2}m(n_{i\uparrow} - n_{i\downarrow}) + \mathcal{O}((\delta n)^2) \end{aligned}$$

where n and m are the average occupancy per spin and average spin polarization, each per unit cell:

$$\begin{aligned} n &= \langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle \\ m &= \langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle \end{aligned}$$

$\langle n_{i\sigma} \rangle = \frac{1}{2}(n - \sigma m)$. The mean field grand canonical Hamiltonian $\mathcal{K} = \hat{H} - \mu \mathcal{N}$, may then be written as

$$\hat{\mathcal{K}} = -t \sum_{\langle ij \rangle} \sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} + \frac{1}{2} \sum_i (n_{i\uparrow}^2 + n_{i\downarrow}^2) - \frac{1}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow})^2 + \mu \sum_i (n_{i\uparrow} + n_{i\downarrow})$$

where we've quantized spins along the direction of \mathbf{H} , defined as $\hat{\mathbf{z}}$. You should take note of two things here. First, the chemical potential is shifted *downward* (or the electron energies shifted *upward*) by an amount $\frac{1}{2}Un$, corresponding to the average energy of repulsion with the background. Second, the effective magnetic field has been shifted by an amount $\frac{1}{2}Um/\mu_B$, so the effective field is

$$H_{\text{eff}} = H + \frac{Um}{2\mu_B}$$

The *bare* single particle dispersions are given by $\epsilon_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} + \sigma \mu_B H$, where

$$\epsilon_{\mathbf{k}} = \sum_{\mathbf{R}} t(\mathbf{R}) e^{-i\mathbf{k} \cdot \mathbf{R}} \quad (5.8.37)$$

and $t_{ij} = t(\mathbf{R}_i - \mathbf{R}_j)$. For nearest neighbor hopping on a d -dimensional cubic lattice, $\epsilon_{\mathbf{k}} = -t \sum_{\mu=1}^d \cos(k_\mu a)$, where a is the lattice constant. Including the mean field effects, the *effective* single particle dispersions become

$$\tilde{\epsilon}_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} - \frac{1}{2}Un + \sigma \left(\frac{1}{2}Um + \mu_B H \right)$$

We now solve the mean field theory, by obtaining the free energy per site, $\varphi(n, T, H)$. First, note that $\varphi = \omega + \mu n$, where $\omega = \Omega/N_{\text{sites}}$ is the Landau, or grand canonical, free energy per site. This follows from the general relation $\Omega = F - \mu N$; note that the total electron number is $N = nN_{\text{sites}}$, since n is the electron number per unit cell (including both spin species). If $g(\epsilon)$ is the density of states per unit cell (rather than per unit volume), then we have¹⁷

$$\varphi = \frac{1}{4}U(m^2 + n^2) + \bar{\mu}n - \frac{1}{2}k_B T \int_{-\infty}^{\infty} d\epsilon g(\epsilon) \left\{ \ln \left(1 + e^{(\bar{\mu} - \epsilon - \Delta)/k_B T} \right) + \ln \left(1 + e^{(\bar{\mu} - \epsilon + \Delta)/k_B T} \right) \right\} \quad (5.8.38)$$

where $\bar{\mu} \equiv \mu - \frac{1}{2}Un$ and $\Delta \equiv \frac{1}{2}Um + \mu_B H$. From this free energy we derive two self-consistent equations for μ and m . The first comes from demanding that φ be a function of n and not of μ , $\partial\varphi/\partial\mu = 0$, which leads to

$$n = \frac{1}{2} \int_{-\infty}^{\infty} d\epsilon g(\epsilon) \left\{ f(\epsilon - \Delta - \bar{\mu}) + f(\epsilon + \Delta - \bar{\mu}) \right\}, \quad (5.8.39)$$

where $f(y) = [\exp(y/k_B T) + 1]^{-1}$ is the Fermi function. The second equation comes from minimizing f with respect to average moment m :

$$m = \frac{1}{2} \int_{-\infty}^{\infty} d\epsilon g(\epsilon) \left\{ f(\epsilon - \Delta - \bar{\mu}) - f(\epsilon + \Delta - \bar{\mu}) \right\}. \quad (5.8.40)$$

Here, we will solve the first equation, eq. [neqn], and use the results to generate a Landau expansion of the free energy φ in powers of m^2 . We assume that Δ is small, in which case we may write

$$n = \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \left\{ f(\varepsilon - \bar{\mu}) + \frac{1}{2} \Delta^2 f''(\varepsilon - \bar{\mu}) + \frac{1}{24} \Delta^4 f''''(\varepsilon - \bar{\mu}) + \dots \right\}. \quad (5.8.41)$$

We write $\bar{\mu}(\Delta) = \bar{\mu}_0 + \delta\bar{\mu}$ and expand in $\delta\bar{\mu}$. Since n is fixed in our (canonical) ensemble, we have

$$n = \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) f(\varepsilon - \bar{\mu}_0), \quad (5.8.42)$$

which defines $\bar{\mu}_0(n, T)$.¹⁸ The remaining terms in the $\delta\bar{\mu}$ expansion of Equation [nexpan] must sum to zero. This yields

$$D(\bar{\mu}_0) \delta\bar{\mu} + \frac{1}{2} \Delta^2 D'(\bar{\mu}_0) + \frac{1}{2} (\delta\bar{\mu})^2 D'(\bar{\mu}_0) + \frac{1}{2} D''(\bar{\mu}_0) \Delta^2 \delta\bar{\mu} + \frac{1}{24} D'''(\bar{\mu}_0) \Delta^4 + \mathcal{O}(\Delta^6) = 0, \quad (5.8.43)$$

where

$$D(\mu) = - \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) f'(\varepsilon - \mu) \quad (5.8.44)$$

is the thermally averaged *bare* density of states at energy μ . Note that the k^{th} derivative is

$$D^{(k)}(\mu) = - \int_{-\infty}^{\infty} d\varepsilon g^{(k)}(\varepsilon) f'(\varepsilon - \mu). \quad (5.8.45)$$

Solving for $\delta\bar{\mu}$, we obtain

$$\delta\bar{\mu} = -\frac{1}{2} a_1 \Delta^2 - \frac{1}{24} (3a_1^2 - 6a_1 a_2 + a_3) \Delta^4 + \mathcal{O}(\Delta^6), \quad (5.8.46)$$

where

$$a_k \equiv \frac{D^{(k)}(\bar{\mu}_0)}{D(\bar{\mu}_0)}. \quad (5.8.47)$$

After integrating by parts and inserting this result for $\delta\bar{\mu}$ into our expression for the free energy f , we obtain the expansion

$$\varphi(n, T, m) = \varphi_0(n, T) + \frac{1}{4} U m^2 - \frac{1}{2} D(\bar{\mu}_0) \Delta^2 + \frac{1}{8} \left(\frac{[D'(\bar{\mu}_0)]^2}{D(\bar{\mu}_0)} - \frac{1}{3} D''(\bar{\mu}_0) \right) \Delta^4 + \dots,$$

where prime denotes differentiation with respect to argument, at $m = 0$, and

$$\varphi_0(n, T) = \frac{1}{4} U n^2 + n \bar{\mu}_0 - \int_{-\infty}^{\infty} d\varepsilon \mathcal{N}(\varepsilon) f(\varepsilon - \bar{\mu}_0), \quad (5.8.48)$$

where $g(\varepsilon) = \mathcal{N}'(\varepsilon)$, so $\mathcal{N}(\varepsilon)$ is the integrated bare density of states per unit cell in the absence of any magnetic field (including both spin species).

We assume that H and m are small, in which case

$$\chi = \chi_0 + \frac{1}{2} a m^2 + \frac{1}{4} b m^4 - \frac{1}{2} \chi_0 H^2 - \frac{\chi_0}{2 \mu_B} H m + \dots,$$

where $\chi_0 = \mu_{\text{ssr}}(B)^{1/2}$, $D(\bar{\mu}_0)$ is the Pauli susceptibility, and

$$a = \frac{1}{2} U \left(1 - \frac{1}{2} U D \right), \quad b = \frac{1}{32} \left(\frac{(D')^2}{D} - \frac{1}{3} D'' \right) U^4, \quad (5.8.49)$$

where the argument of each $D^{(k)}$ above is $\bar{\mu}_0(n, T)$. The magnetization density (per unit cell, rather than per unit volume) is given by

$$M = - \left(\frac{\partial \varphi}{\partial H} \right) = \chi_0 H + \frac{\chi_0}{2 \mu_B} H m.$$

Minimizing with respect to m yields

$$a m + b m^3 - \frac{\chi_0}{2 \mu_B} H m = 0,$$

which gives, for small m ,

$$m = \frac{\chi_0}{2 \mu_B} H \left(1 - \frac{1}{2} U D \right).$$

We therefore obtain $M = \chi H$ with

$$\chi = \frac{\chi_0}{1 - \frac{U}{U_c}}, \quad (5.8.50)$$

where

$$U_c = \frac{2}{D(\bar{\mu}_0)}. \quad (5.8.51)$$

The denominator of χ increases the susceptibility above the bare Pauli value χ_0 , and is referred to as – I kid you not – the *Stoner enhancement* (see Fig. [stencil]).

[stencil] A graduate student experiences the Stoner enhancement.

[stencil] A graduate student experiences the Stoner enhancement.

It is worth emphasizing that the magnetization per unit cell is given by

$$M = - \left(\frac{1}{N_{\text{sites}}} \right) \left(\frac{\partial \mathcal{H}}{\partial H} \right) = \mu_B m.$$

This is an operator identity and is valid for any value of m , and not only small m .

When $H = 0$ we can still get a magnetic moment, provided $U > U_c$. This is a consequence of the simple Landau theory we have derived. Solving for m when $H = 0$ gives $m = 0$ when $U < U_c$ and

$$m(U) = \pm \left(\frac{U}{2b U_c} \right)^{1/2} \sqrt{U - U_c}, \quad (5.8.52)$$

when $U > U_c$, and assuming $b > 0$. Thus we have the usual mean field order parameter exponent of $\beta = \frac{1}{2}$.

Antiferromagnetic solution

In addition to ferromagnetism, there may be other ordered states which solve the mean field theory. One such example is antiferromagnetism. On a bipartite lattice, the antiferromagnetic mean field theory is obtained from

$$\langle n_{i\sigma} \rangle = \frac{1}{2}n + \frac{1}{2}\sigma e^{i\mathbf{Q}\cdot\mathbf{R}_i} m, \quad (5.8.53)$$

where $\mathbf{Q} = (\pi/a, \pi/a, \dots, \pi/a)$ is the antiferromagnetic ordering wavevector. The grand canonical Hamiltonian is then

$$\begin{aligned} & \langle \text{aligned} \rangle \text{CK}^{\text{ssr}}\{\text{MF}\} = -\frac{1}{2} \sum_{\langle i,j \rangle} \text{Big}(\text{cyl}_{\text{d}}\{\text{i}\sigma\} \text{cnd}_{\text{d}}\{\text{j}\sigma\} + \text{cyl}_{\text{d}}\{\text{j}\sigma\} \text{cnd}_{\text{d}}\{\text{i}\sigma\}) \text{Big} - \frac{1}{2} \sum_{\text{un}} \text{Big}(\text{cyl}_{\text{d}}\{\text{i}\sigma\} \text{cnd}_{\text{d}}\{\text{i}\sigma\}) \text{Big} \\ & \text{where } \varepsilon(\mathbf{k}) = -\hat{t}(\mathbf{k}), \text{ as before. On a bipartite lattice, with nearest neighbor hopping only, we have } \varepsilon(\mathbf{k} + \mathbf{Q}) = -\varepsilon(\mathbf{k}). \text{ The above matrix is diagonalized by a unitary transformation, yielding the} \\ & \text{eigenvalues} \end{aligned}$$

$$\lambda_{\pm} = \pm \sqrt{\varepsilon^2(\mathbf{k}) + \Delta^2} - \bar{\mu} \quad (5.8.54)$$

with $\Delta = \frac{1}{2}Um$ and $\bar{\mu} = \mu - \frac{1}{2}Un$ as before. The free energy per unit cell is then

$$\begin{aligned} \varphi &= \frac{1}{4}U(m^2 + n^2) + \bar{\mu}n \\ &\quad - \frac{1}{2}k_B T \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \left\{ \ln \left(1 + e^{(\bar{\mu} - \sqrt{\varepsilon^2 + \Delta^2})/k_B T} \right) + \ln \left(1 + e^{(\bar{\mu} + \sqrt{\varepsilon^2 + \Delta^2})/k_B T} \right) \right\}. \end{aligned}$$

The mean field equations are then

$$\begin{aligned} n &= \frac{1}{2} \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \left\{ f(-\sqrt{\varepsilon^2 + \Delta^2} - \bar{\mu}) + f(\sqrt{\varepsilon^2 + \Delta^2} - \bar{\mu}) \right\} \\ \frac{1}{U} &= \frac{1}{2} \int_{-\infty}^{\infty} d\varepsilon \frac{g(\varepsilon)}{\sqrt{\varepsilon^2 + \Delta^2}} \left\{ f(-\sqrt{\varepsilon^2 + \Delta^2} - \bar{\mu}) - f(\sqrt{\varepsilon^2 + \Delta^2} - \bar{\mu}) \right\}. \end{aligned}$$

As in the case of the ferromagnet, a paramagnetic solution with $m = 0$ always exists, in which case the second of the above equations is no longer valid.

Mean field phase diagram of the Hubbard model

Let us compare the mean field theories for the ferromagnetic and antiferromagnetic states at $T = 0$ and $H = 0$. Due to particle-hole symmetry, we may assume $0 \leq n \leq 1$ without loss of generality. (The solutions repeat themselves under $n \rightarrow 2 - n$.) For the paramagnet, we have

$$\begin{aligned} n &= \int_{-\infty}^{\bar{\mu}} d\varepsilon g(\varepsilon) \\ \varphi &= \frac{1}{4}Un^2 + \int_{-\infty}^{\bar{\mu}} d\varepsilon g(\varepsilon) \varepsilon, \end{aligned}$$

with $\bar{\mu} = \mu - \frac{1}{2}Un$ is the ‘renormalized’ Fermi energy and $g(\varepsilon)$ is the density of states per unit cell in the absence of any explicit (H) or implicit (m) symmetry breaking, including both spin polarizations.

For the ferromagnet,

$$\begin{aligned} n &= \frac{1}{2} \int_{-\infty}^{\bar{\mu}-\Delta} d\varepsilon g(\varepsilon) + \frac{1}{2} \int_{-\infty}^{\bar{\mu}+\Delta} d\varepsilon g(\varepsilon) \\ \frac{4\Delta}{U} &= \int_{\bar{\mu}-\Delta}^{\bar{\mu}+\Delta} d\varepsilon g(\varepsilon) \\ \varphi &= \frac{1}{4}Un^2 - \frac{\Delta^2}{U} + \int_{-\infty}^{\bar{\mu}-\Delta} d\varepsilon g(\varepsilon) \varepsilon + \int_{-\infty}^{\bar{\mu}+\Delta} d\varepsilon g(\varepsilon) \varepsilon. \end{aligned}$$

Here, $\Delta = \frac{1}{2}Um$ is nonzero in the ordered phase.

Finally, the antiferromagnetic mean field equations are

$$\text{where } \varepsilon_0 = \sqrt{\bar{\mu}^2 - \Delta^2} \text{ and } \Delta = \frac{1}{2}Um \text{ as before. Note that } |\bar{\mu}| \geq \Delta \text{ for these solutions. Exactly at half-filling, we have } n = 1 \text{ and } \bar{\mu} = 0. \text{ We then set } \varepsilon_0 = 0.$$

The paramagnet to ferromagnet transition may be first or second order, depending on the details of $g(\varepsilon)$. If second order, it occurs at $\frac{U}{\text{Big}(\text{cyl}_{\text{d}}\{\text{i}\sigma\} \text{cnd}_{\text{d}}\{\text{i}\sigma\})} = 1$, where $\frac{1}{\text{Big}(\text{cyl}_{\text{d}}\{\text{i}\sigma\} \text{cnd}_{\text{d}}\{\text{i}\sigma\})}$ is the paramagnetic solution for $\bar{\mu}$. The paramagnet to antiferromagnet transition is always second order in this mean field theory, since the RHS of Equation (5.8.54) is a monotonic function of Δ . This transition occurs at $\frac{U}{\text{Big}(\text{cyl}_{\text{d}}\{\text{i}\sigma\} \text{cnd}_{\text{d}}\{\text{i}\sigma\})} = 2$.

Note that $\frac{U}{\text{Big}(\text{cyl}_{\text{d}}\{\text{i}\sigma\} \text{cnd}_{\text{d}}\{\text{i}\sigma\})} \rightarrow 0$ logarithmically for $n \rightarrow 1$, since $\frac{1}{\text{Big}(\text{cyl}_{\text{d}}\{\text{i}\sigma\} \text{cnd}_{\text{d}}\{\text{i}\sigma\})} = 0$ at half-filling.

For large U , the ferromagnetic solution always has the lowest energy, and therefore if $\frac{U}{\text{Big}(\text{cyl}_{\text{d}}\{\text{i}\sigma\} \text{cnd}_{\text{d}}\{\text{i}\sigma\})} < \frac{U}{\text{Big}(\text{cyl}_{\text{d}}\{\text{i}\sigma\} \text{cnd}_{\text{d}}\{\text{i}\sigma\})}$, there will be a first-order antiferromagnet to ferromagnet transition at some value $\frac{U}{\text{Big}(\text{cyl}_{\text{d}}\{\text{i}\sigma\} \text{cnd}_{\text{d}}\{\text{i}\sigma\})} = \frac{U}{\text{Big}(\text{cyl}_{\text{d}}\{\text{i}\sigma\} \text{cnd}_{\text{d}}\{\text{i}\sigma\})}$. In Figure 5.8.8, I plot the phase diagram obtained by solving the mean field equations assuming a semicircular density of states $g(\varepsilon) = \frac{2}{\pi} W^{-2} \sqrt{W^2 - \varepsilon^2}$. Also shown is the phase diagram for the $d = 2$ square lattice Hubbard model obtained by J. Hirsch (1985).

Figure 5.8.8: Mean field phase diagram of the Hubbard model, including paramagnetic (P), ferromagnetic (F), and antiferromagnetic (A) phases. Left panel: results using a semicircular density of states function of half-bandwidth W . Right panel: results using a two-dimensional square lattice density of states with nearest neighbor hopping t , from J. E. Hirsch, *Phys. Rev. B* **31**, 4403 (1985). The phase boundary between F and A phases is first order.

Figure 5.8.9: Mean field phase diagram of the Hubbard model, including paramagnetic (P), ferromagnetic (F), and antiferromagnetic (A) phases. Left panel: results using a semicircular density of states function of half-bandwidth W . Right panel: results using a two-dimensional square lattice density of states with nearest neighbor hopping t , from J. E. Hirsch, *Phys. Rev. B* **31**, 4403 (1985). The phase boundary between F and A phases is first order.

How well does Stoner theory describe the physics of the Hubbard model? Quantum Monte Carlo calculations by J. Hirsch (1985) found that the actual phase diagram of the $d = 2$ square lattice Hubbard Model exhibits no ferromagnetism for any n up to $U = 10$. Furthermore, he found the antiferromagnetic phase to be entirely confined to the vertical line $n = 1$. For $n \neq 1$ and $0 \leq U \leq 10$,

the system is a paramagnet¹⁹. These results were state-of-the art at the time, but both computing power as well as numerical algorithms for interacting quantum systems have advanced considerably since 1985. Yet as of 2018, we *still* don't have a clear understanding of the $d = 2$ Hubbard model's $T = 0$ phase diagram! There is an emerging body of numerical evidence²⁰ that in the underdoped ($n < 1$) regime, there are portions of the phase diagram which exhibit a *stripe* ordering, in which antiferromagnetic order is interrupted by a parallel array of line defects containing excess holes (the absence of an electron)²¹. This problem has turned out to be unexpectedly rich, complex, and numerically difficult to resolve due to the presence of *competing ordered states*, such as d -wave superconductivity and spiral magnetic phases, which lie nearby in energy with respect to the putative stripe ground state.

In order to achieve a ferromagnetic solution, it appears necessary to introduce geometric frustration, either by including a next-nearest-neighbor hopping amplitude t' or by defining the model on non-bipartite lattices. Numerical work by M. Ulmke (1997) showed the existence of a ferromagnetic phase at $T = 0$ on the FCC lattice Hubbard model for $U = 6$ and $n \in [0.15, 0.87]$ (approximately).

White dwarf stars

There is a nice discussion of this material in R. K. Pathria, *Statistical Mechanics*. As a model, consider a mass $M \sim 10^{33} g$ of helium at nuclear densities of $\rho \sim 10^7 g/cm^3$ and temperature $T \sim 10^7 K$. This temperature is much larger than the ionization energy of ${}^4\text{He}$, hence we may safely assume that all helium atoms are ionized. If there are N electrons, then the number of α particles (${}^4\text{He}$ nuclei) must be $\frac{1}{2}N$. The mass of the α particle is $m_\alpha \approx 4m_p$. The total stellar mass M is almost completely due to α particle cores.

The electron density is then

$$n = \frac{N}{V} = \frac{2 \cdot M/4m_p}{V} = \frac{\rho}{2m_p} \approx 10^{30} cm^{-3}, \quad (5.8.55)$$

since $M = N \cdot m_e + \frac{1}{2}N \cdot 4m_p$. From the number density n we find for the electrons

$$\begin{aligned} k_F &= (3\pi^2 n)^{1/3} = 2.14 \times 10^{10} cm^{-1} \\ p_F &= \hbar k_F = 2.26 \times 10^{-17} g cm/s \\ mc &= (9.1 \times 10^{-28} g)(3 \times 10^{10} cm/s) = 2.7 \times 10^{-17} g cm/s. \end{aligned}$$

Since $\frac{p_F}{mc} \gg 1$, we conclude that the electrons are relativistic. The Fermi temperature will then be $T_F \sim mc^2 \sim 10^6 eV \sim 10^{12} K$. Thus, $T \ll T_F$ which says that the electron gas is degenerate and may be considered to be at $T \sim 0$. So we need to understand the ground state properties of the relativistic electron gas.

The kinetic energy is given by

$$\epsilon(\mathbf{p}) = \sqrt{\mathbf{p}^2 c^2 + m^2 c^4} - mc^2. \quad (5.8.56)$$

The velocity is

$$\mathbf{v} = \frac{\partial \epsilon}{\partial \mathbf{p}} = \frac{\mathbf{p} c^2}{\sqrt{p^2 c^2 + m^2 c^4}}. \quad (5.8.57)$$

The pressure in the ground state is

$$\begin{aligned} p_0 &= \frac{1}{3} n(\mathbf{p} \cdot \mathbf{v}) \\ &= \frac{1}{3\pi^2 \hbar^3} \int_0^{p_F} dp p^2 \cdot \frac{p^2 c^2}{\sqrt{p^2 c^2 + m^2 c^4}} \\ &= \frac{m^4 c^5}{3\pi^2 \hbar^3} \int_0^{\theta_F} d\theta \sinh^4 \theta \\ &= \frac{m^4 c^5}{96\pi^2 \hbar^3} (\sinh(4\theta_F) - 8 \sinh(2\theta_F) + 12 \theta_F), \end{aligned}$$

where we use the substitution

$$p = mc \sinh \theta, \quad v = c \tanh \theta \implies \theta = \frac{1}{2} \ln \left(\frac{c+v}{c-v} \right). \quad (5.8.58)$$

Note that $p_F = \hbar k_F = \hbar(3\pi^2 n)^{1/3}$, and that

$$n = \frac{M}{2m_p V} \implies 3\pi^2 n = \frac{9\pi}{8} \frac{M}{R^3 m_p}. \quad (5.8.59)$$

Now in equilibrium the pressure p is balanced by gravitational pressure. We have

$$dE_0 = -p_0 dV = -p_0(R) \cdot 4\pi R^2 dR. \quad (5.8.60)$$

This must be balanced by gravity:

$$dE_g = \gamma \cdot \frac{GM^2}{R^2} dR, \quad (5.8.61)$$

where γ depends on the radial mass distribution. Equilibrium then implies

$$p_0(R) = \frac{\gamma}{4\pi} \frac{GM^2}{R^4}. \quad (5.8.62)$$

 [whitedwarf] Mass-radius relationship for white dwarf stars. (Source: Wikipedia).

[whitedwarf] Mass-radius relationship for white dwarf stars. (Source: Wikipedia).

To find the relation $R = R(M)$, we must solve

$$\frac{\gamma}{4\pi} \frac{GM^2}{R^4} = \frac{m^4 c^5}{96\pi^2 \hbar^3} (\sinh(4\theta_F) - 8 \sinh(2\theta_F) + 12 \theta_F). \quad (5.8.63)$$

Note that

$$\sinh(4\theta_F) - 8 \sinh(2\theta_F) + 12 \theta_F = \begin{cases} \frac{96}{15} \theta_F^5 & \theta_F \rightarrow 0 \\ \frac{1}{2} e^{4\theta_F} & \theta_F \rightarrow \infty. \end{cases} \quad (5.8.64)$$

Thus, we may write

$$p_0(R) = \frac{\gamma}{4\pi} \frac{gM^2}{R^4} = \begin{cases} \frac{\hbar^2}{15\pi^2 m} \left(\frac{9\pi}{8} \frac{M}{R^3 m_p} \right)^{5/3} & \theta_F \rightarrow 0 \\ \frac{\hbar c}{12\pi^2} \left(\frac{9\pi}{8} \frac{M}{R^3 m_p} \right)^{4/3} & \theta_F \rightarrow \infty. \end{cases} \quad (5.8.65)$$

In the limit $\theta_F \rightarrow 0$, we solve for $R(M)$ and find

$$R = \frac{3}{40\gamma} (9\pi)^{2/3} \frac{\hbar^2}{G m_p^{5/3} m M^{1/3}} \propto M^{-1/3}. \quad (5.8.66)$$

In the opposite limit $\theta_F \rightarrow \infty$, the R factors divide out and we obtain

$$M = M_0 = \frac{9}{64} \left(\frac{3\pi}{\gamma^3} \right)^{1/2} \left(\frac{\hbar c}{G} \right)^{3/2} \frac{1}{m_p^2}. \quad (5.8.67)$$

To find the R dependence, we must go beyond the lowest order expansion of Equation [cases], in which case we find

$$R = \left(\frac{9\pi}{8} \right)^{1/3} \left(\frac{\hbar}{mc} \right) \left(\frac{M}{m_p} \right)^{1/3} \left[1 - \left(\frac{M}{M_0} \right)^{2/3} \right]^{1/2}. \quad (5.8.68)$$

The value M_0 is the limiting size for a white dwarf. It is called the *Chandrasekhar limit*.

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